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A Novel Approach for Describing MICROMIXING EFFECTS IN HOMOGENEOUS REACTORS

Vemuri Balakotaiah, Saikat Chakraborty
University of Houston • Houston, TX 77204-4004

Reacting flow systems are hierarchical in nature, i.e., they are characterized by multiple length (or time) scales. Scale separation exists in most reactors, however, and these disparate scales are typically characterized by three representative ones, namely, micro (molecular), meso (catalyst particle or tube diameter), and macro (reactor or process) scales. In most cases of practical interest, a strong nonlinear coupling exists between reaction and transport at micro and meso scales, and the reactor performance at the macro scale. As a result, transport limitations at the smaller scales significantly influence the reactor and hence the process performance.

Such effects could be quantified by numerically solving the convection-diffusion-reaction (CDR) equation from the macro down to the micro scale. But the solution of the CDR equation from the reactor (macro) scale down to the local diffusional (micro) scale, using computational fluid dynamics (CFD), is prohibitive in terms of numerical effort and impractical for the purpose of reactor control and optimization. Moreover, even with today’s computational power, it is impractical to explore the different types of bifurcation features and spatio-temporal behaviors that exist in the multidimensional parameter space, using CFD codes. In such cases, low dimensional models are a natural alternative.

Historically, chemical engineers have derived low dimensional models for reactors using a top-down approach, which is based on a priori assumptions on the length and time scales of convection, diffusion, and reaction. The classical ideal reactor (CSTR and PFR) models are examples of such low-dimensional models obtained on the basis of simplified (or oversimplified) assumptions. These assumptions are usually not justified since justification requires comparison of the solution obtained from the simplified models with that obtained from the CDR model.

In order to account for experimental observations that could not be explained by these ideal reactor models, the latter have been modified by introducing the concepts of dispersion coefficients\(^1\) and residence time distribution\(^2\) to account for macro- and micro-mixing effects. Several other reactive mixing models followed in the next forty years: the two- and three-environment model\(^3\), the coalescence-redispersion model\(^4\), interaction by exchange with mean model\(^5\), engulfment-deformation-diffusion model\(^6\) and CFD models using probability density functions (PDF) and direct numerical simulation (DNS).

This article presents an alternative (bottom-up) approach and an elementary treatment of mixing effects on reactor performance. We will present a brief historical review of homogeneous reactor models before discussing this new approach.

BRIEF HISTORY OF HOMOGENEOUS REACTOR MODELS

The most widely used homogeneous reactor models are the three classical ideal reactor models: the plug-flow reactor (PFR) model, the continuous stirred tank reactor (CSTR) model, and the batch reactor (BR) model. While the BR model and the PFR model (which are identical for constant density systems with time replaced by space time or dimensionless distance along the tube) have existed since the late eighteenth century. A conceptual leap came in the form of the CSTR model through the work of Bodenstein and Wohlgast in 1908.\(^1\) Unlike the PFR model, which assumes no gradients in the radial direction and no mixing in the axial direction,
the CSTR model assumes complete mixing at all scales. For constant density systems, the three classical reactor models are described by

**PFR**

\[ \langle u \rangle \frac{d\langle C \rangle}{dx} = -R(\langle C \rangle) \quad \text{with} \quad \langle C \rangle = C_{in} \quad @ \quad x = 0 \]  

**BR**

\[ \frac{d\langle C \rangle}{dt} = -R(\langle C \rangle) \quad \text{with} \quad \langle C \rangle = C_{in} \quad @ \quad t = 0 \]  

**CSTR**

\[ \frac{(\langle C \rangle - C_{in})}{\tau_C} = -R(\langle C \rangle) \]  

where \( \langle C \rangle \) is the spatially (or cross-sectional) averaged reactant concentration, \( C_{in} \) is the mean inlet concentration of the reactant, \( R(\langle C \rangle) \) is the sink term due to the presence of homogeneous reaction, \( x \) is the coordinate along the length of the PFR, \( \langle u \rangle \) is the mean fluid velocity in the reactor, \( t \) is the time, and \( \tau_C \) is the total residence time in the reactor.

Irving Langmuir first replaced the assumption of no axial mixing of the PFR model with finite axial mixing and the accompanying Dirichlet boundary condition \( (\langle C \rangle = C_{in} \quad @ \quad x = 0) \) by a flux-type boundary condition

\[ D_m \frac{d\langle C \rangle}{dx} = \langle u \rangle [\langle C \rangle - C_{in}] \quad @ \quad x = 0 \]  

where \( D_m \) is the molecular diffusivity of the species. The above boundary condition was rediscovered several times in the years that followed: first by Förster and Geib, which was quoted and applied by Damköhler, and then, later, by Danckwerts. Since then it has been known as the "Danckwerts" boundary condition. In his paper, Langmuir dealt with both the limiting cases of "mixing nearly complete" and "only slight mixing."

Thirty years later, Gerhard Damköhler in his historic paper, summarized various reactor models and formulated the two-dimensional CDR model for tubular reactors in complete generality, allowing for finite mixing both in the radial and the axial directions. In his paper, Damköhler used the flux-type boundary condition at the inlet and also replaced the assumption of plug flow with parabolic velocity profile, which is typical of laminar flow in tubes.

Förster and Geib first introduced the concept of residence time distribution (RTD) to study the case of longitudinal dispersion in tubes. Twenty years later, Danckwerts, in his much celebrated paper, devised a generalized treatment of RTD and introduced the concepts of "holdback" and "segregation." Following this, it was Zweierling, who quantified the degrees of mixing with the ideas of "complete segregation" and "maximum mixedness" and brought forth the concept of micromixing, or mixing at the molecular scale in homogeneous reactions.

In the last forty years, a wide range of micromixing models for homogeneous reactors have been formulated. While most of these low-dimensional mixing models are phenomenological in nature, the rigorously derived CFD models are high-dimensional and therefore numerically very expensive, especially for the case of multiple reactions with fast/non-isothermal kinetics. As a result, in spite of the simplifying assumptions present, the century-old ideal classical reactor models (Eqs. 1-3) are still the most popular choices among chemical engineering practitioners (and teachers). The classical ideal reactor models, which are easy-to-solve ordinary differential or algebraic equations with no adjustable parameter, are particularly preferred over the full CDR models (which are partial differential equations in more than one dimension) in case of multiple reactions with complex kinetics.

### Spatial Averaging of Convection-Diffusion-Reaction Equation

The main goal of this article is to illustrate a new approach for deriving low-dimensional homogeneous reactor models, capable of predicting mixing effects. These models are derived through rigorous spatial averaging of the three-dimensional CDR equations over local length scales by using the Liapunov-Schmidt (L-S) technique of classical bifurcation theory. We illustrate this spatial averaging technique using the simple case of laminar flow in a tube with homogeneous reaction. The scalar concentration \( C(r, \theta, x, t') \) in a tubular reactor is assumed to obey the CDR equation

\[ \frac{\partial C}{\partial t'} + u(r) \frac{\partial C}{\partial x} = \frac{1}{r} \frac{\partial}{\partial r} \left( D_r \frac{\partial C}{\partial r} \right) + \frac{1}{r^2} \frac{\partial}{\partial \theta} \left( D_{\theta} \frac{\partial C}{\partial \theta} \right) + \frac{\partial}{\partial x} \left( D_x \frac{\partial C}{\partial x} \right) - R(C) \]  

with accompanying initial and boundary conditions, given by

\[ C(r, \theta, x, t' = 0) = C_0 \quad \frac{\partial C}{\partial r} = 0 \quad @ \quad r = a \]  

\[ C(r, \theta, x, t' = 0) = C(r, \theta + 2\pi, x, t') \]  

\[ D_r \frac{\partial C}{\partial r} = u(r) [C(r, \theta, x, t') - C_{in}] \quad @ \quad x = 0 \]  

\[ \frac{\partial C}{\partial x} = 0 \quad @ \quad x = L \]  

where \( D_r \) and \( D_x \) are the transverse and axial diffusivities, respectively; \( r, \theta, x \) are the radial, azimuthal, and axial coor-
dines, respectively; and \( u(r) \) is the fluid velocity profile. We take \( a \) (radius of the pipe) and \( L \) (length of the pipe) to be the characteristic lengths in the radial and axial directions, respectively; \( \langle u \rangle \) is the cross-sectional average velocity; and \( C_R \) is a reference concentration. Then, we obtain four time scales in the system associated with convection (\( \tau_C \)), radial diffusion (\( \tau_D \)), axial diffusion (\( \tau_x \)), and reaction (\( \tau_R \)), given by

\[
\tau_D = \frac{a^2}{D_L}, \quad \tau_x = \frac{L^2}{D_x}, \quad \tau_C = \frac{L}{\langle u \rangle}, \quad \tau_R = \frac{C_R}{R(C_R)}
\]

and the ratios of these time scales give rise to the dimensionless parameters: \( p \) (transverse Peclet number), \( Pe \) (axial Peclet number), \( Da \) (Damköhler number), and \( \phi^2 \) (local Damköhler number), given by

\[
p = \frac{a^2 \langle u \rangle}{LD_L}, \quad Pe = \frac{\langle u \rangle L}{D_x}, \quad Da = \frac{LR(C_R)}{\langle u \rangle C_R} = \frac{\tau_C}{\tau_R} \]

In dimensionless form, Eq. (5) for the case of constant species diffusivities, can be rearranged as

\[
\nabla^2 c = \frac{1}{\xi} \frac{d}{d\xi} \left( \xi \frac{dc}{d\xi} \right) + \frac{1}{\xi^2} \frac{d^2 c}{d\xi^2} = \left[ \frac{\partial c}{\partial t} - \frac{1}{Pe} \frac{\partial^2 c}{\partial z^2} + \frac{u(\xi)}{D} \frac{\partial c}{\partial z} + Da \tilde{f}(c) \right] \Delta p g(c)
\]

with initial and boundary conditions being

\[
c(\xi,0,0,0) = c_0 \quad \frac{dc}{d\xi} = 0 \quad @ \xi = 1
\]

\[
c(\xi,0,0,0) = c(\xi,0,0,0) + 2\pi, \quad 0 \leq \xi \leq 0
\]

where

\[
t = \frac{t'}{\tau_C}, \quad \xi = \frac{r}{a}, \quad z = \frac{x}{L}, \quad u = \frac{u}{\langle u \rangle}
\]

\[
c = \frac{C}{C_R}, \quad \tilde{f}(c) = \frac{R(C)}{R(C_R)}
\]

The form of the CDR equation (Eq. 8) clearly illustrates that a scale separation exists in the system, with \( p \) being the ratio of the local to the global scale (when \( Pe \) and \( Da \) are of order unity), and spatial averaging over the local scales is possible. It can be seen from Eqs. (8) and (9) that in the limit of \( p \to 0 \), \( \nabla^2 c \to 0 \) and transverse (or small scale) concentration gradients vanish, in which case the equations simplify to the classical one-mode axial dispersion model. If local diffusion time is small but finite compared to convection, reaction, and axial diffusion time, local (transverse) gradients remain small and we can write

\[
c(\xi,0,0,0) = \langle c \rangle + \langle u'c' \rangle
\]

where \( \langle c \rangle \) is the transverse averaged concentration and \( \langle u'c' \rangle \) is the fluctuation about this average, and \( \langle u'c' \rangle \to 0 \) as \( p \to 0 \). (Also, by definition \( \langle c \rangle = 0 \).) Multiplying Eq. (11) by the local velocity profile, \( u(\xi) = \langle u \rangle + u' \), and averaging over the cross-section gives

\[
c_m = \langle c \rangle + \langle u'c' \rangle
\]

where \( c_m \) is the mixing-cup (velocity weighted) concentration. Similarly, transverse averaging of Eq. (8) over the cross-section gives

\[
\frac{\partial c}{\partial t} - \frac{1}{Pe} \frac{\partial^2 c}{\partial z^2} + \frac{u(\xi)}{D} \frac{\partial c}{\partial z} + Da \int_0^{2\pi} \int_0^{2\pi} \xi c(\xi,0,0,0) d\theta d\xi = 0
\]

For the case of a tubular reactor, the spatial (transverse) average and mixing-cup concentrations are defined by

\[
\langle c \rangle = \frac{\int_0^{2\pi} \int_0^{2\pi} \xi c(\xi,0,0,0) d\theta d\xi}{\int_0^{2\pi} \int_0^{2\pi} \xi d\theta d\xi}
\]

and

\[
c_m = \frac{\int_0^{2\pi} \int_0^{2\pi} \xi u(\xi) c(\xi,0,0,0) d\theta d\xi}{\int_0^{2\pi} \int_0^{2\pi} \xi u(\xi) d\theta d\xi}
\]

It may be noted that in all flow reactors, \( c_m \) is the experimentally measured variable. We refer to \( \langle c \rangle \) and \( c_m \) as the two modes of the system and our spatially averaged reactor models as Two-Mode Models (TMMs). Equation 13 is called the global equation, while Eq. (12) is called the local equation. The local equation shows that the difference between \( c_m \) and \( \langle c \rangle \) depends on the local velocity gradients \( u' \) and the local concentration gradients \( c' \) caused by molecular diffusion and reaction at the local scales. Micromixing is captured by the local equation as an exchange between the two modes (scales), \( c_m \) and \( \langle c \rangle \).

In order to determine \( c' \) (and hence the term \( \langle u'c' \rangle \) or the difference between \( c_m \) and \( \langle c \rangle \)), we substitute Eq. (11) in Eq (8) to obtain

\[
\nabla^2 c' = pg(\langle c \rangle + c')
\]
The L-S technique solves Eq. (16) for $c'$ by expanding it in the parameter $p$ as

$$c' = \sum_{i=1}^{n} p_i c_i$$

(17)

and by using the Fredholm Alternative (i.e., the fact $c'$ lies in the function space orthogonal to which $\langle c \rangle$ resides). Such an expansion (Eq. 17) is possible, since for $p = 0$, the transverse diffusion operator in Eq. (8) has a zero eigenvalue with a constant eigenfunction. Thus, $\langle u'c' \rangle$ could be determined to any order in $p$, i.e., closure of the local equation could be accomplished to any desired accuracy. In practice, the leading term (that is of order $p$) is sufficient to retain all the qualitative features of the full CDR equation. For example, for the case of azimuthally symmetric feeding, we have

$$c' = -p \frac{\partial \langle c \rangle}{\partial z} + \frac{1}{12} \frac{5^3}{4} + \frac{5^4}{8} + O(p^2)$$

(18)

Substituting Eq. (18) into Eqs. (12) and (13) gives the two-mode model to $O(p)$ as

$$\frac{\partial \langle c \rangle}{\partial t} + \frac{1}{Pe} \frac{\partial^2 \langle c \rangle}{\partial z^2} + D a \langle c \rangle + O(p^2) = 0$$

(19)

$$\langle c \rangle - c_m = \beta_1 p \frac{\partial \langle c \rangle}{\partial z} + O(p^2)$$

(20)

with boundary and initial conditions given by

$$\frac{1}{Pe} \frac{\partial c_m}{\partial z} = c_m - c_{m, in} \quad @ \quad z = 0$$

(21)

$$\frac{\partial c_m}{\partial z} = 0 \quad @ \quad z = 1$$

(22)

$$\langle c \rangle = \langle c_0 \rangle \quad @ \quad t = 0$$

(23)

where $1/\beta_1$ is called the exchange coefficient, which depends on the local shear rates. For the case of fully developed laminar flows, $D_a = D_s = D_m$ (molecular diffusivity of the species), and $\beta_1 = 1/48$. We refer to this model as the two-mode axial dispersion model. (Further details of the spatial averaging procedure using the L-S technique can be found in Chakraborty and Balakotaiah.14,15)

It should be noted that the spatially averaged CDR equation (Eqs. 19 and 20) retains all the parameters ($p$, $Pe$, $Da$) of the three-dimensional CDR equation (Eq. 8) and hence all the qualitative features of the latter. It should also be mentioned that this model is capable of capturing macromixing effects through the axial Peclet number $Pe$ in the global equation (Eq. 19), as well as micromixing effects through the exchange coefficient $\beta_1^{-1}$ and transverse Peclet number $p$ in the local equation (Eq. 20). In fact, the L-S technique guarantees that the solution of the averaged model (Eqs. 19-23) agrees with the exact solution of the three-dimensional CDR equation to $O(p)$. [Three decimal accuracy is obtained for a second-order reaction for the case of $Pe \rightarrow \infty$ if $\phi^2 < 1$ (see ref. 14).]

Using the spatial averaging technique illustrated above, accurate low-dimensional models could be obtained for different types of reactors and flow profiles. For example, the two-mode model for a tubular reactor with fully developed turbulent flow is the same as Eqs (19) through (23), where $D_\perp$ is the effective turbulent diffusivity and $\beta_1$ is a function of Reynolds number ($Re$) and friction factor $f$. This model is obtained by starting with the time-smoothed (Reynolds averaged) CDR equation, where the reaction rate $R(C)$ in Eq. (5) is replaced by the Reynolds averaged reaction rate (after closure) $R_a(C)$. Spatial averaging by the L-S technique is then performed on the time-averaged CDR equation (i.e., spatial averaging follows time averaging) to obtain the two-mode model (see ref. 15 for details). In the next section, we will present the two-mode models for other types of homogeneous reactors.

**TWO-MODE MODELS FOR HOMOGENEOUS REACTORS**

**Tubular Reactors**

The steady-state two-mode model for a tubular reactor for the case of $Pe \rightarrow \infty$ (i.e., no macromixing present) may be obtained from Eqs. (19) through (21). In dimensional form, it is given by

$$\langle u \rangle \frac{dC_m}{dx} = -R(C) \quad \text{with} \quad C_m(x = 0) = C_{m, in}$$

(24)

$$C_m - \langle C \rangle = -t_{mix} \langle u \rangle \frac{dC_m}{dx} = t_{mix} R(C)$$

(25)

where the local mixing time $t_{mix}$ (in the local Eq. 25 describing micromixing effects) is given by

$$t_{mix} = \beta_1 \frac{a^2}{D_\perp}$$

(26)

where $a$ is the local diffusional length scale over which spatial averaging is performed, $D_\perp$ is the local diffusion coefficient, and $\beta_1^{-1}$ is the exchange coefficient. In the limit of complete micromixing (i.e., $t_{mix} \rightarrow 0$), the two-mode convection model reduces to the ideal one-mode zero-parameter PFR model.

**Loop and Recycle Reactors**

In a loop reactor of length $L$, a flow rate of $q_{in}$, and with an average velocity of $\langle u_{in} \rangle$, enters and leaves the reactor at points $x = 0$ and $x = l$, respectively (where $x$ is the length coordinate along the loop). The total flow rate in the loop is $Q + q_{in}$ between points $x = 0$ and $x = l$, and is $Q$ between...
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points $x = l$ and $x = L$, due to a recycle rate of $Q$. The recycle ratio $\Lambda$ is the ratio of the volume of fluid returned to the reactor entrance per unit time to the volume of fluid leaving the system per unit time, and is given by $\Lambda = Q/q_m$. The two-mode model for such a loop reactor can be obtained as

$$
\langle u_m \rangle \frac{dC_m}{dx} = \begin{cases} 
\frac{-1}{1+\Lambda} R((C)) & 0 \leq x < l \\
\frac{1}{\Lambda} R((C)) & l \leq x \leq L
\end{cases}
$$

(27)

with boundary conditions

$$
C_m - \langle C \rangle = t_{\text{mix}} R((C)) \quad 0 \leq x < L
$$

(28)

For the special case when no reaction occurs between $x = l$ and $x = L$, i.e., $C_m(x=l) = C_m(x=L)$, the loop reactor reduces to a recycle reactor of length $l$, the two-mode model for which is given by

$$
\langle u_m \rangle \frac{dC_m}{dx} = \frac{-1}{1+\Lambda} R((C))
$$

with $C_m(x = 0) = C_{m,\text{in}} + \frac{\Lambda}{1+\Lambda} C_m(x = l)$

(30)

$$
C_m - \langle C \rangle = t_{\text{mix}} R((C)) \quad 0 \leq x < L
$$

(31)

The two-mode loop and recycle reactor models, like the two-mode axial dispersion model, are two-parameter two-mode models. Here, the two parameters are the recycle ratio $\Lambda$, and the local mixing time $t_{\text{mix}}$, which describe macro- and micro-mixing effects in the system, respectively.

Tank Reactors (CSTRs)

It is well known that as the recycle ratio $\Lambda$ of a recycle reactor is increased, the behavior shifts from a PFR at $\Lambda = 0$ (no macromixing) to a CSTR as $\Lambda = \infty$ (perfect macromixing). We use this idea to obtain the two-mode model for a perfectly macromixed CSTR, by integrating Eq. (30) along the length of the reactor $x$ and simplifying the resulting equation for $\Lambda > 1$. This gives the two-mode model for a perfectly macromixed CSTR as

$$
\frac{C_m - \langle C \rangle}{t_{\text{mix}}} = \frac{C_{m,\text{in}} - C_m}{t_{\text{mic}}}
$$

(32)

$$
C_m - \langle C \rangle = t_{\text{mic}} R((C))
$$

(33)

where $t_{\text{mic}}(=V/q_m)$ is the total residence time in the reactor, and $t_{\text{mix}}$ is the characteristic local mixing time, which captures micromixing effects. In the limit of complete micromixing (i.e., $t_{\text{mix}} \rightarrow 0$), the TMM for a CSTR reduces to the ideal one-mode zero-parameter CSTR model.

It should be pointed out that the local equation (eqs. 25, 28, 31, 33) is the same for all reactor types. This is an important observation, which shows that scale separation exists in all types of homogeneous reactors.

**Physical Interpretation of Two-Mode Models**

Using the example of a tank reactor, we present a physical interpretation of the two-mode models. The physical system equivalent to the two-mode model of a CSTR is a tank reactor consisting of two zones, each of size $V$, namely, a non-reacting convection zone (A), represented by $C_m$, and a reaction zone (B), represented by $\langle C \rangle$. Thus, $C_m$ is representative of the convection scale of the system and $\langle C \rangle$ is representative of the reaction scale of the system. The interaction between the two scales (or the two zones A and B) is quantified by an exchange of materials at a rate of $q_m$. This exchange occurs only through local diffusion, and $t_{\text{mic}}(=V/q_m)$, which is the characteristic time scale for this exchange, therefore depends on the local shear rate and diffusion coefficient. Equations (32) and (33) represent the steady-state material balances for zone B and zone A, respectively.

In general, any infinitesimal volume $dV$ inside the tank could be so imagined to consist of two zones/scales, and a corresponding two-mode model could be written (Eqs. 32-33) for the volume $dV$. If macromixing in the tank is complete, the two-mode model for any control volume of the tank could be integrated over the entire volume of the tank to generate a single two-mode model (Eqs. 32-33) for the whole tank.

Macromixing effects are often not negligible in real tanks, however, and are influenced by several factors including the type and speed of impellers (turbines) and the manner of feed distribution. Several macromixing models are available in the literature, e.g., the two-compartment model, recycle model, tanks-in-series model, exchange-with-stagnant-zone model, any of which could be suitably coupled with the TMM to describe both macro- and micro-mixing in tanks. However, if micromixing effects are dominant compared to macromixing ones (as in well-stirred tanks), it could be shown by using L-S reduction in finite dimensions, that these models (i.e., the two-mode n-compartment model, etc.) could be reduced to Eqs. (32) and (33), where the local mixing time $t_{\text{mix}}$ is replaced by an effective mixing time $t_{\text{mic}}$, which captures both macro- and micro-mixing effects. This effective mixing time $t_{\text{mic}}$ now not only depends on the local diffusion time and local shear rates, but also intricately on the tank geometry, type and number of impellers, baffle positions, and power dissipation in the system.
SIMILARITY BETWEEN TWO-MODE MODELS OF HOMOGENEOUS REACTORS AND TWO-PHASE MODELS OF CATALYTIC REACTORS

A striking structural similarity between the two-mode models for homogeneous reactors and two-phase models for heterogeneous catalytic reactors exists. This could be seen more clearly when Eqs. (24) and (25) are rewritten as

\[
\left\langle u_x \right\rangle \frac{dC_m}{dx} = -\frac{C_m - \langle C \rangle}{t_{mix}} = -R\langle C \rangle
\]

with \( C_m = C_{m,\infty} @ x = 0 \) (34)

The two-phase model for a heterogeneous wall-catalyzed reaction in a tubular reactor is given by

\[
\left\langle u_x \right\rangle \frac{dC_m}{dx} = -\frac{C_m - C_s}{t_{TP}} = -R(C_s)
\]

with \( C_m = C_{m,\infty} @ x = 0 \) (35)

It may be noticed that the spatially averaged concentration \( \langle C \rangle \) of the TMM (in Eq. 34) is replaced by the surface (wall) concentration \( C_s \) in the two-phase model (Eq. 35), while the local mixing time \( t_{mix} \) of the TMM is replaced in the two-phase model by a characteristic mass transfer time between the two phases \( t_{TP} \), which is given by

\[
t_{TP} = \beta_{TP} t_D = \frac{1}{Sh_{m,T}} \frac{a^2}{D_m}
\]

where \( t_D \) is the transverse diffusion time scale and \( Sh_{m,T} = 1/\beta_{TP} \) is the two-phase (dimensionless mass) transfer coefficient (asymptotic Sherwood number) that depends on the velocity profile and tube geometry. For the case of fully developed laminar flow in a circular tube, \( Sh_{m,T} = 48/11 = 4.36 \), while its analogue in the TMM (comparing Eqs. 26 and 36) is \( Sh_{m,E} = 1/\beta_{l} = 48 \) (the dimensionless mass exchange coefficient in the TMMs).

As illustrated in the next section, just as the two-phase models can capture the mass-transfer limited asymptote in heterogeneous reactions (which is missed by the pseudo-homogeneous models), so can the two-mode models capture the mixing-limited asymptote in homogeneous reactions, which is rendered inaccessible by the traditional one-mode models. Thus, there exists the following one-to-one correspondence between two-phase models of catalytic reactors and two-mode models of homogeneous reactors: two-phase transfer time \( t_{TP} \) \( \rightarrow \) local mixing time \( t_{mix} \), two-phase transfer coefficient \( Sh_{m,T} \) \( \rightarrow \) two-mode exchange coefficient \( Sh_{m,E} \), surface (wall) concentration \( C_s \) \( \rightarrow \) spatially averaged concentration \( \langle C \rangle \), and mass-transfer limited reaction \( \rightarrow \) mixing-limited reaction.

APPLICATIONS OF TWO-MODE MODELS

Bimolecular Second-Order Reactions

Second-order reactions provide the simplest example of nonlinear kinetics, where micromixing limitations have significant effects on reactant conversion. We use the TMM to determine micromixing effects on conversion of a typical bimolecular second-order reaction of the type

\[
A + B \xrightarrow{k} P \quad \text{with rate} \quad = kC_A C_B
\]

occurring in a CSTR, where \( k \) is the reaction rate constant. For the case of stoichiometric feeding \( (i.e., C_{A,in} = C_{B,in} = C_{in}) \), the conversion \( X \) obtained by using the TMM is given by

\[
X = \frac{1}{1 + \eta} - \frac{\sqrt{4 Da(1 + \eta)} + 1 - 1}{2 Da(1 + \eta)^{2}}
\]

(37)

where \( \eta = \frac{t_{mix}}{t_C} \) is the dimensionless local mixing time, and \( Da = kC_{in}^2 t_C \) is the Damköhler number. Figure 1 shows the variation of conversion \( X \) with \( Da \) for different values of the dimensionless local mixing time \( \eta \). The case of \( \eta = 0 \) corresponds to the ideal CSTR. For \( \eta > 0 \) and \( Da \rightarrow \infty \), the local concentrations \( \langle C_i \rangle \) \((i=A,B)\) approach zero, while the mixing-cup concentrations approach a mixing limited asymptote, given by

\[
\langle C_A \rangle = \langle C_B \rangle = 0 \quad C_{A,in} = C_{B,in} = \frac{\eta}{1 + \eta} \quad X = \frac{1}{1 + \eta}
\]

(38)

As mentioned in the previous section, this mixing-limited reaction...
asymptote for homogeneous reactions is analogous to the mass-transfer limited asymptote for wall-catalyzed reactions. Just as the wall (surface) concentrations approach zero for the case of infinitely fast surface reactions (while the bulk/mixing-cup concentrations remain finite), so do the local concentrations \( C_i \) for infinitely fast homogeneous reactions \( (i=A,B) \). Unlike in catalytic reactions, where exchange between the phases occurs at the solid-fluid boundary, the exchange between modes (scales) in homogeneous reactors occurs over the entire domain.

**Competitive-Consecutive Reactions**

Competitive-consecutive reactions of the type

\[
A + B \xrightarrow{k_1} C \quad \text{and} \quad B + C \xrightarrow{k_2} D
\]

are prototype of many multistep reactions such as nitration of benzene and toluene, diazo coupling, bromination reactions, etc. Experimental observations\(^{[16]}\) show that if the first reaction is infinitely fast as compared to the second one \( (i.e., \frac{k_1}{k_2} \to \infty) \), under perfectly mixed conditions B is completely consumed by the first reaction and the yield of D is zero \( (\text{if A and B are fed in stoichiometric amounts}) \). But it was observed that if the mixing of A and B is not attained down to the molecular scale, the first reaction is not complete and there remains a local excess of B, which can then react with C to produce D. The yield of D increases monotonically as the rate of the second reaction increases, finally attaining a mixing-limited asymptote. We use the TMM for a CSTR to verify this observation. Figure 2 shows the increase in the yield of D, \( Y_D \), with Damköhler number of the second reaction, \( Da_2 \), where \( Y_D = \frac{2C_{mb}/(C_{in} + 2C_{mb})}{C_{Cin}} \), and \( Da_2 = k_2C_{in} \tau C \). The figure corresponds to the case when the first reaction is infinitely fast \( (i.e., \frac{k_1}{k_2} \to \infty) \), and A and B are fed in stoichiometric amounts \( (i.e., C_{Bin} = C_{inin} = C_{in} \text{ and } C_{Cin} = C_{Din} = 0) \). While no D is formed for the case of \( \eta = 0 \) (ideal CSTR), a significant increase in yield of D is obtained if finite micromixing limitations are present in the system. The maximum yield of D, obtained when the mixing limited asymptote is attained also for the second reaction, is

\[
Y_{D,max} = \begin{cases} 
\frac{2\eta}{1+2\eta} & \text{for } \eta \leq 1 \\
\frac{2}{1+2\eta} & \text{for } \eta > 1 
\end{cases}
\]

Thus, in this case, an optimal yield of D is obtained for \( \eta = 1 \).

**CONCLUSIONS**

In the hierarchy of homogeneous reactor models, the classical ideal reactor models stand at one end as the simplest, while the generalized convective-diffusion-reaction (CDR) model stands at the other end as the most detailed one. While the former cannot capture the mixing effects due to local velocity gradients, molecular diffusion and reaction, the latter requires extensive computations, especially for large Schmidt and/or Damköhler numbers, and for multiple reactions with large number of species. The Two-Mode Models (TMMs) proposed here bridge the gap between the two extreme cases of reactor models and provide a practical approach for describing mixing effects on reactor performance. They retain all the parameters present in the full CDR model and therefore all the qualitative features of the latter, and yet their solution requires a numerical effort comparable to that of the classical ideal reactor models.

The analogy between the two-mode models of homogeneous reactors and two-phase models of catalytic reactors could be carried further by noting that for all cases of well-defined flow-fields, where two-phase mass-transfer coefficients \( (S_{Th}) \) can be estimated theoretically, the exchange coefficient \( (S_{Te}) \) or the local mixing time \( (\tau_{mix}) \) of the TMMs could also be estimated. For more complex flow-fields \( (e.g., \text{packed beds}) \), the local mixing time, like the mass-transfer coefficient, could be correlated to Re, Sc, and the geometrical characteristics of the system. Thus, the two-mode models of homogeneous reactors are as general as the two-phase models of catalytic reactors and have a similar range of applicability. (In fact, the classical two-phase models are also two-mode models, the modes being the cup-mixing and the surface (or solid-phase) concentrations. Thus, the two-mode/
two-scale approach may be used to present a unified theory of homogeneous and heterogeneous reactors."

To summarize, the two-mode models are the minimal models that provide a low-dimensional description of mixing, by coupling the interaction between chemical reaction, diffusion, and velocity gradients at the local scales to the macro-scale reactor variables. Due to their simplicity and generality, it is hoped that they will find applications in the preliminary design and optimization of homogeneous chemical reactors, as well as provide an alternative method for teaching micromixing effects in homogeneous reactors.

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REFERENCES


Dear Editor:

I recently used the illustration below to explain the benefits of countercurrent flow to students in a separation process subject that I teach. I've never heard this illustration used before and it seems to be a good one, so I thought it would be good to put it in the public domain for the benefit of other lecturers. However, it is very short and does not warrant being a "peer-reviewed" paper.

Explaining Why Counter-Current is More Efficient than Co-Current

While washing the dishes one night, I realized that this activity provides a useful everyday illustration of why countercurrent mass and heat transfer processes are more efficient than co-current ones.

I asked the students in my class what would be the best way to clean a pile of dirty dishes if they had at their disposal one basin of dirty wash water and one basin of clean wash water. The class quickly reached the consensus that it would be best to first use the dirty water to clean off as much of the dirt as possible and then use the clean water to perform a second-stage clean. The dirty water would remove the bulk of the dirt, minimizing the contamination of the clean water and leaving it in better condition to clean off any remaining stubborn dirt. Putting the dirty dishes straight into the clean water would quickly dilute and waste its cleaning ability.

This is equivalent to having the countercurrent flow of streams in a liquid-liquid extraction or gas-liquid absorption column. The clean solvent is best used to perform the final stage of cleaning, while the used solvent is still able to perform some cleaning of the raw feed stream as it enters the column.

Students seemed to intuitively understand this illustration, and it provides a non-graphical complement to the usual method of explaining the benefits of countercurrent flow, which involves showing how the average concentration (or temperature) difference driving force differs between co-and countercurrent flows.

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INTRODUCING MOLECULAR BIOLOGY TO ENVIRONMENTAL ENGINEERS
Through Development of a New Course

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Historically, applications of biology in chemical and environmental engineering have been approached from different perspectives with different goals. For example, chemical engineering optimizes biochemical reactions of pure cultures of microorganisms in highly controlled bioreactors used for manufacturing (e.g., fermentation), whereas environmental engineering employs mixed microbial communities with minimum controls as least-cost processes for meeting regulatory requirements (e.g., sewage treatment). Although chemical and environmental engineering education often incorporates formal training in biology, the motivation for course selection can be very different. Incremental advances in biological knowledge that can be used to increase manufacturing capability or improve efficiency are useful in chemical engineering practice, and their integration into chemical engineering education is justified.

The same principle does not hold for environmental engineering, however. Once minimum regulatory requirements are met, incremental advances in biological knowledge do not offer the significant cost savings for environmental biological unit operations that are needed to encourage the adoption and integration of the new knowledge into environmental engineering education.

Recently, development of 16S ribosomal ribonucleic acid (16S rRNA)-targeted technology provided researchers in environmental engineering with new tools to identify microorganisms and to study microorganisms in bioreactor environments. As compared to classical techniques for identification and enumeration, 16S rRNA-targeted technology allows in situ examination of the structure (i.e., who is present?) and function (i.e., what are they doing?) of microbial communities without a prerequisite for isolating pure cultures.113 For researchers in environmental engineering, 16S rRNA-targeted technology has been extensively tested, and current research activities have moved beyond the “proof-of-concept” state to widespread applications.23 In contrast, integration of 16S rRNA-targeted technology within the environmental engineering curriculum remains to be fully developed. At the University of Cincinnati, the author has developed and pilot tested a “proof-of-concept” course titled “Molecular Methods in Environmental Engineering.”

The course was designed to teach limited fundamentals of molecular biology in the context of quantitative engineering design and practice. During its first offering, fifteen graduate students in environmental engineering were exposed to “state-of-the-art” technology, including hands-on laboratory exercises following the “full-cycle 16S rRNA approach.”10 Students learned the importance of detailed understanding of microbial communities and microbial-mediated biochemical networks in biological unit operations, natural biological systems, and the global biosphere. The format of the course included a weekly lecture as well as a semester-long series of hands-on laboratory exercises designed to teach students to develop scientific questions, learn appropriate methodology, conduct careful experimentation, analyze data, and draw conclusions worthy of presentation to peers. Thus the final outcome of the course included preparation of peer-review quality manuscripts by each team of students as well as one-on-one interviews with the instructor.

FULL-CYCLE 16S rRNA APPROACH

Traditionally, the identification of microorganisms in environmental samples has relied upon semi-selective culturing or direct microscopic examination. These techniques have led to a rudimentary understanding of the role of microorganisms in the global biosphere as well as the importance of microorganisms in public health and biocatalysis. Recently, the techniques for determinative microbiology have been dramatically expanded to include cultivation-and-morphologic-independent identification and enumeration of microorgan-

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**Figure 1.** Schematic of the principal steps in the “full-cycle 16S rRNA approach.” Genetic material is isolated directly from an environmental sample and the 16S rDNA genes are amplified in a PCR. The product of the PCR is cloned, and recombinants are isolated for extraction of plasmid DNA. Automated sequencing is used to provide the primary nucleotide structure of the clones, and probe design is accomplished using semi-automated procedures and readily available software. Finally, individual microbial cells are visualized through fluorescence in situ hybridization (FISH) with fluorescently labeled 16S rRNA-targeted oligonucleotide probes.

**FORMAT FOR LABORATORY EXERCISES**

**Step 1** • Students arranged themselves into teams of three. The selection of teammates was based both on a common interest in one environmental sample and on an effort to spread previous experience and expertise in molecular biology among the groups.

**Step 2** • Teams identified, evaluated, and proposed an appropriate environmental system for study. Each system se-
lected for the course was novel for the field of environmental engineering and possessed the capacity to stimulate a more extensive research question (e.g., supplemented a research question in an existing/developing MS or PhD degree, or promoted a novel research direction generally underexplored.) A sample was obtained from the selected system. In all cases, preference was placed on samples that were a part of a developing/ongoing research project with significant supplementary information generated from advanced process engineering and chemical/physical analyses (e.g., sample(s) from a novel bioreactor configuration or a bioreactor treating a novel waste stream).

**Step 3** • Each team generated 16S rDNA sequence information from their sample(s). Genomic DNA was extracted using an UltraClean Soil DNA Isolation Kit[7] according to the manufacturer’s instructions. Mechanical lysis of the samples was performed for one minute at the maximum setting of a Mini Beadbeater-8.[13] Genomic DNA was quantified using a Genesys 10uv[15] spectrophotometer assuming that an absorbance reading of 1.0 at a wavelength of 260 nm corresponded to a concentration of 50 mg DNA/l.

The 16S rDNA genes of bacteria present in the sample were amplified by PCR using primer set S-D-Bact-0011-a-S-17 (5’ to 3’ sequence = gTT TgA TCC Tgg CTC Ag) and S-D- Bact-1492-a-A-21 (5’ to 3’ sequence = ACg gYT ACC TTg TTA CgA CTT). [14] The conditions for PCR included: 5 min. at 94°C; 30 cycles of 0.5 min. at 94°C, 0.5 min. at 55°C, and 0.5 min. at 72°C; 7 min at 72°C; and hold at 4°C. Each reaction tube contained: 1.25 U Takara Ex Taq polymerase,[9] 1x Takara Ex Taq reaction buffer, 200 µM of each deoxyribonucleotide triphosphate (dNTP), 0.2 µM of each primer, and 500 ng of genomic DNA. PCR was conducted using a model 2400 thermal cycler.[8]

Agarose gel electrophoresis was used to check the quality of the PCR product. A 1% (wt./vol.) agarose gel was prepared in 1 x tris buffered EDTA (1 x TBE is 90mM tris borate and 2 mM ethylenediameine-tetraacetic acid (EDTA)) according to the manufacturer’s instructions.[19] Electrophoresis was conducted for two hours using a setting of 100 V for the power supply. DNA fragments were visualized with a hand-held UV lamp after staining the agarose gel for ten minutes at room temperature with 4% (wt./vol.) paraformaldehyde prepared in 1 x phosphate buffered saline (1 x PBS is 130 mM NaCl and 10 mM sodium phosphate buffer). The samples were subsequently stored at -20°C in a 50% (vol./vol.) mixture of ethanol and 1 x PBS. The fixed samples were applied in a sample well on a Heavy Teflon Coated microscope slide[21] and air-dried. FISH was performed as previously described.[22] Briefly, each microscope slide was dehydrated in an increasing ethanol series (50, 80, and 95% [vol./vol.] ethanol, one each minute), each sample well was covered with 9 µl of

Two clones from each team were selected for commercial, automated dideoxy terminal sequencing by the DNA Core Facility at the University of Cincinnati. Sequencing primers included M13(-20) forward and M13 reverse[10] as well as S- *-Bact-0343-a-A-15 (5’ TAC ggg Agg CAg CAg 3’), S- *-0519-a-S-18 (5’ gTA TTA CgC Cgg CTg CTg 3’), S- *-Bact- 0907-a-A-20 (5’ AAA CTC A AA TgA ATT gAC gG 3’), and S- *-Bact-a-S-16 (5’ Agg gTT gCT gCT gT g 3’).[18]

**Step 4** • An initial phylogenetic analysis was conducted, and the results were used to design oligonucleotide hybridization probes for fluorescence in situ hybridization (FISH). Assembled sequences were compared to the Ribosome Database Project (RDP) (available at rdp.cme.msu.edu) using Chimera Check and Probe Match. Preliminary phylogenetic affiliation was confirmed using a BLAST (Basic Local Alignment Search Tool) search of GenBank (available at www.ncbi.nlm.nih.gov, follow the links to BLAST). The fluorescently labeled oligonucleotide probes were ordered from a commercial vendor.

**Step 5** • Each team conducted fluorescence in situ hybridization (FISH) analysis of their original samples. Aliquots of the original sample were chemically “fixed” for one hour at room temperature with 4% (wt./vol.) paraformaldehyde prepared in 1 x phosphate buffered saline (1 x PBS is 130 mM NaCl and 10 mM sodium phosphate buffer). The samples were subsequently stored at -20°C in a 50% (vol./vol.) mixture of ethanol and 1 x PBS. The fixed samples were applied in a sample well on a Heavy Teflon Coated microscope slide[21] and air-dried. FISH was performed as previously described.[22] Briefly, each microscope slide was dehydrated in an increasing ethanol series (50, 80, and 95% [vol./vol.] ethanol, one each minute), each sample well was covered with 9 µl of
hybridization buffer (20% [vol/vol.] formamide, 0.9 M NaCl, 100 mM Tris HCl [pH 7.0], 0.1% SDS), and fluorescein-labeled oligonucleotide probe, 1 µl (50 ng), was added to each sample well. Hybridizations were conducted in a moisture chamber for two hours, in the dark, at 46°C. The slides were washed for 30 minutes at 48°C with 50 ml of prewarmed wash solution (215 mM NaCl, 20 mM Tris HCl [pH 7.0], 0.1% SDS, and 5 mM EDTA). Fixed, hybridized cells were mounted with Cargille immersion oil[23] and a cover slip. Probe-conferred fluorescence was visualized with a model E600 upright epifluorescence microscope,[24] and digital images were captured using a Spot-2 charge coupled device (CCD) camera.[25] The results of the FISH analysis included determining the abundance and spatial organization of phylogenetically defined microbial populations identified by unique oligonucleotide hybridization probes.

The students learned the procedures for the laboratory exercises through a video series produced specifically for this course. They were given a laboratory manual at the start of the class, and videos of the laboratory exercises were distributed biweekly in VHS format. The manual outlined all of the procedures for the laboratory and provided step-by-step instructions to complete each exercise. The videos gave the students an opportunity to view the instructor completing all of the steps of each exercise. The laboratory exercises were completed independently by the three-student teams according to a schedule arranged at the start of the class. Approximately the first fifteen minutes of the weekly lectures were dedicated to reviewing the progress of each team toward meeting the schedule for completion of the laboratory exercises.

TOPICS FOR THE LECTURES

Each week, approximately two hours were spent in a lecture discussion format with the entire class. The nine topics that were covered in the pilot course included:

- Overview of methods including the value of different methods and an answer to the question, “Why do Environmental Engineers need to learn molecular biology?”
- Measuring microbial community structure
- Measuring microbial community function
- Quantitative molecular biology for Environmental Engineering versus qualitative molecular biology for Environmental Science
- Troubleshooting the laboratory exercises to improve the course for the subsequent year
- What is this “phylogeny stuff” anyway?
- Historical development of molecular tools in Environmental Science and Engineering
- Success stories for molecular tools in Environmental Science and Engineering
- Principles of microscopic examination

Figure 2 summarizes the results of students’ responses to a demographic survey. Thirteen of the fifteen students enrolled in the course responded to the survey. The class was divided almost equally between male and female students with a median age of 27-30 years old. Five of the students had received significant formal training in biology, previously participating in more than ten biology courses. The majority of the students had already completed their MS degree (eight out of thirteen), but more than 50% of the students had received their degree outside of environmental engineering or environmental science. Most students spent less than six hours per week on the course, but some students spent significantly more time. Overall, the students enrolled in the pilot test of “Molecular Methods in Environmental Engineering” could be categorized as mature students (i.e., in their late twenties working toward their doctoral degrees). Furthermore, the class contained a significant number of students with extensive previous experience in biology. Thus, the students enrolled in the pilot course were well prepared in maturity and previous biology experience to actively participate in this novel course. As the course continues to be offered, I plan to track the success of the course in relationship to the demographics of the enrolled students.

In addition to collecting demographic information, at the end of the class the students were asked to respond to three open-ended questions. In response to the question, “In your opinion, were the objectives of the course met?” students responded:

- The course met some of the objectives, but some students
Graduate Education

are not convinced why we use molecular biology to identify microorganisms in systems that have been proved or have been operating successfully.

- Yes, I am equipped with knowledge about this approach, and I can interpret research results and publications from this developing field.

In response to the question, "What was the best aspect of this course?" students responded:

- Most of the procedures are basic/universal operations in molecular biology which means that we understand how to study biology and biotechnology at the molecular level.
- Experimental work—because it is through applications that a student gets a tight grip on ideas and concepts. In addition, the challenging experiments and the value of the final result make the work more interesting.
- The lectures were interesting and informative. I learned a great deal, and my ideas about environmental engineering and science have been positively affected by the knowledge I have gained.
- Your perspective. We will never see "cutting edge" developments in a book.
- The whole structure of the course is similar to a research project.
- The best aspect was carrying the concepts from the classroom to the lab in a manner relevant to our field. Also, having a class that is new gives a fresh perspective into the future of environmental engineering.

In response to the question, "What part of the course would you suggest improving?" students responded:

- More theoretical basis, especially for the background of molecular biology methods.

From their responses to the open-ended questions, it is apparent that the students felt the pilot course was a success. It is interesting to note that the students appreciated that the pilot course represented an effort to integrate research into the classroom. One of the greatest difficulties for developing a role for molecular biology in an engineering curriculum is discovering a mechanism for moving these "state-of-the-art" research skills into a classroom setting. In the future, we plan to expand the enrollment for "Molecular Methods in Environmental Engineering" to include undergraduate environmental engineering students as well as graduate and undergraduate students from related disciplines, including chemical engineering and biomedical engineering.

CONCLUSIONS

To address the growing national need for integrating genomics and molecular biology into the engineering curriculum, the author developed and pilot tested a new course, "Molecular Methods in Environmental Engineering." Fifteen graduate students were successfully introduced to molecular biology through lectures and hands-on laboratory exercises following the "full-cycle 16S rRNA approach." Although the pilot course can be considered a success, future offerings of this course must be modified to reduce the difficulty of comprehending molecular biology by inexperienced engineering students. One of the most daunting challenges for this type of "state-of-the-art" course is providing a supportive, yet independent learning environment. For highly motivated graduate students, the author demonstrated that the format for this course is successful. To offer this course to undergraduate students or poorly prepared graduate students represents a future challenge. In upcoming course offerings, the author plans to open enrollment for "Molecular Methods in Environmental Engineering" to undergraduate students in environmental engineering as well as students in chemical engineering and biomedical engineering. As genomics and molecular biology become as common to an engineering curriculum as chemistry and physics, engineering faculty need to take the lead in developing courses that introduce these topics from an engineering perspective with a focus upon quantitative approaches and the application of science to find cost-effective solutions to society's problems.

ACKNOWLEDGMENTS

This laboratory course would not have been possible without the commitment of significant resources from the Department of Civil and Environmental Engineering of the University of Cincinnati. For the success of the pilot test, the author is grateful to the Department.

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To the Editor:

This letter is motivated by the paper "An Undergraduate Course in Applied Probability and Statistics" that appeared in the Spring 2002 issue of Chemical Engineering Education. Probability and statistics are difficult subjects to teach to engineering students, and Professor Fahidy is to be congratulated on his efforts in this area.

In this letter we would like to refer to the discussion and examples related to regression analysis. Professor Fahidy discusses in detail the use of numeric information (such as error variance, confidence intervals, correlation coefficient, etc.) for regression analysis, but does not mention graphic information (residual plots) and physical insight for regression analysis. Using the examples presented by Professor Fahidy, we would like to demonstrate the importance of including graphical information and physical arguments in the regression analysis.

Let us refer first to Example 4 in the paper. In this example, the integral method of rate data analysis is used for a (supposedly) first-order reaction. Nonlinear regression can be used

TABLE 1

<table>
<thead>
<tr>
<th>Reaction Order</th>
<th>1st Order</th>
<th>2nd Order</th>
<th>0th Order</th>
<th>2nd Order</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model</td>
<td>logY=k*t</td>
<td>Y=exp(k*t)</td>
<td>Y=Y/a+k*t</td>
<td>Y=Y/a+k*t</td>
</tr>
<tr>
<td>k (value)</td>
<td>0.0039888</td>
<td>0.0038126</td>
<td>-0.0042162</td>
<td>0.0059893</td>
</tr>
<tr>
<td>95% Conf. Interval</td>
<td>±0.0011009</td>
<td>±0.0010816</td>
<td>±0.0012594</td>
<td>±0.0059893</td>
</tr>
<tr>
<td>Y_0 (or 1/Y_0 , value)</td>
<td>-</td>
<td>1.0329275</td>
<td>0.9365288</td>
<td></td>
</tr>
<tr>
<td>95% Conf. interval</td>
<td>-</td>
<td>±0.5865825</td>
<td>±0.1012594</td>
<td></td>
</tr>
<tr>
<td>R^2</td>
<td>0.7620164</td>
<td>0.7770319</td>
<td>0.80362884</td>
<td>0.7757433</td>
</tr>
<tr>
<td>Variance (based on Y)</td>
<td>0.0023055</td>
<td>0.002271</td>
<td>0.0018759</td>
<td>0.0021994</td>
</tr>
</tbody>
</table>

Figure 1. Residual plot for Example 4 in Fahidy paper.

for finding the reaction rate coefficient (k) using concentration (Y) versus time (t) data, on the regression model Y = exp(-kt). Alternatively, this equation can be linearized to yield lnY=-kt, where linear regression can be applied. The results of the linear and nonlinear regression that were obtained using POLYMATH 5.1 are shown in the first two columns of Table 1. Note that these results are different from what is presented in [1], but they are correct and were confirmed by the author of the original article. Looking at the numerical information presented in Table 1 (parameter values, confidence intervals, correlation coefficients, and variances) leads to the conclusion that there is no significant difference between linear and nonlinear regression for determining k (the variances are almost the same, contrary to what is argued in [1]). The same information may also lead to the conclusion that the model fits the data reasonably well. This conclusion, however, is contradicted by the residual plot shown in Figure 1. The residuals are not randomly distributed around a zero value. This may indicate either lack of fit of the model, or that the underlying assumption of a random error distribution for the dependent variables is incorrect.

Physical insight can suggest alternative regression models, but more information regarding the reaction involved is needed. Since no such information is available, we will assume a homogeneous reaction, just for the sake of the demonstration. Assuming 0th order reaction or 2nd order reaction yields the models shown in the third and fourth columns of Table 1, respectively. The numeric information presented in the Table points on the 0th order reaction as the most appropriate one (smallest variance value—note that in order to be on a unique scale, all the variance calculations must be based on Y). The residual plot for the 0th order reaction is not significantly different, however, from that shown in Figure 1; thus, this model is not supported by the residual plot either.

The conclusion from proper analysis of this example is that the data available are insufficient (in quality, quantity, or both) to determine in any certainty the order of the reaction it represents. To obtain a more definite result, additional measurements must be made.

In Example 5, a linear model Y=a+bx is fitted to data of mean fuel consumption rate (Y) versus vehicle mass (x). The numerical results that were obtained for this example, using POLYMATH, are: parameter values (including 95% confidence intervals) a=-0.8695975±2.0733031;
A New Approach to Teaching TURBULENT THERMAL CONVECTION

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At AIChE’s annual meeting in 2000, I gave an oral presentation of an early version of a pair of new expressions, completely free of explicit empiricism, for the prediction of fully developed turbulent thermal convection in all channels and for all thermal boundary conditions. At the same venue, in 2001 I also presented a greatly improved version, although at the expense of a smidgen of empiricism. Both presentations prompted the same question from participants: “Is this approach being taught to current students, and if not, why not?” I explained in both instances that this material is very new and is not in any textbooks, and furthermore, that it may not appear in textbooks for some time to come since the authors of transport textbooks must first become aware of the concept and its results, and then be convinced of its educational (as well as predictive superiority) over the method they are currently teaching. Also, as Anderson[11] has noted, textbooks in chemical engineering seem to have a unique longevity, and the more successful of them are replaced or revised only after long intervals of time.

Undoubtedly with these textbook characteristics in mind, my mentor and departmental chairman, Donald L. Katz, long ago made the suggestion (which to a young assistant professor was virtually an order) that every year I replace at least 20% of the graduate transport course content by embracing new developments in the literature. Throughout my career, that suggestion led to my use of notes incorporating these new segments, together with using a book or books as a supplement rather than the other way around. I conclude, a full half-century later, that this process of annual supplementation and revision has, by virtue of the associated forced self-study and self-learning in the fields of my teaching, more than compensated me (and perhaps my students) for the efforts, and that it is a worthy complement of the new materials most of us introduce periodically from our own research and consulting. I am here taking advantage of the platform provided by Chemical Engineering Education to encourage and assist the process of supplementation for transport teachers with respect to a new approach for the description and prediction of turbulent thermal convection.

In a previous CEE article,[2] I presented a new approach to the description and teaching of turbulent flow with the same objective. For that simpler and more restricted topic, it was possible to include in the presentation a virtually complete set of supplementary notes for direct use by any interested faculty member. For the much more complex process of turbulent thermal convection and the much more complex process of development of the new model, however, the presentation of a working set of supplemental notes in this format is simply not feasible. Rather, this article has the more limited objective of outlining the new approach with the hope that faculty members who teach transport will be inspired to study the more complete documentation in the key references and make the effort to formulate their own supplemental notes. Perhaps I will eventually find the time and motivation to prepare a monograph on this topic, but I do not recommend that anyone procrastinate with that as the excuse.

When an analogue of the approach that was so simple,
straightforward, and successful for turbulent flow was first attempted for the closely related topic of turbulent thermal convection, I anticipated that the path of development would closely parallel the previous one. While convection is inherently more complex than flow in several respects, it is also simpler in the sense that it merely consists of the superposition of a scalar quantity, the temperature, on the flow. The path of development that emerged after considerable trial and error proved to reflect the greater complexity that had been anticipated, and the final results proved to reflect the anticipated greater simplicity.

The predictive equations for turbulent thermal convection that are described in this paper are, by a significant margin, more accurate, fundamentally sound, and general than any prior ones. They also provide better insight into the relationship between flow and convection and a better conception of thermal convection itself that more than compensates for the greater detail. This new material should therefore, as suggested by audience members at the AIChE presentations, be given serious consideration for inclusion in the final portfolios of both our undergraduate and graduate students.

Apart from the merit of the predictive equations for turbulent thermal convection that emerged, the path of their development appears to have merit itself in an educational sense. On the one hand, it provides insight into a creative process of correlation that is within the capabilities of our students. On the other hand, it provides a perspective within which the strengths and weaknesses of all forms of correlation can be evaluated, not only in flow and convection but also in every aspect of chemical engineering. Our students should be made to realize that whatever career they follow after graduation, they will spend considerable time using and/or formulating correlations.

I have a predilection for presentations in narrative and historical contexts under the presumption that the personal characteristics, as well as the triumphs and failures, of our predecessors not only stimulate interest but also provide a mnemonic for students. In this instance, a description of the serendipitous and irregular path of development of a completely new formulation in a relatively mature field may serve a similar role. Teachers who prefer a more orderly and skeletal approach are welcome to eliminate such diversionary material.

Many details concerning origins, proofs, uncertainties, and limitations are deferred to the references, and in particular to Churchill and Zajic. It is, however, essential that the teacher present these details, or perhaps in the instance of graduate students, assign key references as required collateral reading. In either event, students should be encouraged to question the validity of the many assertions and simplifications in this article rather than accept them “on faith.” Undergraduate students may require more guidance than do graduate students with respect to the new approach, but they have the counterbalancing advantage of less to unlearn.

THE NEW APPROACH FOR TURBULENT FLOW

A thorough understanding by students and faculty alike of the new approach for the description and teaching of turbulent flow, as previously described [2], is an essential prerequisite for the complementary new approach presented here for turbulent thermal convection. Because of space limitations, however, only those results that are directly applied or adapted for thermal convection will be reproduced here.

The time-averaged, once-integrated differential equation of conservation for momentum in the radial (negative-y) direction in steady-on-the-mean, full developed flow of a fluid of invariant density and viscosity through a round tube can be represented by

$$
\tau_w \left( 1 - \frac{y}{a} \right) = \mu \frac{du}{dy} - \rho u \nu' 
$$

Here, $\tau_w$ is the shear stress on the wall, $y$ is the distance from the wall, $a$ is the radius of the pipe, $u$ is the time-averaged velocity, and $u'$ and $v'$ are the fluctuating components of the velocity in the $x$ and $y$ directions, respectively. The superbar designates the time-average of their product, while $\mu$ and $\rho$ are the dynamic viscosity and specific density of the fluid. (Aside to teachers: The origin of this expression and the physical meaning of the several variables and terms, including the signs of the latter, should be described or reviewed as appropriate. Any uneasiness of the students in this regard can be expected to persist in what follows. Of course, this warning applies to some extent to subsequent details as well.)

Equation (1) can be rewritten in terms of the dimensionless “wall” variables of Prandtl, namely

$$
u^+ = u^+ / \tau_w = u^+ / \left( \frac{\rho}{\tau_w} \right)^{1/2}
$$
$$y^+ = y(\tau_w \rho)^{1/2} / \mu
$$
$$a^+ = a(\tau_w \rho)^{1/2} / \mu
$$

and one new variable, namely the fraction of the transport of momentum (or the total shear stress) due to the turbulent fluctuations $(u'v')^+$ as

$$
\left( \frac{1 - y^+}{a^+} \right) \left( 1 - \frac{u^+}{a^+} \right) = \frac{du^+}{dy}
$$

Equation (1), with $y^+/a^+$ replaced by 1-R, can be integrated formally to obtain the following expression for the radial distribution of the time-averaged velocity:

$$
\frac{u^+}{2} = \frac{u^+}{2} \int \frac{1}{R} \left[ 1 - (u'v')^+ \right] dR^2
$$
The velocity distribution can in turn be integrated over the cross-section to obtain, after utilizing integration by parts, the following integral expression for the mixed-mean velocity and thereby the Fanning friction factor:

\[
\frac{1}{2} \left( \frac{2}{f} \right)^{1/2} = u_m^+ = \int_0^1 u^+ dR^2 = a^+ \int_0^1 \left[ 1 - (u'v')^+ \right] dR^4 \tag{4}
\]

Equations (1) through (4) are exact insofar as the restrictions mentioned above with respect to Eq. (1) are fulfilled. In order to implement Eqs. (3) and (4), an expression is required for \((u'v')^+\) in terms of \(y^+\) and \(a^+\). For this purpose, Churchill\(^4\) proposed the following semi-empirical expression:

\[
\left[ (u'v')^+ \right]^{-8/7} = \left[ 0.7 \left( \frac{y^+}{10} \right)^3 \right]^{-8/7} + \exp \left\{ \frac{-1}{0.436y^+} + \frac{1}{0.436a^+} \right\}^{-8/7} \tag{5}
\]

It is essential for the students to be aware of the origins and uncertainties of Eq. (5) since this expression has a critical role, both numerically and functionally, in all of the developments that follow for both flow and convection. The third-power dependence on \(y^+\) for small values of \(y^+\) was originally postulated on the basis of asymptotic analyses, but has since been confirmed by \textit{direct numerical simulations}, which have also produced a theoretical value of approximately \(7 \times 10^{-4}\) for the numerical coefficient. The exponential term for moderate values of \(y^+\), as well as the deductive term for \(y^+\to a^+\), were both derived by speculative analysis, but the coefficients of 0.436 and 6.95 were determined from recent, improved experimental data for the time-averaged velocity distribution. The power-mean form of Eq. (5) is arbitrary and the combining exponent of \(-8/7\) is based on experimental data for \((u'v')^+\).

**AN ASIDE ON A GENERIC CORRELATING EQUATION**

Equation (5) is a particular application of the generic correlating equation proposed by Churchill and Usagi\(^5\) for two regions, namely

\[
y^b = y_0^b + y_b^+ \tag{7}
\]

Here, \(y = y(x)\), \(y_0 = \{x \to 0\}\), \(y_b = y(x \to \infty)\), and \(b\) is an arbitrary exponent. Either \(y_0\) or \(y_b\) or both are necessarily functions of \(x\) rather than fixed values. For three regions, Eq. (7) can be extended either directly as

\[
y^b = \left( y_0^b + y_b^+ \right)^q + y_m^b \tag{8}
\]

or in staggered form as

\[
y^b = \left( y_0^b + y_b^+ \right)^q + y_m^b \tag{9}
\]

Here, \(y_0\) is an intermediate asymptote and \(q\) is a second arbitrary exponent. The reverse order of combination of \(y_0\), \(y_b\), and \(y_m\) leads to equally valid and, in general, fundamentally different representations. Equations (7) through (9) have been introduced here to avoid interrupting the continuity of the development in which they are used.

**DEVELOPMENT OF A NEW FORMULATION FOR TURBULENT CONVECTION**

The analogue of Eq. (1), with the additional idealization of negligible viscous dissipation, is

\[
\frac{j}{L} = -k \frac{\partial T}{\partial y} \tag{10}
\]

and that of Eq. (2) is

\[
\frac{1}{j_w} \left[ \frac{1}{(T'v')^+} \right] = \frac{\partial T^+}{\partial y} \tag{11}
\]

Here, \(j\) is the heat flux density in the \(y\)-direction, \(T\) is the temperature of the fluid, \(j_w\) and \(T_w\) are their values at the wall, \(T^+ = k(\tau_{w0})^{1/2} (T_w - T) / j_w\). \(T'v'\) is the time-averaged product of these fluctuating quantities, \((T'v')^+ = pcT'v' / j\) is the fraction of the radial heat flux density due to the turbulent fluctuations, and \(k\) is the thermal conductivity of the fluid. The terms \(j/w\) and \((T'v')^+\) in Eq. (11) depend on two parameters, namely the Prandtl number \(Pr = \mu c_p / k\) and the mode of heating at the wall, as well as on \(y^+\) and \(a^+\).
From an energy balance over an inner cylindrical segment of the fluid stream, it follows that

\[
\frac{\dot{\jmath}}{\dot{\jmath}_w} = \frac{1}{R} \int_0^{R^2} \frac{u_m}{u} \left( \frac{\partial T}{\partial x} / \frac{\partial T_m}{\partial x} \right) \, dR^2
\]  

(12)

Here, \(T_m\) is the mixed-mean temperature of the fluid stream. As contrasted with \(\tau / \tau_w\), which may be inferred from Eq. (1) to vary linearly with \(R\), \(\dot{\jmath}/\dot{\jmath}_w\) varies non-linearly because of its dependence on the velocity distribution and in some instances on the temperature distribution as well. Also, as can be inferred from Eq. (12), \(T\) varies with \(x\) as well as with \(y\), even in fully developed thermal convection, whereas \(u\) varies only with \(y\) in fully developed flow. Fully developed thermal convection is ordinarily defined by two criteria, namely

\[
\begin{align*}
\frac{\partial}{\partial x} \left( \frac{T_w - T}{T_m - T_w} \right) &= 0 \\
\frac{\partial h}{\partial x} &= 0
\end{align*}
\]

where \(h \equiv \dot{\jmath}_w / (T_m - T_w)\) is the local heat transfer coefficient.

Equation (11) can be put in a more tractable form for both formal and numerical solution by introducing new variables \(\gamma\) and \(Pr_1\) defined as follows, in place of \(\dot{\jmath}/\dot{\jmath}_w\) and \(\overline{(T'v')}^{++}\)

\[
1 + \gamma = \frac{\dot{\jmath}_w}{\dot{\jmath}_w / \tau} = \frac{1}{R^2} \int_0^{R^2} \frac{u_m}{u} \left( \frac{\partial T}{\partial x} / \frac{\partial T_m}{\partial x} \right) \, dR^2
\]  

(13)

and

\[
\frac{Pr_1}{Pr} = \frac{Pr}{1 - \overline{(u'v')}^{++}} \left( \frac{\overline{(u'v')}^{++}}{\overline{(T'v')}^{++}} \right)
\]  

(14)

The result is

\[
\frac{(1 + \gamma)R}{1 + \frac{Pr}{Pr_1} \overline{(u'v')}^{++}} \left( \frac{\overline{(u'v')}^{++}}{\overline{(T'v')}^{++}} \right) = \frac{dT^+}{dy^+}
\]  

(15)

The use of \(\gamma\), the perturbation of the heat flux density distribution from that of the shear stress distribution, was suggested by Reichardt. The variable \(Pr_1\) was originally introduced in connection with modeling in terms of the eddy viscosity and eddy conductivity, and accordingly, by analogy with the corresponding ratio of molecular quantities, was called the turbulent Prandtl number. Although the redefinition of \(Pr_1\) in terms of \(\overline{(u'v')}^{++}\) and \(\overline{(T'v')}^{++}\) avoids these heuristic variables, the traditional name and symbol for this quantity are retained herein out of respect for its historical origin. It should be noted that \(Pr_1\) is not necessarily proportional to \(Pr\) since \(\overline{(T'v')}^{++}\) is, in general, a function of \(Pr\).

Equation \(-\) can be integrated formally to obtain

\[
T^+ = \frac{a^+}{2} \frac{1}{R^2} \int_0^{R^2} \left( \frac{1}{1 + \frac{Pr}{Pr_1} \overline{(u'v')}^{++}} \right) \left( \frac{1}{\overline{(u'v')}^{++}} \right) \, dR^2
\]  

(16)

Then \(T^+\), weighted by \(u^+ / u^+_m\), can be integrated over the cross section to obtain

\[
\frac{Nu}{T_m^+} = \frac{2a^+}{Pr_1 \overline{(u'v')}^{++}}
\]  

(17)

For uniform heating at the wall, it follows from the criteria for fully developed thermal convection that \(\partial T / \partial x = \partial T_m / \partial x\). It then follows from the corresponding reduced form of Eq. (13), together with Eqs. (3) and (4), that \(\gamma\) is a function only of \(\gamma^*\) and \(a^*\). Equation (17) can then by virtue of the same considerations, be integrated by parts to obtain

\[
Nu = 8 \int_0^{(1 + \gamma)^2 \overline{(u'v')}^{++}} \left( \frac{1}{1 + \frac{Pr}{Pr_1} \overline{(u'v')}^{++}} \right) \, dR^4
\]  

(18)

Equation (18) can be reduced for three special cases. For \(Pr = 0\), it can be expressed as

\[
Nu_0 = Nu(Pr = 0) = \frac{2}{(1 + \gamma)^2 \overline{(u'v')}^{++}} = 8(1 + \gamma)^2 \overline{(u'v')}^{++} \overline{(T'v')}^{++}
\]  

(19)

while for \(Pr_1 = Pr\), it can be reduced by virtue of Eq. (4) to

\[
Nu_1 = Nu(Pr = Pr_1) = \frac{8}{(1 + \gamma)^2 \overline{(u'v')}^{++}} = \frac{8}{(1 + \gamma)^2 \overline{(u'v')}^{++}} \overline{(T'v')}^{++}
\]  

(20)
Here, as can be inferred, \((1 + \gamma)^2\) designates the integrated-mean value over \(R^1\), and \((1 + \gamma)^2\) the integrated-mean value weighted by \(1 - (u'v')\). Both quantities may readily be evaluated numerically, using Eqs. (3), (4), and (5), and the reduced form of Eq. (13). For \(Pr \rightarrow \infty\), the temperature field develops almost completely very near the wall where \((u'v')\) can be approximated by \(0.7 (\gamma/10)^3\) and \(\gamma\) can be neglected. Equation (16) can then be integrated in closed form to obtain

\[
Nu = Nu\{Pr \rightarrow \infty\} = 3^{3/2} (0.0007)^{1/3} \frac{a^+ (Pr/Pr_1)^{1/3}}{\pi} = 0.07343 \operatorname{Re}(f/2)^{1/2} (Pr/Pr_1)^{1/3} \quad (21)
\]

For uniform wall temperature, the criteria for fully developed convection require that

\[
\frac{dT}{dx} = \frac{dT_m}{dx} \equiv T^+ / T_m^+
\]

Integration of Eq. (17) by parts is no longer possible, but from the limiting form of Eq. (16) for \(R = 0\), it follows that

\[
Nu_0 = 4 \left( \frac{T_c^+}{T_m^+} \right) / \left( 1 + (\gamma) \right)_{\text{mR}} \quad (22)
\]

and

\[
Nu_1 = 4 \frac{u_m^+}{u_c^+} \left( \frac{T_c^+}{T_m^+} \right) \frac{\operatorname{Re}(f/2)}{(1 + (\gamma)_{\text{mR}})_{\text{R}}} \quad (23)
\]

Here, \(T_c\) is the temperature at the axis of the pipe. Equation (21) remains applicable as is. The determination of numerical values of \(\gamma, T_c^+,\) and \(T_m^+\) from Eqs. (13), (16), and (17) now requires iteration, but the functional forms of Eqs. (22) and (23) are adequate for the development herein.

On the basis of the previous experiences with various aspects of turbulent flow, I anticipated that Eqs. (19) through (23) could be combined in appropriate pairings in the form of Eq. (7) to construct satisfactory correlating equations for \(Pr \geq Pr_t\) and for \(Pr \leq Pr_t\), or alternatively, in appropriate triplets in the form of Eq. (8). All such attempts failed, however. I then found (somewhat serendipitously) that a successful correlating equation for turbulent thermal convection could be devised by using a particular analogy between momentum and energy transfer in which the exact solutions for three particular values of \(Pr\) occur in the form of Eq. (9). Accordingly, a brief and very selective review of such analogies is appropriate at this point.

**SELECTIVE ANALOGIES**

Reynolds\(^7\) postulated that the transport of both momentum and energy between a turbulent stream and its confining surface occurred wholly by means of a mass flux of eddies and thereby derived the equivalent of

\[
Nu = Pr \operatorname{Re}(f/2) \quad (24)
\]

Prandtl\(^8\) improved upon the Reynolds analogy by postulating an added resistance due to linear molecular diffusion of momentum and energy across a viscous boundary layer of thickness \(\delta\) in series with transport by the eddies of Reynolds in the turbulent core, thereby obtaining the equivalent of

\[
Nu = \frac{Pr \operatorname{Re}(f/2)}{1 + \delta^+ (Pr - 1)(f/2)^{1/2}} \quad (25)
\]

Equation (25), just as Eq. (24), is inapplicable for \(Pr < 1\), owing to neglect of thermal conduction in the turbulent core, and also for \(Pr >> 1\), owing to neglect of eddy transport within the viscous boundary layer. Even so, it represents a great advance in that it correctly predicts a coupled, non-power dependence on both \(Pr\) and \(Re\), in the latter case by virtue of the dependence of \(f\) on \(Re\). Of the many analogies that have been proposed to eliminate the deficiencies of the Prandtl analogy for large and small values of \(Pr\) (see, for example, Churchill\(^9\)), only two need to be examined here.

Reichardt\(^6\) eliminated \(dy^+\) between the equivalents of Eqs. (2) and (15) and made several ingenious approximations that allowed him to integrate the resulting combined equation in closed form. Churchill\(^10\) assembled the fragments of this solution into a single expression for \(Nu\) and corrected the erroneous expression used by Reichardt for the shear stress near the wall, thereby obtaining

\[
\frac{1}{Nu} = \left( \frac{1 + \gamma}{\text{mR}} \right) \left( \frac{T_m^+}{T_c^+} \right) \left( \frac{u_r}{u_\text{m}} \right) \left( \frac{Pr_t}{Pr} \right) + \frac{13.62}{\operatorname{Re}(f/2)^{1/2}} \left( \frac{T_m^+}{T_c^+} \right) \left( 1 - \frac{Pr_t}{Pr} \right)^{1/3} \quad (26)
\]

Equation (26) is limited in applicability to \(Pr \geq Pr_t\) by virtue of one of the simplifications made by Reichardt in order to be able to integrate analytically.

Churchill\(^10\) (also Churchill and Zajic\(^13\)) followed a completely different path to derive an expression, which for \(Pr \geq Pr_t\) is exactly equivalent to Eq. (26) except for replacement of the term \(1 - Pr/Pr_t\) by \(1 - (Pr/Pr_t)^{1/3}\). In retrospect, the difference in these expressions is a consequence of the approximation of Reichardt of \(du^+\) by \(dy^+\) in the differential term leading to the right-most term of Eq. (26).

**FINAL FORMS**

The final predictive expressions for turbulent thermal convection emerged from the various expressions above by means of the following lengthy series of insights, postulates, and inferences, all of which were essential.

Churchill, et al.,\(^11\) recognized that Eq. (26) was equivalent, with \(T_m^+ / T_c^+\) evaluated at the limiting conditions, to
They further recognized that when Eq. (17) was rearranged as

$$\frac{\text{Nu} - \text{Nu}_1}{\text{Nu}_\infty - \text{Nu}_1} = \frac{1}{1 + \frac{\text{Nu}_\infty}{\text{Nu}_1} \left( \frac{\text{Pr}_t}{\text{Pr}} - 1 \right)}$$

it had the form of Eq. (9), with

$$b = -q = 1$$
$$y_0 = \text{Nu}_1$$
$$y_\infty = \text{Nu}_\infty$$
$$y_1 = \frac{\text{Nu}_1}{\text{Nu}_\infty} \left( \frac{\text{Pr}_t}{\text{Pr}} - 1 \right)$$

The staggered independent variable, $\text{Pr}/\text{Pr}_t - 1$, has the essential role of converting $\text{Nu}_1$ from a particular value to an asymptote. According to Eq. (28), Nu goes through a sigmoidal transition from $\text{Nu}_1$ to $\text{Nu}_\infty$, a nuance of behavior that had previously been overlooked. In retrospect, correlation in terms of Eq. (7), that is, direct interpolation between $\text{Nu}_1$ and $\text{Nu}_\infty$, was doomed to fail. The relationship provided by the Reichardt analogy was essential to the derivation of Eq. (27).

The identification of Eq. (28) with Eq. (9) suggested that the analogue of Eq. (28) in terms of $\text{Nu}_0$ and $\text{Nu}_1$ might be applicable for $\text{Pr} \leq \text{Pr}_t$. That concept led to an expression with a discrete step in the derivative of Nu with respect to $\text{Pr}/\text{Pr}_t$ at $\text{Pr} = \text{Pr}_t$, but elimination of this discontinuity by means of an arbitrary but ultimately vanishing coefficient resulted in

$$\frac{\text{Nu} - \text{Nu}_0}{\text{Nu}_1 - \text{Nu}_0} = \frac{1}{1 + \frac{\text{Nu}_1}{\text{Nu}_\infty} \left( \frac{\text{Nu}_\infty - \text{Nu}_1}{\text{Nu}_1 - \text{Nu}_0} \left( \frac{\text{Pr}_t}{\text{Pr}} - 1 \right) \right)}$$

where $\text{Nu}_\infty = \text{Nu}_0 \{\text{Pr} = \text{Pr}_t\} = 0.07343 \text{Re}(f/2)^{1/2}$.

The absence of any allusion to geometry or to the thermal boundary condition suggested that Eqs. (28) and (29) might be applicable for all geometries and all thermal boundary conditions. Plots of numerically computed values of Nu versus $\text{Pr}/\text{Pr}_t$ for round tubes with uniform heating and uniform wall temperature, and for parallel-plate channels with equal uniform heating and with unequal uniform temperatures, confirmed the validity of this speculation.

These plots in logarithmic coordinates appeared to provide an excellent overall representation for all values of $\text{Pr}/\text{Pr}_t$, for all values of $a^*$ or $b^*$ (where $b$ is the half-spacing of the parallel plates) greater than 145, which is the lower limit for the existence of fully turbulent flow, for all geometries, and for all thermal boundary conditions. The more critical test provided by arithmetic plots, however, reveal errors in Nu of up to 20% for both $\text{Pr}/\text{Pr}_t = 0 (10)$ and $\text{Pr}/\text{Pr}_t = 0 (0.01)$. After many attempted correctives, substitution of the analogy of Churchill for that of Reichardt to obtain

$$\frac{1}{\text{Nu}} = \left( \frac{\text{Pr}_t}{\text{Pr}} \right) \frac{1}{\text{Nu}_1} + \left[ 1 - \left( \frac{\text{Pr}_t}{\text{Pr}} \right)^{2/3} \right] \frac{1}{\text{Pr}}$$

was found to result in an almost perfect representation for the dependence of Nu on $\text{Pr}/\text{Pr}_t$.

The analogue of Eq. (30) for $\text{Pr} < \text{Pr}_t$, corrected as was Eq. (29) to remove the singularity in the derivative, and with the arbitrary inclusion of the empirical factor $(\text{Pr}_t/\text{Pr})^{1/8}$, is

$$\frac{\text{Nu} - \text{Nu}_0}{\text{Nu}_1 - \text{Nu}_0} = \frac{1}{1 + \left( \frac{\text{Pr}_t}{\text{Pr}} - 1 \right) \left( \frac{\text{Nu}_0 - \frac{2}{3} \text{Nu}_1}{\text{Nu}_1 - \text{Nu}_0} \right) \text{Nu}_\infty}$$

This expression results in almost exact representations for $\text{Pr} < \text{Pr}_t$ for all of the previously mentioned conditions—thereby it is a complement in every respect to Eq. (30).

**IMPLEMENTATION**

The numerical calculation of values of Nu for specified values of Re and Pr and for particular geometries and boundary conditions requires numerical values or expressions for $f$, $\text{Nu}_0$, $\text{Nu}_1$, and $\text{Pr}_t$. For a round tube, values of $f$ of sufficient accuracy can be determined from Eq. (6) by noting that $\text{Re} = 2a^* u_m^*$. Values of $\text{Nu}_0$ and $\text{Nu}_1$ can be calculated from Eqs. (19) and (20), but an array of such values has already been calculated for representative values of $a^*$, and correlating equations have been devised for interpolation. The slight inaccuracy associated with Eq. (5) is totally negligible when it is used in conjunction with Eqs. (19) and (20). Equivalent expressions for $f$, and values and expressions for $\text{Nu}_0$ and $\text{Nu}_1$ are also available or can readily be derived and calculated for other geometries and thermal boundary conditions. Equation (21) is directly applicable as an asymptote for large values of Pr for all geometries and conditions. Current correlating and predictive equations for $\text{Pr}_t$ are quite uncertain (see, for example, KayS[12] or Churchill[13]). However, Nu as predicted by Eqs. (30) and (31) is fortuitously insensitive to the expression used for $\text{Pr}_t$, and the following purely empirical equation

$$\text{Pr}_t = 0.85 + \frac{0.015}{\text{Pr}}$$

appears to be adequate for that purpose. The dividing value
of Pr with respect to the use of Eq. (30) or (31), that is, the value of Pr for which Pr = Prc, is 0.867 according to Eq. (32). Other correlating equations for Pr give only slightly different numerical values for the pivotal value of Pr. Either Eq. (30) or Eq. (31) can be used without serious error for 0.45 < Pr < 1.7, which suggests that Eq. (30) is a sufficient expression for all fluids other than liquid metals.

SUMMARY

Equations (30) and (31), together with Eq. (32), predict values of Nu within 1% or 2% of numerically calculated values for all geometries and conditions in the fully turbulent regime. This is to be compared with deviations of 10% to 40% on the mean for all expressions in current use, many of which are greatly restricted with respect to range and conditions (see Churchill and Zajic[13]). The remarkable improvement in accuracy for Pr ≥ Prc, as provided by Eq. (27), is a consequence of using the Reichardt analogy, which is free of any explicit empiricism. This expression fails in exactness only due to some minor mathematical simplifications made in its derivation. This slight inaccuracy is in turn virtually eliminated by use of the analogy of Churchill. On the other hand, the greatly improved accuracy of Eq. (31) for Pr ≤ Prc is a consequence of the identification of the structure of the analogy of Reichardt with that of the generic correlating equation of Churchill and Usagi for three regimes in staggered form, together with a minor empiricism. This same identification revealed a virtual regime and a point of inflection for Pr ≤ Prc, and another such pair that had never before been recognized for Pr > Prc. The existence of these virtual regimes explains the numerical and functional failures of most prior correlating equations.

The generality of the new expressions for all geometries and thermal boundary conditions is a consequence of the recognition that the analogy of Reichardt could be expressed in terms of Nu0, Nu1, Nu1’, and Prc/Pr. The supplementary expressions for Nu0, Nu1, and Nu1’, which are exact insofar as Prc is independent of y*, follow directly from formulation of the equations of conservation in terms of the fraction of the transport due to the turbulent fluctuations. They could have been derived using eddy diffusional models, but not so simply.

Implementation of the new expressions for specified values of Re and Pr and for particular geometries and thermal boundary conditions, is not onerous since the entire calculation can be preprogrammed.

The path of development leading to Eqs. (30) and (31) could now be streamlined, but the description of the irregular path that was actually followed has educational value in that all students and practicing engineers should be concerned with the evaluation if not the construction of correlating equations.

Although the process of derivation of the new relationships for thermal convection is much more complicated, and the relationships themselves are slightly more complicated to employ, these deficiencies appear to be a small price to pay for their greater accuracy, sounder rationale, and broader applicability.

Students should be prompted to question any of the assertions and non-obvious steps that were made in the abbreviated development herein and not expanded upon by the teacher. Justifications may generally be found in the references.

REFERENCES


Chemical Engineering Education

Dear Editor:

Late last year, you published our Letter to the Editor regarding a survey we were carrying out on the use of Inherently Safer Design (ISD), meant to make the process industry a lot safer. Several of your readers downloaded our questionnaire and sent their responses to us. We got responses from eleven countries world wide.

The findings of the survey have just been published under the title “Inherently Safer Design: Present and Future” in the Transactions of the Institution of Chemical Engineers, Process Safety and Environmental Progress, 80, Part B, May 2002.

We are pleased to enclose a copy of the publication for
your reference. Further, the following is a brief summary of the survey paper. It’s appearance would be a fitting finale to the effort that started with the initial publication of our letter in your journal.

**Summary**

A recent survey of the current use of Inherently Safer Design (ISD) concepts attracted responses from 63 people in 11 countries. These included industrialists, consultants, regulators, and academics. The salient results of the survey are noted below in bullet form to focus attention, followed by recommendations to expedite the adoption and spread of ISD.

- Almost everyone responding knows of ISD. Their knowledge stems from specialized lectures, short courses, books, conferences, and training videos.
- ISD has been practiced by some for decades, whereas others started only recently.
- ISD is used in almost all stages of chemical process development, design, and operation.
- ISD is used during the manufacture of a whole range of products.
- Almost all hazards have been targeted, both on-shore and off-shore.
- The above attests to the universality of ISD applications.
- There is a favorable impact on balance sheets.
- It is important to use “Management of Change” when implementing ISD to avoid introducing any new hazards.
- There is very little additional cost if implemented early. Payback is fast.
- Some applications/practitioners have won awards.
- ISD is included in lectures at several institutions. More will do so now.
- Many are not familiar with the current Inherent Safety (IS) indices. Those familiar with them have used them sparingly. A simple, realistic index is needed that also shows economic benefits. Detailed examples of use at different stages of process development are necessary.
- ISD concepts can influence R&D in various areas of chemical engineering and chemistry.
- ISD should encompass inherent safety, health, and environment (ISHE).
- ISD concepts, suitably modified, can be used for other branches of engineering such as mining, construction, transport, etc.
- Current regulations do not force the use of ISD.

**Recommendations**

The sad truth is that ISD is applied when an ISD enthusiast is on the team and not otherwise. Implementation of the recommendations below might encourage the uptake of ISD.

- Every chemist and chemical engineer should be trained in ISD. Academics and professional bodies should lead in this.
- Other scientists and engineers should be given introductory lectures in ISD with examples from different industries.
- IChemE should make ISD a part of its approved degree syllabus. Subsequently, it should persuade other engineering and science accrediting societies to do likewise.
- There is a need to teach IS to management and financial people also since their role is crucial in encouraging applications of ISD.
- Dedicated funding by government and industry for research and teaching in ISD will encourage many academics to take it up.
- Incentives by the government to cost share demonstration plants and provide tax breaks for ISD.
- Expand ISD to encompass ISHE since the environment and occupational health are day-to-day concerns. It may eventually be extended to ISHEQ (Q for Quality) since improvements in SHE will decisively impact quality of product.
- Companies should provide examples of ISD use in various situations and the economic benefits reaped in order to convince other industries, regulators, government, the media, the public, academics, R&D funding agencies, etc.
- Involve the mainstream print and audiovisual media to favorably impact public opinion.
- Amend regulations to enforce the use of ISD.
- Insistence by international agencies to include ISD in projects that they fund in the same way that the World Bank now insists on environmental impact assessment studies in projects funded by it.

**Some expected results**

- Tall columns of chemical plants will be reduced to one- or two-story heights. This will improve the image of the chemical industry.
- Increased investment in process industry.
- Less restrictive regulations.
- Greater enrolments in UG and PG courses.
- Significantly enhanced funding for R&D.
- Adoption of ISD by other engineering disciplines, especially the more accident-prone ones such as construction, mining, transportation, etc.

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NOVEL CONCEPTS FOR TEACHING PARTICLE TECHNOLOGY

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Particle technology is an interdisciplinary subject dealing with disperse systems, including all types of solid particles (aerosols, suspensions), liquid particles (drops, emulsions), and gaseous particles (bubbles). The main focus of our current research and curriculum, however, is on solid particles.

The goal of particle technology is producing and handling disperse materials under economical and ecological constraints. The materials are produced due to a surplus value of the product properties. Typical examples for these properties are the taste of chocolate, the color of pigments, the strength of concrete, or the electrical properties of semiconductors. Consequently, this is also a key point in our curriculum.

In order to prepare a young engineer for his possible tasks in industry and research, we have organized the curriculum to reflect the structure of the field (see Figure 1). The field can be structured generally in four levels. The first and most fundamental level covers the elementary processes, i.e., the physical fundamentals. They include the statistical foundations of particle technology, multiphase flow, bulk mechanics and powder flow, interfacial phenomena, and the interactions of dispersed matter with electromagnetic radiation. On the second level, we apply the fundamentals to machines and unit operations. In our curriculum, we concentrate on separation processes, further strengthening students’ capabilities in multiphase flow phenomena. The third level considers whole processes. Here, we teach the concept of product engineering, i.e., how to tailor product properties. Consequently, we have a close link to the applications, which are actually very broad:

- Materials science (e.g., all ceramics manufacturing is in fact applied particle technology)
- Life science (e.g., proteins may be treated as small particles in some respects, drug delivery)
- Information technology (e.g., quantum dots, clean room technology, chemical mechanical polishing)
- Environmental engineering (e.g., particle separation)

Traditionally, chemical engineering has been taught in Germany using the unit-operations concept. In most universities, teaching particle technology has followed the concept of Hans Rumpf, who stressed the physical fundamentals in the basic course, which is followed by courses in agglomeration, solid-liquid separation, or particle characterization, to name just a few. Unfortunately, in the USA particle technology is taught extensively in only a few universities. Students learn how to design machines and processes that either keep the particle size constant (i.e., separation, mixing) or change the particle size (i.e., size reduction and size enlargement). In the past, only mechanical means to produce and handle par-
particles were considered; therefore, particles larger than approximately 1µm were mainly dealt with while the non-mechanical methods of particle synthesis (e.g., crystallization, gas phase processes) that lead to submicron particles were neglected.

By introducing product properties, we address the overall goal of a chemical process, i.e., the production of well-defined product properties under economical and ecological constraints. The concept of product engineering transcends goal of a chemical process, e.g., studying methods of particle synthesis (e.g., photocatalysis were considered; therefore, particles larger than approximately 1µm were mainly dealt with while the non-mechanical methods of particle synthesis (e.g., crystallization, gas phase processes) that lead to submicron particles were neglected.)

**Figure 1. Structure of particle technology curriculum and courses offered at Munich University of Technology.**

**Figure 2. Property functions of a typical pigment.**

**Figure 3. Teaching concept and new topics (gray).**

**Educati0n in Particle Technology at TU Munich**

**Teaching Concept and New Topics**

The particle technology courses are a part of the chemical engineering and process engineering ("Verfahrenstechnik" in German) curricula at the Munich University of Technology. On one hand, the traditional education of chemical engineers prepares students for well-known applications such as the design of cyclones or heat exchangers, but many of the traditional applications have reached the point where their economic success is decreasing. On the other hand, new opportunities are evolving in areas that are less familiar to engineers, e.g., information technology or various aspects of ma-
The question is: How can the new areas be included in the curriculum without disregarding the conventional ones? In our opinion, the only answer is that teaching the fundamentals is even more important, but the examples given to the students should change.

In Figure 3, our approach is shown schematically. We explain the whole picture to the students by showing them the progression from molecular precursors to the whole process, which actually covers many orders of magnitude in both geometrical dimensions and time scale. In other words, we pave the way from feed materials to end-product properties—this is the horizontal line. In the vertical, depth is gained by explaining certain aspects in a detailed way. By reflecting the first three levels of Figure 1, we stress particulate interfaces (fundamental level) since we believe that this aspect has not been sufficiently covered in the past. Moreover, with the advent of nanotechnology, interfacial aspects have become increasingly important. The second level, comprising unit operations, is handled in a more-or-less traditional way, although new aspects such as CFD modeling are included. On the process level, disperse systems have to be treated mathematically by means of population balance equations, which have so far not been covered in traditional particle technology curricula.

Courses

The courses are organized into three levels. The first and most fundamental level comprises a two-semester course in “Fundamentals of Particle Technology” (see Figure 4). In this course, the important foundations (ranging from statistics, motion of particles in fluids, fracture mechanics, to dimensional analysis) and their implication in mechanical process engineering are covered. In addition, new elements such as population balances (which are increasingly used in industry) and interfacial phenomena are introduced. The latter comprise the fundamentals of interactions between molecules and particles, characterization of particulate interfaces and aspects of nanoparticle technology (e.g., coagulation and stabilization of colloidal suspensions).

The second level stresses unit operations. Here, we concentrate on “Particle Separation” (see Figure 5). This course is principally organized in the traditional way, focusing on separation of particles from gases as well as solid-liquid separation. Different unit operations in gas-solid separation are introduced systematically by focusing on common principles, i.e., on transport mechanisms of particles to the collecting surfaces of the respective separators. In this way, various unit operations are treated very efficiently, which allows for introduction of new, modern methods such as CFD and its use for optimizing such apparatuses. We also offer a complementary course.
dealing with “Downstream Processing of Biotechnological Products” that focuses primarily on different unit operations for separation, disintegration, and purification of bioproducts as well as their interactions in the whole production process. In several aspects, bioproducts such as proteins can be regarded as nanoparticles, although the limits of this point of view should be kept in mind.

A completely new course is being offered in product engineering (see Figure 6). The key question is how to produce the physical properties that define the product property, from the point of view of both handling and application. Examples for property functions are presented together with various methods for producing the particles (e.g., comminution and classification, gas phase synthesis of nanoparticles, crystallization, and precipitation). Handling and formulation topics round out this course. The students learn key concepts for formation of structured solids, product design, and powder processing systems. In this context, the systems engineering approach is important. There is also a course in particle characterization that teaches the main principles in characterizing particle properties, e.g., concentration, size, shape, surface, and zeta potential (see Figure 7). The purpose of this course is to enable the students to choose an appropriate setup for arbitrary particle characterization tasks. This is accomplished by emphasizing the basic aspects of a measuring technique (e.g., physical principle, signal recording, conditioning, and evaluation) as well as a complete measurement system (including sampling, transport, and preconditioning). These principles are explained in conjunction with a choice of the most important measurement techniques.

Whereas Fundamentals of Particle Technology I and II are mandatory for all chemical engineering students, Particle Separation is one of a group of three courses (together with Process and Plant Design and Design of Thermal Processes) from which the students must choose two. The remaining courses are elective.

**Methodology and Didactics**

The course in particle technology follows several guidelines:

- The key item is the product property approach, i.e., particles have physical properties such as particle size distribution, particle shape, or particle morphology that are closely related to product properties.
- Although it is difficult to describe complete process chains, we enhance the student’s awareness of the complete process.

From a methodological point of view, we believe that teaching should follow a double-tracked approach. On one hand, the teacher should stress the important physical foundations, since excellent skills in the fundamental principles will be essential for the students throughout their studies and their professional lives. This implies that a large num-
ber of facts have to be taught, thus assigning an important role to the teacher. On the other hand, to promote the students' understanding of the underlying principles as well as to sharpen their view of the complete process, active learning appears to be a key issue.\cite{3,5,6} We try to support this active learning in different ways (see Figure 8).

Lab and virtual experiments are conducted so that students can apply and transfer their acquired knowledge and get involved with more realistic problems. This is accomplished by a mandatory lab course (one semester) as well as lab components that are integrated into the courses described above. The lab experiments include a wide field of exemplary tasks that include, for example, dust separation in cyclones, filtration, mixing, and particle characterization by laser diffraction as well as the investigation of the stability of colloidal suspensions by dynamic light scattering. Furthermore, a completely new virtual lab is currently being established in the course Product Engineering, with computer simulations of disperse systems (e.g., crystallization, comminution) based on population balances using commercial software (e.g., LabView and Parsival).

We also encourage the students to take an active role throughout the courses wherever it is appropriate, for example, in the particle characterization course. After introducing the basic principles and the important characteristics of a measurement systems (e.g., assessed equivalent particle size, signal recording, conditioning and evaluation, necessary sample preparation, etc.) as well as discussing their application to the most important measurement techniques, the students are arranged in small groups. Each group is then assigned the task of analyzing one measurement technique that is so far unknown to them. They also have to prepare a presentation of their results that will relay the most important facts to their fellow students. The groups are supposed to work autonomously, with the teacher playing a more passive role and only giving guidelines or help when asked. In this way, several goals can be achieved.

- The students work and access information autonomously, e.g., from literature in a foreign language.
- The group work necessitates that students find their roles in a group and work together productively.\cite{7}
- Finally, the students are given the chance to prepare and give a presentation. Even listening and assessing the presentation of other groups increases their ability in this respect. This is a capability that is not practiced enough.\cite{8}

By actively preparing a small part of the course, the students not only acquire valuable technical knowledge, but they also get a chance to increase their "soft skills." Personal development is often neglected in a university education. Students should concentrate on both their technical skills and their personal growth (see Figure 9). This includes an ability for self-organization and focusing on defined targets, intrinsic motivation to reach goals, and an ability to communicate results. On a deeper level, internal self-reflection is indispensable for accepting personal strengths and weaknesses as well as those of others. This is a precondition for all social skills.

**CONCLUSIONS**

Particle technology is a much wider field than many people realize since it also comprises biochemical, chemical, and thermal processes dealing with particles. Hence, it is not only of the utmost importance in the chemical industry, where about 60-70\% of all products are fabricated in dispersed form, but also for a number of other fields, such as materials science and information technology. Product properties and the subsequently developed product engineering approach is at the center of our considerations. With a continuously growing number of applications for dispersed systems, we feel a need to stress the fundamental aspects even more. With the generally observed trend toward finer particle sizes, new topics such as particle interactions and population dynamics have been included in order to prepare our students for newly developing areas such as nanotechnology. The technical courses are complemented by various activities to strengthen the soft skills of the students.

Recently, suggestions have been made by Cussler, et al.,\cite{9} on how to change chemical engineering curricula. Considering the shift in industrial practice from large-scale processes producing commodities toward more specialized product design, we feel that particle technology and particle design methods deserve a prominent place in the curriculum.

**ACKNOWLEDGMENTS**

The authors would like to thank Professor Helmar Schubert from the University of Karlsruhe for very valuable discussions.

**REFERENCES**


Chemical Engineering Education
Letter to the Editor
Continued from page 262.

b=8.5164364±1.5315505; the error variance s^2=0.467503; and correlation coefficient R^2=0.953603. Professor Fahidy advises not to put too much faith in the linear regression model, in spite of the relatively large R^2 value, because of the extremely wide confidence intervals on the parameter a. The fairly random distribution of the residuals (see Figure 2) suggests, however, that the linear model may be the correct one. Furthermore, both physical considerations (fuel consumption should be zero for a zero mass vehicle) and the wide confidence intervals on the free parameter a, indicate that the model can be improved by setting the free parameter at zero. Indeed, carrying out the regression while setting a=0 yields: b=7.892916±0.3599903; s^2=0.4641509, and R^2=0.9481781. Thus, this model is now acceptable, even with respect to the confidence interval values.

One of Professor Fahidy's objectives in presenting this example was to warn against accepting relatively large R^2 values as proof of good linear relationship between the dependent and independent variables. The limitations of the R^2 statistics in this respect can be most strikingly demonstrated using residual plots. Shacham, et al.,[3] for example, fitted vapor pressure data of 1-propanol with the two-parameter Clapeyron equation. This regression yields the values: R^2=0.9998818 and s^2=1.659E-09 (based on log P). Such a high value of R^2 can be interpreted as a perfect fit. But the residual plot (seen in Figure 3) shows that the vapor pressure data set exhibits a curvature, which is not predicted by the Clapeyron equation. Indeed, using the four-parameter Riedel equation for representation of the same data yields: R^2=1; s^2=1.327E-09 and randomly distributed residuals.

The last example, given in the Appendix of the article deals with a linear model for representing coded effectiveness indicators versus catalysts containing various coded platinum mass units. Analysis of this example shows that if the free parameter, a, is set at zero (as suggested by the wide confidence intervals on a and physical considerations) the linear model is appropriate to represent the data with b=1.6437659±0.0845917, R^2=0.8860414, and s^2=0.8508906.

We can conclude that teaching statistical analysis of data and regression models is very important, but interpretation of numeric statistical indicators must be complemented by graphical analysis and consideration of the physical nature of the model in order to arrive at the correct conclusions.

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Ben-Gurion University of the Negev

Neima Brauner
Tel-Aviv University

References

Author's Response

I am delighted at Professor Shacham's interest in my paper. I also fully concur with the argument that the residual plots are an important and integral part of regression analysis. This is now standard textbook material, and I do routinely discuss this subject in my course. Although my intention was to keep the article from being too long, in retrospect I should have spent a paragraph or two on residual analysis, and I regret the omission.

In Example 4 it was stated that the reaction mechanism was first-order irreversible, but perhaps not strongly enough to imply an a priori knowledge of non-statistical origin, so that 0th and 2nd order models are beyond consideration. With limited data and given a physically correct model, the method that provides regression parameters relating data to model with the smallest error variance may be acceptable in lack of something better, even if the residual plot does not show randomness of a desired degree. The quest for additional measurements is almost universal in the case of limited-size data.

My views about R^2 versus confidence intervals for true regression parameters do not fully coincide with the respondents', but may I point out the redundancy of seven-digit values, computer printouts notwithstanding. An R^2=0.8860414 is not more meaningful than R^2=0.89

Thomas Z. Fahidy
The School of Chemical Engineering at Cornell University recently undertook an evaluation of its Masters of Engineering program to assess the curriculum and the amount of value added to the student’s education by their participation in the program. One conclusion that we reached was that students in a professional masters program were most likely to go on, at least initially, to some kind of a position in a corporate environment. To increase the likelihood of their success in those early years on the job, we felt that some level of knowledge of how a business unit works and how an engineer fits into such a unit would be of significant importance to their careers.

With this in mind we added a requirement that all M. Eng. Candidates take a course that would give them some insight into these areas. While there are a number of different courses at Cornell that deal with related topics, there was no one course that covered all of the areas that we thought were relevant. This led to the development of a new course, primarily for Masters of Engineering students, titled “Managing New Business Development.”

The course is an attempt to explain the business development process as it is likely to be carried out in a major corporation. It deals with concept development, feasibility assessment, front-end analysis to select the best implementation strategy, tactics to take the concept forward, implementation of the selected strategy, and ongoing improvement of the process once it is implemented to either increase or maintain profitability.

The students are exposed to a number of different concepts. As the course advances, they are asked to demonstrate their knowledge through several case studies. The first case study involves producing plans for executing a feasibility study to introduce a new line of cosmetics in a newly opened overseas market. The second involves maximizing value from a feedstock that contains a number of different components.

One of the concepts we found particularly difficult to get across to the students was pricing strategy. To provide a means for hands-on experience with this concept, we developed what we call the “gas station game.” Unlike most games in business schools that generally involve multiple inputs and focuses at sitewide or businesswide optimization in a qualitative manner, this is a quantitative pricing game that aims at illustrating market forces at work. Since most people in the U.S. regularly deal with the fluctuation of gas prices, it is easy for the students to relate to it. We play this game every time the class meets.

THE GAS STATION GAME

In the game, students are divided into four groups, with each of them managing a gas station. Operating under different restrictions (“mom and pop” versus “big chain”), students are asked to decide on their business goals and facility sizes, which in turn lead to pricing structure and marketing tactics. We found that it is generally effective to have students per-
maximizing an individual player’s revenue did not necessarily mean defeating the others. And, in fact, the most favorable revenue picture is one in which all participants were able to share the market in some fashion.

We found that within approximately ten iterations, the students were able to arrive at the conclusion that a shared market created more revenue and that cutthroat competition was unlikely to succeed. With this realization, the students go on to develop pricing strategies that allow each of them to sell close to their facility’s capacity and to maximize their individual revenues.

Figure 2 shows a typical adjustment process based on root-mean-squared deviations in prices and revenues, as compared to values at the last iteration. At around the tenth iteration, prices begin to converge to the range where a reasonable profit is sustained among all stations. The revenues continue to fluctuate, on the other hand, since students often react to price changes of the other stations after their demands have changed, instead of anticipating the behavior of the others. These fluctuations are likely to stabilize if we carry the game further.

CONCLUSION

We think this game provides an easy way to teach pricing strategy in a fairly simplistic business model, and we are happy to pass along this game for your interest and use.

APPENDIX A

Assignment Sheet for the Gas Station Pricing Game

There are four gas stations on Rt. 13, coming into Ithaca. They are about a block apart, as indicated in the figure below.

<table>
<thead>
<tr>
<th>I</th>
<th>II</th>
<th>IV</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Rt. 13 to Ithaca</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>III</td>
</tr>
</tbody>
</table>

Figure 1A: Map of the four gas stations

Preliminary market research indicates a demand of about 120 cars/hr in the day and 20 cars/hr at night, at 10 gals/car. While some percentage of the drivers go to the first gas station in sight, most make that decision based on things such as price, convenience (credit card/speed pass), and brand name. They also have the choice of getting gas from the next town if they feel prices are too high.

Your first task is to decide on the amount of investment, level of service, and pricing strategy for your gas station. Your decision will depend on the nature of your company (mom/pop vs. chain), as listed in Table 1. Table 2 lists the available gas station configurations.

The supply trucks come every seven days to refill the underground gas tanks. If you sell more gas than your designed capacity, the extra gas will be available at 115% x Max gas price in Ithaca.

The goal of this exercise is to achieve the highest return on investment among all groups, with a minimum acceptable ROI at 12% per year. You will be able to change your prices (and only prices) every week, depending on the market situation.

TABLE 1

| Differences between Mom/Pop Operations and Chain Companies |
|-----------------|-----------------|-----------------|-----------------|
| Investment | Supply Cost | Personnel | Service |
| Mom/Pop | $300,000 | $1.45/gal | 1 @ $5/hr | 12 hr |
| Chain | Unlimited | $1.47/gal | 2 @ $5/hr | Speed pass |

TABLE 2

| Gas Station Configurations and Costs |
|-----------------|-----------------|-----------------|-----------------|-----------------|
| Capacities | 20,000 gal | 25,000 gal | 30,000 gal | 40,000 gal |
| Capital Cost | $200,000 | $300,000 | $400,000 | $500,000 |
| Operating Cost | $56/day | $84/day | $111/day | $138/day |
form cash flow analyses for different scenarios. (The project assignment is shown in Appendix A.) The cost parameters are approximated and tested to produce realistic profit figures in the end. Capital costs include the storage tank material and installation, gas pumps, land requirement, engineering costs, etc. The operating costs are estimated as 10% of the capital investment, assuming a ten-year project lifetime.

When the students are ready for the actual price bidding, a simulation is used to determine the demand in each station, based on the four stated prices (see Figure 1). The simulation is modified from the Monte Carlo Gillespie algorithm from reaction kinetics. Simply, the probability of customers visiting each gas station is inversely proportional to the price difference between that particular station and the minimum bidder. The simulation then uses a random number generator to determine the exact demand for each station. An extra station with a fixed price is added to model gas stations from outside this town.

To account for different levels of service provided by each station (e.g., method of payment that is accepted), the prices are adjusted before the probabilities are calculated. These adjustment amounts are based on polls conducted among students regarding their own consumer preferences. The simulation also includes some proportion of cars that stop at the first gas station in sight instead of comparing prices, which again is determined using a Gillespie algorithm with a predetermined probability.

The profit of each company is calculated based on the number of gallons sold minus operating costs of the gas station. As mentioned before, each group decides in advance what the suitable underground storage capacity will be, which gives rise to certain capital costs and operating costs. In the event that the gas station sells more gas than its capacity allows, it will have to obtain extra gas at 115% of the maximum price among the four gas stations. In this way, each gas station is equally profitable if the right price relative to each other is found.

**RESULTS AND DISCUSSIONS**

The results of the game are quite encouraging. We are trying to teach the concepts of customer perception of product value, convenience, and price differentiation based on those perceptions. We are also trying to show that the strategy of

---

**Figure 1.** The gas station game simulation in action.
SPEAKING OF EDUCATION – III

RICHARD M. FELDER
North Carolina State University • Raleigh, NC 27695

There is a theory which states that if ever anyone discovers exactly what the Universe is for and why it is here, it will instantly disappear and be replaced by something even more bizarre and inexplicable. There is another theory which states that this has already happened.

(Douglas Adams)

A lecture is a process by which the notes of the professor become the notes of the students without passing through the minds of either.

(R.K. Rathbun)

A teacher who is attempting to teach without inspiring the pupil with a desire to learn is hammering on a cold iron.

(Horace Mann)

Teachers who cannot keep students involved and excited for several hours in the classroom should not be there.

(John Roueche)

If a professor can be replaced by a CD-ROM, he/she should be.

(Jack Wilson)

I’m sure the reason such young nitwits are produced in our schools is because they have no contact with anything of any use in everyday life.

(Petronius, d. ~66 AD)

Times are bad. Children no longer obey their parents, and everyone is writing a book.

(Cicero)

What’s on your mind, if you’ll forgive the overstatement?

(Fred Allen)

Everything should be made as simple as possible, but not simpler.

(Albert Einstein)

In theory, there is no difference between theory and practice; in practice, there is.

(Chuck Reid)
Engineering educators have done a great job of teaching students engineering science and engineering design. In addition, engineering schools are beginning to address the development of “soft skills” such as communications, teamwork, and ethics. In the current environment, it is increasingly important for the engineering education system to also find ways of teaching entrepreneurship and motivating students toward such activities. This conference will set the stage for a continuing and fruitful dialog between engineering educators and the business community.

The conference will assemble entrepreneurs, engineering educators, and business school faculty to discuss:

- What are the attributes of successful entrepreneurs?
- What are models of successful programs teaching entrepreneurship to engineers?
- What is the culture at a university that fosters a spirit of innovation and entrepreneurship?
- How can engineering faculty become role models of innovation and entrepreneurship?

The outcomes of the conference will be a set of recommendations to engineering faculty, curricular integration options, model programs available for replication, and contacts between academic and business that will be published in the journals of various professional societies.

The Chairs of the Conference are Eleanor Baum of The Cooper Union and Carl McHargue of the University of Tennessee.

Additional information about this Conference, and a registration form, can be found at the Conference’s web site:

<http://www.engconfintl.org/3as.html>

Engineering Conferences International offices are located at:
6 MetroTech Center, Brooklyn, NY 11201
Telephone at 212-591-8144 — Fax at 212-591-8145
e-mail at bhconf@poly.edu

This conference will provide a forum for exchange of ideas on methods of enhancing the global perspective of engineering students, identify the key obstacles, and discuss progress toward eliminating the obstacles. The conference is jointly sponsored by Engineering Conferences International, Ordem dos Engenheiros, Portugal, and E4 (Enhancing Engineering Education in Europe). Thematic Network is financed by the European Commission under SOCRATES II and co-financed by the University of Florence. Contact
<e4@ing.uniflo.it> for more information
or go to
<http://www.ing.unifl.it/te4>.

The conference will focus on the recognition that exposure to other cultures brings personal enrichment to individuals and can be an important component of the educational experience. With the increased globalization of economies, the need extends beyond personal enrichment and has become an important asset to student mobility. Among the issues that must be addressed are compatibility of degree systems, accreditation of courses and/or degrees, quality assurance, an accepted credit system, language of instruction, and legal and social issues such as visas, taxation, and financial support.

The Chairs of the Conference are Carl McHargue of the University of Tennessee and Eleanor Baum of The Cooper Union (New York, NY). The Co-Chairs are Antonio Salgado Baros of the Ordem dos Engenheiros (Portugal), G. Augusti of the University of Rome (LaSapienza, Italy), and C. Borri of the University of Florence (Italy).

Additional information about this conference, and a registration form, can be found at the Conference’s web site:

<http://www.engconfintl.org/3ai.html>

Engineering Conferences International (ECI) is the successor to the United Engineering Foundation Conferences. ECI offices are located at 6 MetroTech Center, Brooklyn, NY 11201
Telephone at 212-591-8144 — Fax at 212-591-8145
e-mail at bhconf@poly.edu — web at www.engconfintl.org.
To state a theorem and then to show examples of it is literally
to teach backwards.

(E. Kim Nebeuts)

Setting an example is not the main means of influencing
another, it is the only means.

(Albert Einstein)

Education is what happens to the other person, not what
comes out of the mouth of the educator.

(Miles Horton)

Education is the ability to listen to almost anything without
losing your temper or your self-confidence.

(Robert Frost)

Lack of education is an extraordinary handicap when one is
being offensive.

(Josephine Tey)

Education is one of the few things a person is willing to pay
for and not get.

(William Lowe Bryan)

Education is what survives when what has been learned has
been forgotten.

(B.F. Skinner)

A graduation ceremony is an event where the commencement
speaker tells thousands of students dressed in identical caps
and gowns that individuality is the key to success.

(Robert Orben)

There is a legend that the difference between classes of
freshmen and post-graduates is that if you say “Good
Morning” to the first, they reply “Good Morning.” But the
graduate students write it down.

(Donald Bligh)

I used to keep my college roommate from reading my
personal mail by hiding it in her textbooks.

(Joan Welsh)

Predicting the future is easy. It’s trying to figure out what’s
going on now that’s hard.

(Fritz Dressler)

If I knew what I was looking for, it wouldn’t be research,
would it?

(Richard Feynmann)

If I accept you as you are, I will make you worse; however if
I treat you as though you are what you are capable of
becoming, I help you become that.

(Goethe)

Teaching is the greatest act of optimism.

(Colleen Wilcox)

Try not to have a good time...this is supposed to be educa-
tional.

(Charles Schulz)
I believe phase equilibrium thermodynamics is the most conceptually difficult undergraduate chemical engineering class. Even students who perform calculations satisfactorily seem confused over the meaning of what they have learned.

Phase equilibrium is the single undergraduate chemical engineering class in which abstract concepts are presented to the near exclusion of practical applications. Table 1 gives examples of practical or physically intuitive subject matter found in classes that students typically consider abstract, theoretical, or mathematical. These actually contain some balance of theory and practice, giving students a point of reference to physical processes and equipment. Calculations such as bubble and dew points are needed for practical design, of course, but most phase equilibrium courses do not connect these to real processes or equipment. Practical applications of the material are taught as part of unit operations, mass transfer, or distillation courses.

Students frequently have more intuition about the physical meaning of abstract quantities in classes other than phase equilibrium. Heat transfer students could define the Prandtl number as $C_p\mu / k$, give a physical interpretation for all three variables, and potentially recognize related facts. For example, “The Prandtl number could be derived by applying the Buckingham Pi theorem to a heat transfer problem,” or “Larger Prandtl numbers result in larger convective heat transfer coefficients.” They know that the Prandtl number for liquid water at 100 atm and 150°C is unlikely to be 100 or 0.01.

When phase equilibrium students define chemical potential, it is typically in terms of other abstract concepts—free energy, standard states, fugacity, and activity. They are unlikely to know whether a certain chemical potential is positive or negative, nor what practical significance its sign would have. Without doing a calculation, how many phase equilibrium students know whether the fugacity of liquid water at 100 atm and 150°C is closest to 5 atm, 50 atm, or 500 atm? Most are at a complete loss when asked to apply abstract quantities such as activity coefficients to practical questions, e.g., “Is ethanol more likely to form an azeotrope with n-hexane or n-octane?” Lacking qualitative understanding, their only approach for answering this question is detailed quantitative calculation.

### STRATEGIES FOR BUILDING INTUITION

Prausnitz, et al.,[1] describes the phase equilibrium problem as a three-step process. First, a real problem is translated into an abstract mathematical problem. Second, the mathematical problem is solved. In the final step, the mathematical solution is translated back into physically meaningful

![Michael Misovich](image)

Michael Misovich will be Associate Professor in the Physics and Engineering Department of Hope College in August, 2002. His research interests include thermodynamic property predictions from equations of state, physical chemistry of polymer solutions, chemical engineering education, and its assessment.

### TABLE 1

Content of “Theoretical” ChE Classes

<table>
<thead>
<tr>
<th>Class</th>
<th>Theoretical Concepts</th>
<th>Practical Concepts</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fluid Mechanics</td>
<td>Shear stress tensor, Dimensional Analysis</td>
<td>Pumps, Valves, Piping</td>
</tr>
<tr>
<td>Mass Transfer</td>
<td>Fluxes of all sorts</td>
<td>Packed absorption towers</td>
</tr>
<tr>
<td>Transport Phenomena</td>
<td>Partial differential equations, Dimensionless Greek variables</td>
<td>Viscometers, Heat transfer with free convection, Wetted wall columns</td>
</tr>
<tr>
<td>Phase Equilibrium</td>
<td>Chemical potential fugacity, activity</td>
<td>Bubble and Dew Points, Flash, Solubilities</td>
</tr>
</tbody>
</table>

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TABLE 2
Common Intuition about Chemical Engineering Data

- High molecular weight compounds have high boiling points
- A substance with a density order of magnitude less than water is probably a gas
- A Reynolds number in the laminar range for flow of water in typical process piping is not typical
- Convective heat transfer coefficients are very low for gases as compared to liquids

TABLE 3
Uncommon Intuition about Phase Equilibrium Data

- The fugacity of a liquid is approximately its vapor pressure, as long as the pressure is not extremely high
- The fugacity of a component in an ideal gas mixture is its partial pressure
- Substances we consider noncondensible gases have fugacity coefficients larger than one; liquids and condensible vapors have fugacity coefficients smaller than one
- Substances with large differences in boiling points are unlikely to form azeotropes; substances with very close boiling points are almost certain to form them
- Activity coefficients larger than approximately seven indicate that liquid-liquid phase separation is possible
- The dilute component in either of two nearly immiscible phases obeys Henry's Law up to its solubility limit

TABLE 4
Comparison of Graphical Figure Use in ChE Textbooks

<table>
<thead>
<tr>
<th>Textbook</th>
<th>Graph Figures</th>
<th>Non-graph Figures</th>
<th>Pages</th>
<th>Graphs per 100 pages</th>
<th>Percent Graph Figures</th>
</tr>
</thead>
<tbody>
<tr>
<td>Introduction to Chemical Engineering Thermodynamics (Chapters 10-15)</td>
<td>107</td>
<td>44</td>
<td>568</td>
<td>19</td>
<td>71</td>
</tr>
<tr>
<td>Chemical and Process Thermodynamics (Chapters 9-13)</td>
<td>116</td>
<td>60</td>
<td>541</td>
<td>21</td>
<td>66</td>
</tr>
<tr>
<td>Transport Phenomena (Chapters 35, 37-40)</td>
<td>69</td>
<td>105</td>
<td>711</td>
<td>10</td>
<td>40</td>
</tr>
<tr>
<td>Elementary Principles of Chemical Processes (Chapter 6)</td>
<td>17</td>
<td>15</td>
<td>587</td>
<td>3</td>
<td>53</td>
</tr>
<tr>
<td>Momentum, Heat, and Mass Transfer (Chapters 35, 37-40)</td>
<td>159</td>
<td>106</td>
<td>773</td>
<td>21</td>
<td>60</td>
</tr>
</tbody>
</table>

*Graph figures include all two- and three-dimensional coordinate plots and nomographs. Any figure that included both graphical and nongraphical information was treated as a graph figure. Only numbered, captioned figures in text and examples were counted; figures with problems and in appendices were excluded.

*Pages include all text, examples, questions, and problems but exclude appendices.

Thermodynamics and unit operations texts contain more graphs and a higher proportion of figures that are graphs, as opposed to schematic diagrams and other drawings. Within each text, the chapters more typically, this step consists of transforming highly abstract variables into physically significant ones.

Chemical Potential → Fugacity → Activity → Composition

Each transformation results in a less abstract variable than the previous step. Students do not seem to recognize this, perhaps because we do not teach it explicitly. Instead, they see chemical potential, fugacity, and activity as equally nebulous and abstract concepts upon which a rote series of mathematical operations will hopefully produce a physically meaningful variable such as composition, pressure, or temperature.

One of my principal goals in teaching phase equilibrium thermodynamics is to help students develop an intuitive understanding of the topic. I point out to them in the beginning that this class deals with techniques for generating data to use in other classes to the nearly total exclusion of applications. Since students will not be able to rely on processes or equipment to provide intuition, I emphasize understanding the data and its significance. This type of intuition about data, rather than equipment, occurs in other classes as the Prandtl number example above and as similar examples in Table 2 indicate.

To promote this, I emphasize calculation and use of data having an obvious physical interpretation, e.g., temperature, pressure, volume, vapor pressure, composition, and enthalpy. When concepts such as free energy, chemical potential, fugacity, and activity are presented, the focus is partly on their use in solving for the more physical variables. Whenever possible, I encourage students to examine how the abstract variables affect the physical variables, and thus to develop some intuition about the significance of the abstract variables. Examples are given in Table 3; these are sometimes present, but not frequently emphasized, in phase equilibrium texts.

More so than in many chemical engineering classes, phase equilibrium data are most useful and understandable when presented graphically. This is evident from observations given in Table 4 of how frequently graphical material is presented in textbooks.
closely related to phase equilibrium have a higher proportion of graphs than the text as a whole, as indicated by the numbers in parentheses in Table 4.

Furthermore, many students have a visual learning style. These students may struggle with equations and textual information, especially in an abstract context, and it is crucial that they see data presented graphically and also learn how to prepare data in a format that is most comprehensible to them. Hence, students need to make the connection between calculations and equations discussed in class and graphical presentation of phase equilibrium data. To assure they are capable of both understanding and generating graphical data, I assign a significant number of computer problems requiring this, as explained in further detail later in this article. Computer spreadsheets have been previously suggested for use in solving phase equilibrium and equation-of-state calculations, and they are well suited both for the calculations and for subsequent graphical presentation. One recent text includes a number of example spreadsheets that may be used for applications similar to those described in this article, although I prefer to have students write their own spreadsheets.

DETAILS OF PHASE DIAGRAM COMPUTER ASSIGNMENT

As an illustration of such assignments, consider the construction of a binary Pxy diagram for an ideal solution at some constant temperature. Figure 1 is an example generated by repetitive dew point pressure and bubble point pressure calculations. Taking liquid mole fraction $x_1$ as the independent variable, and assuming component vapor pressures $P_{1}^{\text{sat}}$ and $P_{2}^{\text{sat}}$ at are known, Eqs. (1-3) allow calculation of all dependent variables in the problem. To generate the diagram, allow $x_1$ to vary over the range 0.0 to 1.0. These calculations are easily done using computer spreadsheet software.

$$x_2 = 1 - x_1$$  \hspace{1cm} (1)
$$P = x_1 P_{1}^{\text{sat}} + x_2 P_{2}^{\text{sat}}$$  \hspace{1cm} (2)
$$y_1 = \frac{x_1 P_{1}^{\text{sat}}}{P}$$  \hspace{1cm} (3)

Figure 2 shows the general organization of this spreadsheet. The upper rows contain headings and constants such as the vapor pressures. The middle rows are used for calculations. The leftmost column is initially filled with values between 0 and 1 at intervals of 0.01, or a suitable small increment. (This should be done using spreadsheet commands or formulas; occasionally, a student will attempt to enter the numbers manually and become frustrated that using the computer apparatus makes solving the problem too time-consuming.) Fill the remaining three columns in the middle rows of the spreadsheet with formulas given by Eqs. (1-3). If these formulas are entered correctly in the first of the middle rows, a single copy/paste command generates the entire table through the remaining middle rows.

There may be one complication in producing a graph from these results. In a conventional Pxy diagram, pressure is taken as the vertical coordinate twice. With liquid composition as the horizontal coordinate, a bubble point curve is produced, then with vapor composition as the horizontal coordinate, a dew point curve is produced. To do this on the spreadsheet, a single y-coordinate must be paired with two different x-coordinates. At one time, few spreadsheet packages included this capability, but many recent versions (including Microsoft Excel) now allow it. If using an older package without this...
capability, set up the lower rows of Figure 2 as shown, then define the first column as the x-coordinate for graphing and each of the two columns containing pressure values as separate y-coordinates. The lower rows of Figure 2 can be omitted when using current versions of Excel and other spreadsheets that allow multiple xy pairs to be graphed.

ADDITIONAL COMPUTER ASSIGNMENTS

Table 5 lists other thermodynamic data graphs prepared using computer spreadsheets. A very brief discussion of each follows. Many were prepared by students as homework assignments using techniques similar to those outlined for the Pxy diagram. Copies of these assignments are available upon request. Some graphs were not assigned but were generated by the instructor and presented during class discussion.

The same spreadsheet data used to produce a Pxy diagram as described above could be used to plot an xy diagram at constant temperature. Pxy and Txy are the predominant representations of VLE data in phase equilibrium classes, but xy is probably the most frequently used format of the phase equilibrium data in other classes, e.g., distillation, absorption, mass transfer.

Using the method described above, generating Pxy data for an ideal binary system at constant temperature does not require trial and error. Calculation of a single Txy datum for an ideal binary system at constant pressure requires iteration or trial and error since the vapor pressures are functions of temperature. But generating a Txy diagram for such a system—the locus of dew and bubble point temperatures for all possible compositions—does not require trial and error. Taking temperature as the independent variable rather than liquid composition, all other variables can be calculated directly by Eqs. (1-3). Selecting a range of temperatures in increments between the pure-component boiling points generates the diagram. Plotting y versus x instead of T versus y and T versus x produces an xy diagram at constant pressure from the same data.

For nonideal binary mixtures, activity coefficients are functions of liquid composition and possibly temperature. Pxy and xy diagrams at constant temperature are generated in a straightforward fashion without iteration since temperature is fixed and liquid composition is taken as the independent variable for generating the table as described above.

Iteration cannot be avoided when generating Txy and xy diagrams at constant pressure for nonideal binaries. To find activity coefficients and vapor pressures, liquid composition and temperature are needed. Only one can be assumed. Direct calculation of liquid composition from vapor pressure, as in the ideal case, is not possible. If temperature is used as the independent variable, as suggested for the ideal case, a unique composition may not result because azeotropes are possible. I recommend using liquid mole fraction as the independent variable ranging from 0 to 1, as in the Pxy diagrams. Iteration can be performed by circular recalculation on the spreadsheet. Unfortunately, spreadsheets vary significantly in their implementation of circular recalculation, even from version to version, and it is difficult to give a "recipe" that works in all cases. Often, particular rearrangements of equations or ordering of the columns is necessary. No matter what package was being used, however, I have always been able to find some method that eventually worked.

Thermodynamics textbooks commonly contain graphs of excess and partial excess properties such as volume and enthalpy for binary solutions. In the volumetric properties assignment, students generate similar graphs for ethanol-water using density data as a function of composition taken from

| TABLE 5 |
| Graphs Prepared Using Spreadsheets for Phase Equilibrium Class |

| Binary phase diagrams for ideal solutions |
| Pxy<sup>a</sup> |
| Txy<sup>b</sup> |
| xy<sup>c</sup> |

| Fugacity versus pressure |
| Numerical integration of PV data<sup>a</sup> |
| Generalized virial coefficient<sup>b</sup> |
| Redlich-Kwong equation of state<sup>b</sup> |

| Volumetric properties of binary nonideal solutions |
| Excess volume<sup>a</sup> |
| Partial molar excess volumes<sup>b</sup> |

| Activity coefficients in binary solutions versus composition |
| Margules<sup>a</sup> |
| Van Laar<sup>b</sup> |
| Wilson<sup>a</sup> |

| Infinite dilution activity versus temperature |
| Wilson<sup>a</sup> |

| Phase diagram for nonideal azeotrope forming binary mixture |
| Pxy<sup>b</sup> |
| Txy<sup>b</sup> |
| xy<sup>b</sup> |

| Excess free energy of homogeneous azeotrope forming binary mixture versus composition |
| Experimental data<sup>a</sup> |
| Margules equation (fit to azeotrope data)<sup>a</sup> |
| Margules equation (best fit to VLE data)<sup>a</sup> |
| Wilson equation (literature constants)<sup>b</sup> |

| Excess free energy of heterogeneous azeotrope forming binary mixture versus composition |
| Experimental data<sup>a</sup> |
| Margules equation (best fit to VLE data)<sup>a</sup> |
| Margules equation (best fit to LLE solubility data)<sup>a</sup> |

<sup>a</sup>Prepared by students as homework assignment
<sup>b</sup>Prepared by instructor for class discussion

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Continued on page 291.
The Chem-E-Car competition has been run for undergraduates by the AIChE for the past three years with finals at the AIChE annual meetings. The idea is for teams of undergraduate students to design and build a small car powered by a chemical reaction. The objective is for the car to travel a certain distance and then stop. The distance to be traveled and the weight to be carried by the car are not announced until the day of the competition. The emphasis is on control of a chemical reaction, with a keen eye on safety and the environmental impact of the design. The winner is the team whose car stops nearest to the required distance. In addition to designing and building the car, each team must make a poster that describes the car’s operation and include a safety and environmental assessment.

Having witnessed the enthusiasm of the participating students and spectators at the AIChE Chem-E-Car Competition finals held in Dallas and Los Angeles, I decided to organize a Chem-E-Car competition here in Australia. Early in 2001, I contacted all chemical engineering departments in Australia and New Zealand, sent them copies of the rules (for the AIChE competition), and invited them to join. Six departments responded enthusiastically, and within a couple of months teams of students were working away. The original plan was to have local competitions within each department, with these competitions generating finalists for the grand Australasian final. University work and the difficulty of the Chem-E-Car task took its toll, however. Several teams fell by the wayside, including the team from my department. As time went on, it became clear that the grand final would be a fight between five teams—four from Australia and one from the National University of Singapore, who, upon hearing about the competition, asked if they could take part. The grand final was held on day three of the World Congress of Chemical Engi-

Figure 1. The NUS car (a) with bodywork removed to reveal the inner detail and (b) in motion.

Figure 2. The UNSW car drifting through its self-generated mist.
neering at the Melbourne Exhibition Centre in late September.

THE TEAMS AND THE CARS

National University of Singapore (NUS)

The NUS car (Figure 1) used the decomposition of 15% hydrogen peroxide solution with dilute potassium permanganate solution as a catalyst to generate oxygen, which was stored in the stainless steel reactor. Opening the ball valve at the rear of the reactor released the contents in short order, propelling the car along. The car was stopped by friction. The distance traveled was controlled by adjusting the quantities of reactant used and the time for reaction.

During the test runs prior to the competition, this car announced itself with a loud bang and blew away the plastic sheeting that had been specially erected as a splashguard behind the start line. Race helpers hurriedly modified and reerected the splashguard. The valve on the rear of the reactor was equipped with a lengthened handle. Starting the car involved swinging an oversized pair of laboratory tongs, golf-iron style, to hit the handle and swiftly open the valve. The swipe with the tongs only happened at the precise time, dictated by the reaction countdown.

On its first official competition run, the team member wielding the tongs was either a little too enthusiastic or had poor aim; the result was that the car turned onto its side within a few meters of the start line.

University of New South Wales (UNSW)

The UNSW car, named “Cold Power,” was powered by a 1.5-3V electric motor running from an electrochemical cell. The cell used solutions zinc sulfate and copper sulfate with zinc and copper electrodes. The electrodes were made from 1 mm sheet, totaling around 200cm² for each metal. The distance was controlled using a switch that involved measuring the speed of sublimation of solid carbon. A quantity of solid carbon dioxide was placed in a container on one side of a pulley. On the other side were a number of counterweights such that the solid carbon dioxide container rested on a metal electrode, which completed the circuit. As the solid carbon dioxide vaporized, the weight on that side of the pulley decreased until it was outweighed by the counterweights. Once this occurred, the solid carbon dioxide container lifted off the electrode and cut the power to the motor. The amount of solid carbon dioxide initially placed in the container (anywhere from 20g to 50g) was determined by the distance to be traveled. The UNSW car was interesting to observe as it glided along in a white cloud generated by the subliming carbon dioxide (see Figure 2).

Sydney University

The Sydney University car (see Figure 3) was designed and built by a team of first-year engineering students (mechanical and chemical). It was driven by an electric motor powered by an electrochemical cell comprised of 1.8M sulfuric acid and potassium dichromate solution (1g/100ml) with zinc electrodes. This car had three wheels and a low center of gravity. It...
was able to travel well in a straight line. The inventory of acid was only 5ml, and the cell was enclosed to minimize spillage problems in the event of a crash. The first run of the Sydney team was good, but unfortunately, it started without the required weight.

**Newcastle University Team One**

The Newcastle Team One car was driven by a small 3.5V 1A motor and powered by a zinc/copper copper sulfate battery, using 1M copper sulfate solution and 1M sulfuric acid. This car made a promising start, getting third closest to the line on its first run. Technical problems (a broken electrical connection to the motor), however, prevented it from leaving the starting line on its second run (see Figure 4).

**Newcastle University Team Two**

The Newcastle Team Two car (see Figure 5) was driven by a 3V electric motor via a six-speed gearbox. The motor was powered by a battery of four cells each producing 1.45V-two section of solder wire incorporated into the cell wiring and connection to the motor), however, prevented it from leaving the starting line on its second run (see Figure 4).

Reports from faculty involved in supervising the local department competitions suggested that the students benefited greatly from the experience. To get to the start line with a car that was competitive and worked according to the rules, each team had to solve the series of specific engineering problems. Several teams went beyond mere functionality and considered aesthetics. The concentration and enthusiasm of the participants was palpable, and I was privileged to witness it. It is not often that our students engage in something that is fun and also a great learning exercise. The Chem-E-Car Competition was this and more.

The Chem-E-Car Competition will be held again next year with the grand final in Christchurch, New Zealand, at the CHEMeca 2002, the annual conference of chemical engineers in Australia and New Zealand.
User-Friendly Phase Equilibrium

Continued from page 287.

handbooks.[10,11] By doing this assignment, students can develop a better intuitive understanding of the meaning of such excess property data because they see where the data came from. Additionally, the magnitude of the variation of activity coefficient with pressure is related to the partial molar excess volume. Using these results, students can prove to themselves why activity coefficients are typically assumed pressure-independent.

Before using activity coefficients in VLE calculations, students prepare a few plots of activity coefficient versus composition or of infinite dilution activity coefficient versus temperature. When they produce graphs similar to those in the textbook, students reinforce their concept of what "shape" these functions should have. Also, by plotting results from several different equations on one graph, students see that it makes little difference which correlation is chosen in most cases. For subsequent VLE and LLE calculations, they typically use the Margules equation because it is the most simple mathematically.

In conjunction with VLE phase diagrams, students produce plots of excess free energy functions. These plots can be used to determine constants in an activity coefficient correlation. For example, a plot of $G^\circ/RTx_1x_2$ versus $x_1$ can be used to determine Margules equation parameters by a straight-line fit. When constants determined by several methods are used to plot an $xy$ diagram, students learn the fit of the data is as important as which equation is used.

Phase separation and LLE are analyzed with graphs of free energy of mixing versus liquid composition. For LLE, it is the shape of these curves—convex or concave—that is the determining factor in phase stability. As with the VLE data, students generate plots of these functions from experimental data points and, by fitting activity coefficient correlations in various ways, compare the results.

Phase equilibrium and chemical reaction equilibrium are often taught in one course. I have also successfully used computer spreadsheet assignments or demonstrations for class discussion in the reaction equilibrium portion of the course.

It is a fundamental belief of mine that students will choose to use the computer and specific software in cases where it makes a problem easier to solve. When I assigned these problems, I did not require the use of specific software. (In fact, I did not require the use of a computer at all, but with the availability of computing resources and the students' familiarity with computers, no hand-plotted solutions have been submitted in about ten years!) I typically discussed how to structure a spreadsheet for the assignment and frequently had the students work through a hand calculation for a single data point as an in-class exercise.

The majority of students "follow the path of least resistance" and complete the assignment using the standard spreadsheet package, currently Microsoft Excel. The specific choice of spreadsheet has little effect. Students have solved the problems using Quattro Pro, Lotus 1-2-3, SuperCalc, and the Smart Spreadsheet in past years. Moreover, it is unnecessary to use a spreadsheet, as a few students have demonstrated by solving the problems using programming languages (FORTRAN, C), graphics packages, and math solvers (Mathcad, Maple).

All students eventually gravitated to spreadsheets by the end of the class, however. The only warning I give to students who use nonstandard computer software is that I may not be able to assist them with computer-related problems if they are using a package with which I am unfamiliar.

CONCLUSIONS

In teaching phase equilibrium thermodynamics, I have attempted to promote understanding and intuition of the course material. Initial explanation that the goals of the class relate mainly to data handling and generation, unlike other chemical engineering classes, prevents confusing expectations from developing. Meaning and consequences of data are emphasized, particularly for abstract quantities such as activity coefficients for which interpretation is not necessarily explicit. Widespread presentation and students' use of graphical data is made convenient using computer spreadsheet software.

ACKNOWLEDGMENTS

These computer assignments were developed over a series of courses taught at Michigan State University and Villanova University.

REFERENCES

Laboratory exercises are essential towards the development of a good chemical engineering graduate with desirable skills such as independent learning, interdependent learning, problem solving, critical thinking, creative thinking, interpersonal skills, teamwork, leadership, integration, communication, and change management. The standard laboratory exercise in chemical engineering, however, revolves around an apparatus that remains unchanged for several years and can lead to unethical practices among students such as submission of data/reports from previous years. Moreover, the application of thought, which is crucial for laboratory work and developing the skills mentioned above, is almost nonexistent in the standard laboratory exercise. From an instructional-objectives viewpoint, most laboratory exercises are designed to be at Bloom level 2 (comprehension) out of the possible six levels. This leads to severe resentment toward laboratory work among students and professors alike. Students consider lab courses as a formality to be completed, while faculty treat them as poor cousins of theory courses, relegating the entire responsibility for lab courses to lab supervisors or teaching assistants.

We believe that if students are challenged to think critically on laboratory exercises and encouraged to be creative, their interest in and respect for laboratory work would improve, and in turn, the faculty would be further motivated to offer better laboratory courses/projects. With this belief, a laboratory course consisting of both dual-step laboratory exercises and a recommendation/innovation exercise was conceived and assigned to third-year (junior) undergraduate students taking the fluid mechanics laboratory at the Indian Institute of Technology, Bombay.

Our laboratory guidelines state that the overall aim of this laboratory course is to inspire students to appreciate the underlying themes of the experimental aspects/approaches to engineering/science with fluid-flow aspects as a model subject. The goal is to develop students' abilities to "think with their hands." Another purpose of this course is to improve understanding of fluid-flow principles, to develop a physical feel for some fluid-flow situations, to develop a familiarity with some commonly used fluid-flow equipment, to inculcate a concern for safety, to improve communication of experimental results, to improve the quality of analysis and inquiry, and to kindle the spirit of discovery in students. Further, we expect the exercise to develop some of the above-mentioned skills in a chemical engineering graduate.

The laboratory exercises consisted of dual-step laboratory experiments (performed by student groups) and a recommendations report (an individual activity).

The Dual-Step Laboratory Exercise

Each laboratory experiment was conducted over two lab sessions. During the first session, student groups were expected to follow the procedures given in the manual to carry out the experiment. Students were expected to become comfortable with the equipment and the experiment, and the first-session experiments were designed accordingly. After the first session, students were required (as homework) to analyze the data taken during the lab session based on the theoretical principles in the lab manual/fluid mechanics textbook/notes and examine whether the results obtained were as expected.

The recommendations report (an individual activity) was designed to challenge students to think critically on lab data/observations and incorporate their inputs into the laboratory manual to improve future experiments. Each student was expected to propose some suggestions/innovations to improve the equipment/apparatus, the experimental procedure, the safety aspect of the laboratory, communication of experimental results, and improvement in experimentation. The report was to be submitted along with the final experiment results. Each student was also expected to improve the quality of analysis and mathematical modeling of the experiment. The students’ suggestions/innovations were expected to be reviewed by the faculty and the necessary changes were made to the experimental setup to improve future lab results.

In conclusion, the implementation of these innovative laboratory exercises and the incorporation of the recommendations report have provided many students with opportunities to create, innovate, and contribute to the laboratory manuals. The students have shown interest in these exercises and have expressed a desire to continue the process of improvement in laboratory experiments. The faculty member has also been motivated to offer better laboratory courses/projects in the fluid mechanics laboratory.

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expected. The following ensued:

a) If the experimental results matched the expected results, students were expected to think of additional experiments, preferably new ones, that could be done with the same (or slightly modified) setup. But the additional experiments need to be done within the time frame of the second lab session. We believe that working with these practical constraints would help students acquire “street smarts,” which are useful in handling real-world problems.

b) If the experimental results did not match the expected results, students were required to form hypotheses based on the results and design ways to experimentally (with certain calculations) prove or disprove their various hypotheses in the second lab session. The emphasis was on the technical/scientific rigor in proofs. The students were also warned that their theories could be proved false by their experiments and that it was acceptable to admit they did not understand the reasons for disagreement within the time available to them and therefore, additional study would be required.

After the second lab session, each student group was expected to submit a single report in the regular format, i.e., (a) Aim and Objectives, (b) Methodology, (c) Results and Discussion (which was required to be significant), (d) Conclusions, and (e) the original data sheets. The reports were graded on the following bases:

If the actual results matched the expected results:
- Ability to follow procedures 10%
- Data analysis (1st session) 15%
- Discussion (1st session) 15%
- Creativity/originality aspects (2nd session) 20%
- Data analysis (2nd session) 15%
- Discussion (2nd session) 15%
- Presentation (mainly communication) 10%

Reports that addressed novel aspects to study in their second session were rewarded handsomely in grading the creativity/originality criterion (see the student examples presented later).

If the actual results did not match the expected results:
- Ability to follow procedures 10%
- Data analysis (1st session) 15%
- Discussion 15%
- Clarity in thought and situation/problem analysis (2nd session) 20%
- Rigor (2nd session) 15%
- Discussion (2nd session) 15%
- Presentation (mainly communication) 10%

Reports that were well developed on both the possible reasons for the disagreement between actual and expected data and the experiments to prove or disprove them were given high marks for the clarity-in-thought criterion. The difficulty level in problem analysis was also recognized in that criterion—reports that fully analyzed a difficult situation received higher marks than those that, as a matter of chance, analyzed a simple, easy-to-identify situation. Also, reports that unequivocally proved or disproved their points received high marks for the rigor criterion. Other criteria, such as data analysis, discussion, and presentation, carry their usual weight.

The Recommendations Report

Over the duration of the course, each student was expected to think about an experiment or a set of experiments that could be done in the fluid mechanics lab. Students were encouraged to be as creative as possible. Near the end of the course (a week before the last day of classes), each student was expected to submit a detailed report on this experiment (or set of experiments) and the equipment and instruments needed.

The reports were evaluated on the following bases:
- Creativity/originality aspects 30%
- Clarity in thought 20%
- Detail 30%
- Doability 10%
- Presentation (mainly communication) 10%

The dual-step exercises evaluated through the reports carried a 70% weight, and the recommendation report carried a 30% weight toward the final grade.

IMPLEMENTATION OF DETAILS /RATIONALE

In the beginning of the semester before the experiments began, the instructor met the class and discussed the exercises and recommended strategies. In addition to experimental details for the first session, the laboratory manual carried information on safety procedures for the lab, error analysis, technical writing, and the unacceptability of academic dishonesty, all of which were seriously discussed in the initial meeting. The instructor also emphasized the need for safety procedures whenever he observed lapses during the lab sessions. Student groups were asked to select their own leaders who would assign duties for the group members and be generally responsible for the group’s activities. This ensured that an avenue for the development of teamwork and leadership skills existed. Also, on many occasions, the instructor communicated to the groups through their leaders.

Before the start of the first session, the groups were advised to familiarize themselves with the details for each experiment using the lab manual and the textbook. The first-session experiments were designed as shorter versions of the experiments given in the usual lab course, and students were encouraged to spend the additional time becoming comfortable with the setup and the various equipment used. For example, the instructor encouraged the students to raise questions regarding the equipment or the reasoning behind the various experimental steps, which the students normally took for granted. The students took the first session seriously because they knew they had to consider the setup, the experimental methods, and the underlying theory in order to have an interesting second session. During the experiment (both sessions), groups were advised to record the data in duplicate
using a carbon sheet, and the members were asked to sign each data sheet. The duplicate copy was submitted to the instructor at the end of each session, and non-submission would result in a grade of zero for that session. The instructor has never had to give a zero over the past two years for this reason.

After the data analysis for the first session, the groups were required to meet the instructor to discuss their plans for the second session. This meeting was not to guide the students on what they could do in the second session, but for the instructor to listen and comment on the possibility of doing the experiments. This meeting was normally scheduled a few days before the second session, primarily to address any special requirements for the experiment that needed to be communicated to the lab superintendent. Also, this meeting helped the instructor ensure that the second-session experiments were of proper scope (neither too large nor too small) and reasonably well thought out, especially if the actual data matched the expected data in the first session. In addition, it was communicated to the students at the beginning of the semester that no complete dismantling of the set-ups would be allowed, except in rare cases. This encouraged the students to think of “non-invasive” means for testing their theories. Also, this precaution was necessary because some piping networks in our lab had packings to prevent leaks that would be difficult for an inexperienced person to reassemble.

The lab reports for the dual-step exercises were due before the start of the next experiment; the instructor graded them and offered constructive criticism and feedback within a week of submission. Students appreciated the timely feedback.

The grading of the recommendations report was time consuming (three to four consecutive, full days). As long as grades are important, some students may cheat to get the best grade; therefore, a significant amount of time was spent establishing the originality of submitted reports. This was achieved through one-on-one interviews with students who had submitted “doubtful” reports. During an interview, it was easy to ascertain whether cheating had taken place by asking relevant questions, most of which were on the experiment submitted.

All experiments were run on existing equipment; therefore, this dual-step exercise does not require additional funds for equipment. It can be run anywhere, even in the face of fund crunches. It also provides a greater probability for disagreement between actual and expected data, and thus helps students develop lateral-thinking abilities while forming hypotheses for the disagreement. Therefore, the dual-step laboratory exercise provides a way to turn a seeming disadvantage in running an existing laboratory course into an advantage of improving thought in students.

**SAMPLES FROM STUDENT EXERCISES**

**Samples from the Dual-Step Laboratory Exercises**

**Agreement Between Actual and Expected Data** • An experiment for the lab involved studying the relationship between Power number and Reynolds number in an agitated system. One of the groups found good agreement between actual and expected data and therefore had to think of additional experiments to do on the same setup. They decided to compare the relationship between Power and Reynolds numbers for an aqueous system with and without a surfactant. They found that the Power number for the corresponding Reynolds number was lower for the system with surfactant than for plain water. Therefore, they concluded that the power requirements for an aqueous system with surfactant are lower than that for plain water. They also provided qualitative explanations for the observed results from a molecular viewpoint.

Another experiment involved studying two-phase flow characteristics in a vertical transparent tube such as the relationships between slug length and slug velocity and between pressure drop and void fraction, etc. The group that obtained results as expected decided to study the relationship between the radius of curvature of the slug’s leading edge and its length. They developed a theory based on geometrical considerations for the variation of the leading-edge curvature with slug length; they also showed correspondence between the theoretically expected results and measured data.

**Disagreement Between Actual and Expected Data** • Another experiment involved a piping network with various types of pipes, fittings, and valves. The objectives for the first session included determination of the frictional losses across the pipe fittings and valves. The experiment required recording readings from manometers attached to the pressure taps across relevant fittings or valves and determining the water flow rate using the pressure difference measured across the orifice meter.

The first group that worked on the experiment found that the friction loss constants obtained for the various fittings on the network were higher by almost an order of magnitude than literature values. Therefore, the group first postulated that scale formation led to higher loss constants. To test the postulate, they arranged for the network to be cleaned thoroughly and repeated the experiment in the second session. This did not yield significantly different loss constants, thereby partly disproving the postulate that the scale formation alone resulted in the discrepancy. Students in one of the other groups that worked on the experiment postulated that the water-flow rate measurements using the calibration curve for the orifice meter may not have been correct; they noticed
a discrepancy between flow rates measured using a measuring jar/stop watch arrangement and the orifice meter readings. So, the students prepared a fresh calibration graph for the orifice meter and found it to be different from the existing, erroneous calibration chart. They also proved that the friction loss constants obtained using the new calibration graph were comparable to the values found in the literature.

**Samples from the Recommendations Report**

A student named Nikhil Agarwal suggested an inexpensive, simple method for determining the viscosity of a solution by allowing it to flow over a smooth, inclined flat plate from a reservoir and taking measurements. Using suitable balances, Nikhil expressed the viscosity as a function of measurable parameters (with origins from the thickness of the liquid layer) as:

\[ \mu = \frac{\rho \delta^3 \cos \beta}{3Q} \]

where \( \rho \) is the fluid density, \( g \) is the acceleration due to gravity, \( \delta \) is the film thickness, \( \beta \) is the angle between the plate and the vertical, and \( Q \) is the flow rate. He carefully considered the details and limitations of the experimental procedure and suggested a method to study the variation of viscosity with temperature using the same setup.

Another student, Sikander Siraj, using input from a friend in electrical engineering, suggested a photoelectric diode-based (PED) device for the measurement of slug lengths in the two-phase flow experiment. The idea had its origins in the burglar alarm principle. For the measurement, he used the deviation caused by the refraction of the infrared beam when it passes through media of different refractive indices.

**STUDENT AND STAFF FEEDBACK**

The students were asked to send their comments through e-mail to their class representative, who removed details pertaining to the authors of the comments, compiled without editing, and forwarded the comments as a single file to the instructor. For the improved version of the lab, comments from 82 out of 83 students were received, and all except nine explicitly stated that the lab was useful to them. They said that their learning included fluid-mechanics principles, application of thought to a lab, leadership qualities, thinking creatively, and working in a group. Some positive comments over the past two years include, "Due to this lab alone, I can say that I know some chemical engineering," and "This is the first time I feel what a lab course is all about." Also, many students suggested minor changes in equipment, etc., to improve the lab. Of the nine students who did not state their liking for the lab, seven were neutral, and the other two said that the lab was not useful to them.

The staff associated with the lab were enthusiastic about fulfilling the requirements of the lab. They also said that they enjoyed setting up the various experiments although it involved additional time.

**INITIAL CHALLENGES**

The first time it was offered, almost all students expressed that the lab demanded a lot of their time. We believe this was because students compared it with previous editions of the same course. In addition, the same experiments that were given in previous editions were packaged into a two-session (dual-step) format, significantly increasing the work. Therefore, in the next edition of the course, the experiments were consolidated into half the original number, with all other details unchanged. Afterwards, there were very few comments (3 out of 83) that there was too much work.

The first time the course was offered, the groups were assigned according to student roll numbers, which the students hated. The next time, the students were asked to form their own groups with the average cumulative performance index (CPI) of the group members being close to the class average CPI; this incorporates cooperative learning elements. Complaints about unsuitable groups were almost eliminated.

The remaining challenge is group size. Six students in a group is nonideal and should be reduced. We intend to reduce the number by running the experiments more frequently in the future. The logistics constraint needs to be addressed first, however.

In short, a focus on developing the critical thought process in students made the laboratory course interesting to both students and instructors and also developed students' respect for experimental work.

**ACKNOWLEDGMENTS**

We would like to thank the students of CL333 for their enthusiastic participation in the exercise as well as O.S. Sawarkar, V.B.V. Nair, V. Ramachandran, and A.D. Kadam for their contributions.

**REFERENCES**

On three occasions in recent years, I have taught an elective course at the University of Notre Dame for chemical engineering seniors titled “Topics on Ecology and the Environment.” I developed the course because I felt it was important for our students (and myself as well) to have a greater appreciation—from a chemical engineer’s perspective—for the workings of Earth’s natural processes, both biotic and abiotic, and a knowledge of how human and industrial activities are disturbing or might disturb them.

One of the significant components is a module on the carbon cycle—the subject of this article. In gathering and developing material for this module and others in the course, I was struck by these observations:

- Many of the Earth’s processes, including the carbon cycle, though fundamentally very complex in detail, can be represented by simple models that are useful for study purposes and even for quantitative estimates, at least as a first approximation.
- The development, analysis, and application of models are well within the scope of an undergraduate chemical engineering curriculum.
- The subject matter, or bits and pieces of it, can be integrated advantageously, straightforwardly, and nearly seamlessly into core chemical engineering courses.

My objectives in this article are to demonstrate all of this, using the carbon cycle as the means, and to provide convenient material for others who may be persuaded by my third observation.

Of the biogeochemical cycles of the six major “life” elements, C, N, P, S, O, and H, the carbon cycle receives the lion’s share of the attention in the literature. That’s no surprise inasmuch as most of our energy needs are met by the burning of carbon-based fuels and inasmuch as the consequent increasing level of atmospheric carbon dioxide and its potential effect on the Earth’s climate is a frequent focus of attention in technical and nontechnical publications. What’s more, chemical engineers will have opportunities to play a prominent role in any steps taken to moderate that level, whether those steps be toward alternate energy sources or toward sequestering or otherwise preventing emissions directly into the atmosphere.

THE CONCEPTUAL MODEL

Carbon is found in all of Earth’s compartments or reservoirs—in the biota and in the atmosphere, hydrosphere, and lithosphere. Mathematical models describing the cycle account for the movement of carbon among and within those reservoirs and for anthropogenic disturbances, which are principally due to fossil fuel burning and deforestation (i.e., mainly burning of removed trees) for land use changes.

Figure 1 presents a schematic diagram of a conceptual model of the carbon cycle consisting of six reservoirs, numbered one through six. (A seventh reservoir for fossil fuels enters dynamically into the model later only as a disturbance to the six-reservoir natural cycle.) Other reservoirs, including sediments, marine biota, and lakes, rivers, and streams, are omitted for reasons given later. In one way or another, all models are based on this starting picture, which is sometimes

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modified to include one or more of the omitted reservoirs. Models differ primarily in the extent of detail and correspondingly in the objectives of the modeler. For example, highly detailed climate studies employ general circulation models based on fundamental transport equations to describe processes in the atmosphere and/or ocean reservoirs and several types of vegetation to describe the atmosphere-biota exchange. At the other extreme, so-called “box” (or “compartment” or “lumped”) models that are intended to give estimates of global averages of carbon in major reservoirs, are based on spatially aggregated descriptions, often with no more detail, sometimes even less, than that shown in Figure 1. Except to allude to the structure of high-end models and their purposes (and sometimes to compare results), I choose to work with simple box models in the course. In short, as tools for study, they have suited my purposes. Further, if properly calibrated and tuned, they have proven useful for quantitative purposes so long as the principal interest is in global averages, particularly in atmospheric carbon dioxide levels.

The conceptual model represented in Figure 1 and the mathematical description to follow are amalgamations of several box models that I have studied and used in the course. The version presented here is closely patterned after, but not identical to, that described in a recent publication by Lenton. I usually have the students go through the development of other models as complementary outside work.

**THE REFERENCE PRE-INDUSTRIAL STATE**

The quantities shown in parentheses in the boxes in Figure 1 represent estimates of the “pre-industrial” distribution of carbon (i.e., the mass of element C in all of its compounds) in petagrams (PgC, 1 Pg = 10¹⁵g.) These are typical reference values presumed to represent the balanced (steady-state) conditions around the year 1850—early in the industrial revolution when there was little or no observable change from year to year.

The numbers in parentheses beside the arrows in Figure 1 represent estimates, in petagrams of carbon per year (PgC/ y), of the transport (commonly termed “fluxes” in the relevant literature) of carbon between reservoirs. Such fluxes are adjusted so that each box is balanced at a steady state, where it would remain unless disturbed. There is no common agreement on the values of the reference pre-industrial masses and fluxes, or even on the reference year (generally between 1800 and 1860), but the variation from one reference source to another is of little significance. The values shown in Figure 1 are in line with those used in the references cited above.

Mₜ, the mass of carbon in the atmosphere reservoir can be taken to be entirely in the form of CO₂. The 612 PgC in that reservoir corresponds to a CO₂ concentration of 286 ppmv (parts per million by volume) —the concentration unit used in most illustrations to follow. (The conversion factor of 2.128 PgC/ppmv is based on a total atmosphere mass of 5.14 x 10¹⁷ with a molecular weight of 29.)

Notice the notation in Figure 1. M, stands for the mass of carbon in box i; F, for the flux of carbon from box i to box j. The anthropogenic disturbance flux Fᵣ moves carbon from a nonrenewable fossil fuel reservoir to the atmosphere. The other anthropogenic disturbances, Fₐ and F, take carbon from the renewable terrestrial biota reservoir to the atmosphere (deforestation) and from the atmosphere to the terrestrial biota (reforestation), respectively. (There is increasing interest in sequestering part of Fᵣ by redirecting it to cavities in the lithosphere and/or to the deep ocean. Those slight but interesting variations to the model will be mentioned in suggested exercises near the end.) The following list gives a succinct description of the other fluxes:

- Fᵣ accounts for all carbon emissions to the atmosphere except those due to deforestation. It is commonly termed "emissions due to fossil fuel burning" —a term that I shall use throughout. Other industrial sources, such as cement manufacturing, account for only a few percent of the total.
The mathematical description of the box model of Figure 1 consists of a set of carbon balance equations. For the atmosphere, box 1, for example

\[
\frac{dM_1}{dt} = F_{21} - F_{12} + F_{13} + F_{51} - F_{15} + F_{61} + (F_{t} + F_{d} - F_{r})
\]

In general

\[
\frac{dM_j}{dt} = \sum_{i=1}^{6} (F_{ji} - F_{ij}) + \text{disturbances}
\]

If a particular \( F_{ij} \) does not appear in Figure 1, its value in Eq. (2) is zero. The disturbances, as represented in Figure 1, appear only in the balances for boxes 1 and 5.

To keep account of the fossil fuel supply, a seventh box is added, an out-of-cycle, nonrenewable reservoir of the carbon in fossil fuels. The following balance describes the depletion of that reservoir:

\[
\frac{dM_7}{dt} = -F_t
\]

All terms in these equations have units of petagrams of carbon per year (PgC/yr).

The initial conditions are the reference pre-industrial reservoir levels in 1850. I use 5300 PgC for the initial value of \( M_7 \), somewhat arbitrarily, but based on rather common statements that while the total carbon stored in fossil fuels is about 10,000 PgC, only about half of it can actually be recovered for use.

Since most of the reservoirs undergo relatively small changes over periods of interest, as later simulations will show, the fluxes can be related to the reservoir masses by first-order processes. That is

\[ F_{ij} = k_{ij}M_i \]

Such relationships are frequently employed in box models of the biogeochemical cycles, including the carbon cycle, with three exceptions: \( F_{15}, F_{21}, \) and \( F_{31} \). For the others, the numerical value of \( k_{ij} \) can be obtained readily from the reference data given in Figure 1.

If the carbon in the ocean were present simply as carbon dioxide in aqueous solution, we would expect all four of the \( F \)'s connecting the ocean surface waters to the atmosphere to be describable by Eq. (4)—under the safe assumption that Henry’s law applies to the dilute CO₂ solution. The situation is complicated, however, by the fact that CO₂ is a weak acid and solution enters into equilibrium chemical reactions involving carbonate and bicarbonate forms. Therefore, while the fluxes \( F_{21} \) and \( F_{31} \) can be related linearly to aqueous CO₂, they are not linearly related to the total C; that is, to \( M_2 \) and \( M_3 \). The relationship to the total carbon in solution is complicated. It is affected by all of the factors that affect acid-base equilibrium in ocean water—total alkalinity, salinity, temperature, and dissolved salts of weak bases, such as boron. A rigorous treatment requires linking a set of equations for ocean chem-
istry dynamics to the above set. Some studies have followed that procedure, as have in some instances. Others have opted for a simpler empirical approach that uses the following relationships:

\[ F_{21} = k_{21}M_2^{\beta_2} \quad F_{31} = k_{31}M_3^{\beta_3} \]  

(5)

Values of the exponents \( \beta_2 \) and \( \beta_3 \), called buffer factors or Revelle factors, can be obtained from charts of the type given in the book by Butcher, et al. They can also be obtained by delving into the intricacies of ocean chemistry dynamics and correlating results of calculations. I used the latter approach to obtain the values shown later, but to save space and to stay on track, I shall spare further detail.

My testing has shown that results of computations using constant values of the \( \beta \)'s hardly differ from those obtained by appending detailed ocean dynamics to the model, so long as changes in \( M_1 \) and \( M_2 \) are relatively small, generally less than 5%. The numerical values of \( \beta \) range between 9 and 15; the nonlinearity is surprisingly strong. Notice that with values of \( \beta_2 \) and \( \beta_3 \) given, numerical values of the rate constants \( k_{21} \) and \( k_{31} \) can be determined from the reference conditions given in Figure 1.

The rate of photosynthetic uptake, \( F_{15} \), of carbon from the atmosphere cannot be represented realistically as a linear function of \( M_1 \). The basic reason is that the function should account for a saturation effect with regard to the nutrient \( \text{CO}_2 \). That is, the rate increases with increasing \( \text{CO}_2 \) but approaches a limit. For small changes in \( M_1 \), the function may be approximated by a linear relationship, but as a later illustration will show, changes in \( M_1 \) are large over the periods of interest.

There seems to be no clear consensus as to what form to use for \( F_{15} \) in models of this type. Whatever the specific form, a common feature is a dependence on atmospheric carbon that suggests an ultimate saturation. The particular one chosen does not seem to be a critical matter so long as the constants are calibrated or tuned to fit existing data. Nevertheless, this is a fertile item for classroom discussion, debate, and outside work. Here I shall use the form employed by Lenton:

\[ F_{15} = \begin{cases} k_{15}M_8 \frac{M - \gamma}{M_1 + \Gamma} & \text{for } M_1 > \gamma \\ 0 & \text{for } M_1 \leq \gamma \end{cases} \]  

(6)

where

- \( \gamma \) is the threshold value of \( M_1 \) (I used Lenton’s value of 62 PgC)
- \( \Gamma \) is a saturation parameter (Lenton used it as a tuning parameter and arrived at a value of 194 PgC. By methods described later, I arrived at a value of 198 PgC.)
- \( k_{15} \) is a rate coefficient to be calculated from the reference state.
- \( M_8 \) is a function that depends on the disturbances \( F_r \) and \( F_d \) as explained and described below. In short, it accounts for changes in the Earth’s capacity for terrestrial biota.

The role of the function \( M_8 \) is important but not obvious at first glance, and definitions and explanations do not come easily. Let me first define it by way of the following equation and then offer brief explanations.

\[ M_8(t) = 1 + \int_{1850}^{t} \frac{(k_rF_r - k_dF_d)dt}{M_{5,\text{ref}}} \]  

(7)

where

- \( k_r \) is the fraction of forested area or mass (or forest capacity) that cannot be reforested (is not available for regrowth) following deforestation activities—for example, forest areas cleared for urban development.
- \( k_d \) is that fraction of the reforested area or mass that increases the Earth’s capacity for terrestrial biota. (This is sometimes termed “aforestation” as opposed to “reforestation” that directly renews deforested areas.)
- \( M_{5,\text{ref}} \) is a normalizing factor inserted arbitrarily to make \( M_8 \) dimensionless. I take it to be the initial value of \( M_8 \).

Lenton used this form but did not include \( k_d \) and \( F_d \) explicitly in his formulation. Reforestation can be accounted for without those factors if \( F_d \) is allowed to have negative values. I prefer to show \( F_r \) and \( F_d \) separately for clarity in simulations later.

Simply stated, the integral in Eq. (7) accounts for permanent effects of the disturbances \( F_d \) and \( F_r \). Were that integral not included, the model equations would lead to the following illogical conclusion, among others: If \( F_r = 0 \) and if \( F_d \) and \( F_r \) eventually settle to zero, the ultimate steady state of carbon in the reservoirs would be identical to the starting reference state; the effects of the temporary nonzero values of the disturbances would die away, according to the model. But obviously the effects of some land use changes must persist—for example, if forest areas are cleared and urbanized with no offsetting reforestation. With the integral included in \( M_8 \), with \( k_d = 0 \) and \( F_d = 0 \), such land use change would permanently affect the distribution of carbon, not its total amount. Other illustrations can be given to justify the form of \( M_8 \), but perhaps further explanation, if needed, is better sought in student exercises later.

An alternate form of the integral equation above is this differential equation:

\[ \frac{dM_8}{dt} = \frac{k_rF_r - k_dF_d}{M_{5,\text{ref}}} \]  

with initial condition \( M_8(1850) = 1 \) (8)

The numerical value of the coefficient \( k_{15} \) in Eq. (6) can be calculated from the reference values shown in Figure 1, given values for \( \Gamma \) and \( \gamma \) and taking \( M_8 = 1 \) (its initial state).

With Eq. (8) added to the material balance equations, the complete mathematical model consists of the following set of eight ordinary differential equations:
\[
\begin{align*}
\frac{dM_1}{dt} &= -(k_{12} + k_{13})M_1 - k_{15}M_8 \frac{M_1 - \gamma}{M_1 + \gamma} + k_{21}M_2^2 \\
&\quad + k_{31}M_3^2 + k_{51}M_5 + k_{61}M_6 + F_f(t) - F_f(t) \\
\frac{dM_2}{dt} &= k_{12}M_1 - (k_{23} + k_{24})M_2 - k_{21}M_2^2 + k_{43}M_4 \\
\frac{dM_3}{dt} &= k_{13}M_1 + k_{23}M_2 - k_{34}M_3 - k_{31}M_3^2 + k_{43}M_4 \\
\frac{dM_4}{dt} &= k_{24}M_2 + k_{34}M_3 - (k_{42} + k_{43})M_4 \\
\frac{dM_5}{dt} &= k_{15}M_8 \frac{M_1 - \gamma}{M_1 + \gamma} - (k_{51} + k_{61})M_5 - F_f(t) + F_f(t) \\
\frac{dM_6}{dt} &= k_{56}M_5 - k_{61}M_6 \\
\frac{dM_7}{dt} &= -F_f(t) \\
\frac{dM_8}{dt} &= \left[ k_dF_d(t) - k_rF_r(t) \right] / M_{5,ref}
\end{align*}
\]

Numerical values for the constants are given in Table 1. Determining the values of the k's, as described earlier, calibrates the model to the data for the reference year 1850. The value for \( \gamma \) is taken from Lenton’s model. The value for \( k_d \) is somewhat arbitrary and could be adjusted by tuning the model, but I have taken it to be constant throughout at \( 0.23 \). (Lenton used a value of \( 0.27 \).) I have arbitrarily chosen a value of unity for \( k_r \). My method for determining the value for \( \Gamma \), the only tuning parameter, will be described in the next section. The values for \( \beta_2 \) and \( \beta_3 \) were determined as described earlier.

Implicit in this development is the assumption that the carbon cycle is independent of all other state variables, or that all others are constant, such as temperature, moisture, and other nutrient levels. That assumption is frequently invoked, but it may be an oversimplification if the model results are to be applied to global climate dynamics, for example. In the aforementioned work of Lenton\( ^3 \) the carbon cycle is coupled to the Earth’s energy balance, and in that of Ver et al.\( ^7 \) to other nutrient cycles.

**TUNING AND TESTING WITH HISTORICAL DATA**

Extensive historical records are available for testing and tuning the model. Figure 2 shows data on emissions due to fossil fuel consumption, \( F_f \), taken from Marland et al.\( ^{11} \) and deforestation, \( F_d \), taken from Houghton and Hackler,\( ^{12} \) as well as the total of the two over the period 1850 through 1990. (I used 1990 as the endpoint because the deforestation data given by Houghton and Hackler are not tabulated beyond that year. We can safely assume that reforestation, \( F_f \), has been negligibly small in the past.) The dramatic increase in fossil fuel emissions since the middle of the twentieth century is evident.

The solid curves in Figure 2 show my empirical fit of the reported data. In order to get a rather precise representation I used separate functions over four segments of \( F_f \) and over six segments of \( F_d \). This detailed fitting may seem to be overkill. I simply wanted to eliminate an inaccurate

---

**TABLE 1**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>( k_{12} )</td>
<td>0.0931</td>
<td>( y^{-1} )</td>
</tr>
<tr>
<td>( k_{13} )</td>
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</tr>
<tr>
<td>( k_{14} )</td>
<td>147</td>
<td>( y^{-1} )</td>
</tr>
<tr>
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<td>( 58 (730\text{PgC}) )</td>
<td>( \text{PgC} (1.09) y^{-1} )</td>
</tr>
<tr>
<td>( k_{16} )</td>
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<td>( y^{-1} )</td>
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<tr>
<td>( k_{17} )</td>
<td>0.0164</td>
<td>( y^{-1} )</td>
</tr>
<tr>
<td>( k_{18} )</td>
<td>( 18 (140\text{PgC}) )</td>
<td>( \text{PgC} (1.09) y^{-1} )</td>
</tr>
<tr>
<td>( k_{24} )</td>
<td>0.714</td>
<td>( y^{-1} )</td>
</tr>
<tr>
<td>( k_{26} )</td>
<td>0.00189</td>
<td>( y^{-1} )</td>
</tr>
<tr>
<td>( k_{27} )</td>
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<td>( y^{-1} )</td>
</tr>
<tr>
<td>( k_{28} )</td>
<td>0.0862</td>
<td>( y^{-1} )</td>
</tr>
<tr>
<td>( k_{29} )</td>
<td>0.0862</td>
<td>( y^{-1} )</td>
</tr>
<tr>
<td>( k_{30} )</td>
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<td>( y^{-1} )</td>
</tr>
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<td>( \beta_2 )</td>
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</tr>
<tr>
<td>( \beta_3 )</td>
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</tr>
<tr>
<td>( \gamma )</td>
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</tr>
<tr>
<td>( \Gamma )</td>
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<td>( \text{PgC} )</td>
</tr>
<tr>
<td>( k_d )</td>
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<td></td>
</tr>
<tr>
<td>( k_r )</td>
<td>1.0</td>
<td></td>
</tr>
</tbody>
</table>

---

**Figure 2.** Historical record of carbon emissions to the atmosphere. Symbols represent reported data; \( ^{11,12} \) solid curves are empirical fits.
representation of the disturbance record as an explanation for any model failure.

With this representation of the historical disturbances and the model constants in Table 1, the system of ordinary differential equations in Eq. (10) can be solved readily, by numerical routines available in a number of software packages, to obtain a model-generated record of carbon in the reservoirs from 1850 through 1990. (I used Mathcad for this particular exercise and extensively throughout the course.) The solid curve of Figure 3 shows the result for atmospheric CO$_2$; the data points are reported estimates or measurements from the Worldwatch Institute database.$^{[13]}$ The good agreement between model results and reported data was assured over a portion of the curve, at least by my method of determining the value of $r$. Its value of 198 PgC, as given in Table 1, was determined by an iterative search aimed at minimizing the total squared difference between model results and reported data over the period 1980-1990. Admittedly, the good agreement over the early years was also virtually assured because model constants were calculated to give a perfect fit of the reference data of 1850. Over the other years, the maximum disagreement, which occurs around 1925, is less than 1.3%. All such things considered, this test of the model lends legitimacy to its use in predicting carbon distributions through some years ahead.

Table 2 lists the calculated 1990 levels of carbon for all reservoirs. Notice that changes in the five of the six reservoirs have been relatively small over the 140-year period, according to the model. The terrestrial biota in box 5 increased only from 577 to 580 PgC owing to the offsetting effects of decreases by deforestation and increases by atmospheric CO$_2$ fertilization. The atmospheric reservoir increased by 23% by 1990 and is obviously destined to go higher, but changes in others have amounted to about 2% or less.

A total of 214 petagrams of new carbon was injected into the cycle from the fossil fuel reservoir and distributed among the other reservoirs over the period 1850 through 1990. Eventually most of that will reside in the deep oceans, box 4, but by 1990 that reservoir has increased by only 71 petagrams. Atmospheric carbon increased by 141 petagrams. Some of that redistribution of carbon, but not any of the increase in the total, is due to deforestation with a nonzero value of $k_d$.

In the simulations to follow, the ending values of the $M$'s for 1990, given in Table 2, are used as the initial state.

**SIMULATIONS**

The simulations described in this section engage the students in the use of the model and exhort them to learn about current trends, issues, and possible future actions—and to become informed about likely consequences regarding future disturbances to the carbon cycle. The principal interest is in the prediction of atmospheric carbon dioxide levels through the 21st century. Such predictions, based on models of varying degrees of complexity, have been reported in a number of recent studies.$^{[1,3,5,7,14]}$

**Disturbance Scenarios**

Postulated scenarios for future carbon emissions over a century of time when human activities, worldwide economies, and international politics are involved are naturally laden with uncertainty, the effects of which, in fact, probably overshadow the effects of the assumptions and simplifications in the model itself. Notwithstanding such, predictions through simulations require inserting the disturbance functions $F_r, F_{ct},$ and $F_r$ into the model equations.

The most commonly employed scenarios for carbon emissions are those in a set of five that were suggested in a 1992 report to the International Panel on Climate Change, IPCC.$^{[3,15]}$

$^a$ The list given in the References section is only a small sample. The interested reader will be led to a much larger assortment of models and related subjects simply by entering the keyword "carbon" on a web browser.
Known by the names IS92a, IS92b, ... IS92e, they are based on likely or possible trends in population changes, economic growth, energy supplies, etc. in developed and developing countries. There is also a Kyoto protocol, which, if enacted according to Article 3 of the agreement, would call for a worldwide decrease in emissions to 95% of the 1990 level by the year 2012.[16]

Shown in Figure 4 are slightly modified versions of three of the IS92 scenarios for total carbon emissions for 1990 onward, including the most pessimistic (IS92e) and the most optimistic (IS92c) cases, and what’s usually referred to as the “business-as-usual” scenario (IS92a). The latter is the most commonly used version, and as its description implies, is based on the assumption that carbon emissions can be predicted from current trends with no major changes in policies and practices.

Also shown in Figure 4 is a representation of the scenario for the Kyoto protocol, based on the assumption that emissions would be held constant after 2012. (Ver., et al., used a similar representation.[17]) The IS92 scenarios break down the anticipated emissions into fossil fuel use and deforestation. All of them use the same deforestation pattern, which declines to zero by 2100. A curve showing the modified deforestation scenario is also included in Figure 4. The differences between that curve and the others in the figure are the fossil fuel components. Reforestation is not included in the scenarios as a separate disturbance.

Some Results

I use two different approaches for simulations, each having certain advantages over the other. One is a straightforward numerical solution of the differential equations using Mathcad—basically similar to the method used to generate the historical curve in Figure 3. It’s the workhorse that I incorporate into classroom presentations and the major tool used by the students for assigned work. I constructed the other using LabVIEW®** to give a convenient user interface, a virtual laboratory, for certain classroom demonstrations and student experiments. It provides the user with hands-on control of the disturbances during a simulation, showing effects of manipulations “live” on virtual strip-chart recorders and digital displays. (Actually, I’ve used the LabVIEW simulation for classroom demonstration at the very beginning of the module because it is illustrative and serves to introduce goals and what the appetite for learning about model development and simulations.) Space limitations prohibit a full description of the LabVIEW simulator and its operation here, but the gist of it is shown in the photo of the user’s panel in Figure 5 and the brief description in the caption. Notice that those features afford the user an option of sequestering carbon by reforestation and by capturing a fraction of emissions, $F_r$, in the deep ocean and geologic reservoirs.

Figure 6 presents an example of the results of Mathcad simulations using the four scenarios of Figure 4. (For those simulations, I used linear interpolation between the data points shown in Figure 4 for the period 1990-2100.) The results in Figure 6 are based on the parameters listed in Table I except that here the values used for $\beta_2$ and $\beta_3$ are 11.0 and 12.3, respectively. (As I mentioned above, those values depend on the total carbon in the surface ocean reservoirs. I used the 1990 values of $M_s$ and $M_C$ given in Table 2 as a basis for the new $\beta$ values for the period 1990-2100.) $F_r$ is taken to be zero.

Notice that the model predicts atmospheric CO$_2$ would increase to 702 ppm by the year 2100 if the IS92a business-as-usual scenario were followed. Based on that scenario, predictions by models used by others[1,3,14] range between 697 and 724 ppmv. Over the entire 110-year period, the maximum difference in atmospheric CO$_2$ between any two of the four models (the three cited above and the present one) is about 4%, an observation that buttresses confidence in discussions of quantitative results from the model at hand. Notice the wide range of predicted CO$_2$ levels in 2100 resulting from the different scenarios for carbon emissions. The highest is nearly twice the lowest; both are probably unrealistic extremes. Business-as-usual would result in nearly doubling the 1990 CO$_2$ level by the year 2100, according to the model prediction.

---

* I modified the IS92 scenarios for both the fossil fuel and deforestation components in order to bring the 1990 values of the scenarios in agreement with the data actually reported for that year.[11,12] This amounted to adding 0.1 PgC to all of the IS92 fossil fuel quantities and increasing all of the deforestation values by about 30%. These modifications are more for refinement and fastidiousness than for any significant effect on calculations.

** LabVIEW, developed by the National Instruments Corporation in Austin, Texas, is graphical programming software developed mainly for data acquisition and instrument control. It also serves as a powerful tool for constructing virtual laboratories.

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**Figure 4. Carbon emissions to the atmosphere; historical data and possible future scenarios.**
Additional Work

Using Mathcad and LabVIEW simulations, students obviously can be involved in examining all sorts of questions, model variations, and parameter effects. Here is a partial list of exercises that I have used, some of which require consulting outside references.

- Extend simulations beyond 2100 to address a number of questions raised about the ultimate steady state. (Actually, I ask the students to use the steady-state forms of the equations to address some of these.) What would that ultimate state be if emissions were halted immediately?

What would it be if all carbon in the fossil fuel reservoir were eventually used? How long will it take to approach a steady state if carbon emissions to the atmosphere are halted at a certain time?

- Carry out simulations to clarify, if necessary, the roles and effects of \( k_{i} \), \( k_{r} \), and \( M_{s} \)—or to test entirely different forms of \( F_{1} \), the rate of photosynthetic uptake of carbon.

- What is a realistic mathematical description for the disturbance, \( F_{r} \), if reforestation begins with new trees that require a number of years for maturation?

- Examine the predicted changes in the strengths of the terrestrial and oceanic sinks (or sources?) of atmospheric carbon over the 21st century.

- It is sometimes suggested that the most realistic goal that can be achieved regarding the control of atmospheric \( \text{CO}_2 \) is to “stabilize” it at twice the pre-industrial level by the year 2100. Try to achieve that goal by manipulating the emissions (or by fabricating an emissions scenario) in such a way that atmospheric \( \text{CO}_2 \) lines out at about 1224 PgC (572 ppmv) by the year 2100. (This is an ideal exercise—even an entertaining one—for the LabVIEW simulator. In fact, the data shown on the digital displays and charts in Figure 5 are the end states of this exercise.) Notice that the difference between the emissions level so achieved in 2100 and that dictated by the IS92a sce-
DETERMINING THE FLOW CHARACTERISTICS OF A POWER LAW LIQUID

JAMES R. HILLIER, DALE TING, LISA L. KOPPLIN, MARGARET KOCH, SANTOSH K. GUPTA
University of Wisconsin • Madison, WI 53706

Non-Newtonian liquids present unique problems with respect to their flow behavior. These problems are seldom addressed in undergraduate courses in chemical/mechanical engineering and are possibly covered only through a single experiment in one of the laboratory courses. Tjahjadi and Guptal extended the work of Walawender and Chen[2] and developed an experimental scheme that illustrates how the apparent viscosity, \( \eta \), of a pseudoplastic liquid (dilute aqueous solution of Na-CMC) decreases with increasing shear rate, \( \dot{\gamma} \). They also suggested performing additional experiments after adding some sodium chloride to the CMC solution, to observe a dramatic decrease in \( \eta \) and relate it to the contraction of the polyelectrolyte molecules in an ionic medium.

Although the results had considerable educational value, the equations used were quite complex and cumbersome to use, with the result that a student obtained little insight into the method of analysis—this limits the value of their experiment.

In the present work (developed as part of the “informal” experiments[3] at the Summer 2000-I laboratory at the University of Wisconsin-Madison), a much simpler experiment has been developed that uses the easily understood macroscopic energy balance (the engineering Bernoulli equation[4]) to obtain experimental results.

A 0.07% (by weight) solution of a sodium salt of carboxymethyl cellulose (Na-CMC; weight average molecular weight \( = 7 \times 10^5 \); DS = 0.9; Aldrich Chemicals, Milwaukee, WI) in deionized water was used for our study. CMC was selected because of its pseudoplastic nature over a range \( (1 - 10^5 \text{ s}^{-1}) \) of shear rates. In addition, CMC is an inexpensive, nontoxic, biodegradable, water-soluble polymer, commonly used in mining applications, food thickeners, adhesives, and textiles.

The results obtained could also be compared to existing values in the literature[1] for consistency.

EXPERIMENTAL SET-UP

The experimental set-up is similar to that used for studying the flow characteristics of Newtonian liquids, as described by Crosby.[5] Flush-mounted glass capillaries (in one case, a copper tube) of different diameters and lengths are used with a drain tank,[5] as shown in Figure 1. Two different kinds of experimental units were made so as to vary the shear rate over a reasonable range. The detailed dimensions are provided in Table 1.

PROCEDURE

The CMC solution to be used in all the experimental runs was prepared using laboratory-grade carboxymethyl cellulose powder. A solution of 0.07 wt% CMC in deionized wa-
Figure 1. Experimental set-ups for Phases 1 and 2.

**a and b,** 50 ml graduated tube (buret with lower end cut) connected to aligned glass capillaries, flush-mounted to minimize entrance losses.

c, 5 lit SS tank (diameter - 0.158 m) with sight glass to measure h, used. Glass or Cu capillaries/tubes used. Details provided in Table 1.

<table>
<thead>
<tr>
<th>TABLE 1</th>
<th>Details of the Experimental Runs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Run No.</td>
<td>Set-Up Used</td>
</tr>
<tr>
<td>(Fig. No.)</td>
<td>m^2</td>
</tr>
<tr>
<td>1</td>
<td>la</td>
</tr>
<tr>
<td>2</td>
<td>la</td>
</tr>
<tr>
<td>3</td>
<td>la</td>
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<td>4</td>
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<td>lb</td>
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<td>12</td>
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<tr>
<td>13</td>
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<tr>
<td>14</td>
<td>lc (glass)*</td>
</tr>
<tr>
<td>15</td>
<td>lc (glass)*</td>
</tr>
<tr>
<td>16</td>
<td>lc (Cu)*</td>
</tr>
</tbody>
</table>

* Glass capillary or Cu tube used
+ See Figures 1 a-c
++ See Eq. (2)

The solution was prepared well in advance to guarantee the homogeneity of the solutions. The solution was heated to 30-50°C for about 4 to 8 hours and stirred for over 24 hours. Homogeneity of the solution was confirmed by observing its clarity against a very bright light source.

In each experimental run, a specified amount of polymer solution was added to the holding tank. The initial values, h₀, of the level of solution in the tank (see Figure 1) are given for the different experimental runs (Table 1). Flow was started, and data on h was recorded over time, t, starting at the calibration mark. This allowed flow patterns to establish so that data would not be altered by flow development. Experimental runs were stopped prior to complete efflux of the liquid from the tank, so as to reduce the significance of end effects.

**THEORY**

Since CMC solutions behave like pseudoplastic, their apparent viscosities, η, decrease with increasing shear rates, γ. The general dependence of η on γ is quite complex, but over small ranges of the shear rate, γ, the following power law model is followed quite well:

\[ τ = Kγ^n \tag{1} \]

where τ is the shear stress. In Eq. (1), the constant, K, is referred to as the consistency index, and the exponent, n, is the power law index. The apparent viscosity is then given by

\[ η = \frac{τ}{γ} = Kγ^{n-1} \tag{2} \]

A macroscopic (mechanical energy balance for this system leads to (see Appendix 1 for details)

\[ ρg(L + h) = 2KL \left( \frac{3n + 1}{n} \right) v^n \frac{1}{r_0^{n+1}} \tag{3} \]

In Eq. (3), ρ is the density of the solution, r₀ and L are the (inner) radius and length of the capillary (Figure 1), h is the height of the solution above the capillary entrance at time, t, g is the acceleration due to gravity, and v is the mass-average velocity inside the capillary at time t.

The mass-average velocity of the solution inside the capillary can be obtained using the continuity equation

\[ v = \left( \frac{R}{r_0} \right)^2 \left( \frac{-dh}{dt} \right) \tag{4} \]

where R is the inner radius of the drain tank. A second
The primary advantage of the present study is that analysis of the raw data can be performed using equations that are easily understood by juniors in chemical engineering, and standard computer packages can be used...

or third degree polynomial can be fitted to data on h(t). This gives excellent values of the coefficient of determination of about 0.999 and higher. This polynomial is then used with Eq. (4) to obtain v. Eqs. (3) and (4) can be combined and integrated for Newtonian fluids (n = 1) to give the standard equation for the efflux time for a vertical tank-pipe assembly under laminar-flow conditions. The students find these derivations easier to comprehend (in fact, they can make the derivations themselves) than the equations described by Tjahjadi and Gupta.

The validity of the assumption of laminar flow should be confirmed by calculating the Reynolds number for the pseudoplastic liquid using

\[ \text{Re} = 2^{3-n} \left( \frac{n}{3n+1} \right)^n \frac{D^n \rho v^{2-n}}{K} \]  

For pseudoplastic flows present in the laminar region, as in this study, the sudden contraction/entrance losses are expected to be negligible. In the more general case where the entrance losses are important, the Bagley correction can be used. This could be a possible avenue of further study for a student.

Equation (3) can be rewritten as

\[ \log [\rho g(L + h)] = \log \left[ \frac{2KL}{\alpha \rho_0^n \left( \frac{3n+1}{n} \right)^n} \right] + n \log (v) \]  

An appropriate log-log plot of Eq. (6) gives n (slope). K can then be obtained using n and the intercept, \( \alpha \), using

\[ K = \exp \left[ \frac{\alpha \rho_0^n \left( \frac{3n+1}{n} \right)^n}{2L} \right] \]  

Once values are obtained for both n and K, the shear rate (at the wall of the tube, \( r = r_w \)) can be evaluated using

\[ \dot{\gamma} = \left( \frac{\rho g(L + h)\rho_0}{2LK} \right)^{1/n} \]  

The apparent viscosity, \( \eta_a \), can then be evaluated (at this wall shear rate) using Eq. (2). Equation (8) assumes that the power law dependence is valid, and so the value of \( \dot{\gamma} \) obtained is inferred from the data-fitting procedure.

Unfortunately, use of the power law assumption, though helpful in simplifying the experiment at the undergraduate level, can give a false idea of the complexity of the method of analysis routinely used by professional, non-Newtonian rheologists (who commonly use the Rabinowitsch technique). An alternative procedure of data analysis that is not as difficult and that can be attempted by an undergraduate student, is the use of the Schummer approximation described in Appendix 2. Such an analysis preserves, to some extent, the physics of mechanical energy balance and closely follows the steps that would be employed in the professional rheological evaluation of non-Newtonian viscosity. One set of experimental data generated herein is analyzed later to compare the results using the power law and the Schummer approaches.

RESULTS AND DISCUSSION

Details of the several experimental set-ups and runs are given in Table 1. These experiments were designed and performed in two phases—Runs 1 and 11 through 16 in Table 1 comprising the first phase, followed by Runs 2-10. The results of the first phase were analyzed and used to help improve the designs for Phase 2. Figure 2 shows data from Phase 1. It demonstrates the decrease of the apparent viscosity with increasing shear rates. Although the viscosity vs. shear rate diagram is incomplete, the shear-thinning effect characteristic of pseudoplastic fluids is quite evident. The straight-line segments on this log-log plot confirm the validity of the power-law model over small ranges of shear rate. The data overlap in some regions, which confirms the accuracy of the results. The value of the power law index varies from about 0.3 to 1.0 (see Table 1). The range of shear rates covered extends over almost two decades, and the data appears to fall

![Figure 2. Apparent viscosity vs. shear rate for a 0.07 wt% Na-CMC aqueous solution, assuming power law behavior of the liquid. Phase 1 results shown with Runs indicated. Results from Ref. 11 also shown for comparison. Temperature = 23°C.](image-url)
on a smooth curve over this range.

The data is also found to be consistent with some earlier work[11] performed using the same solution, using a stainless steel tank with a copper tube, similar to that used in Run No. 16. Our data is also consistent with the earlier data[1] on a 0.07 wt% Na-CMC solution having a slightly larger weight-average molecular weight of 7.5 x 10^5 (the apparent viscosity at 1000 s⁻¹ was about 7 cP earlier, and is about the same in Figure 2). The replicability of our results was found to be excellent.

It should be mentioned here that an interesting activity would be to confirm the experimental results obtained here with those using more sophisticated capillary-flow or Couette viscometers available in research laboratories. Use of the former would also illustrate the use of the more exact Rabinowitsch technique of analysis.[9]

The experimental results shown in Figure 2 were then used to design a few additional experiments (Phase 2) so as to extend the range of shear rates. The corresponding plot for the apparent viscosity vs. shear rate for these runs is given in Figure 3, and the values of K and n in Table 1. It was found that the data for the two sets of experimental runs, in the range of shear rates of about 300 to 1000 s⁻¹, superposed very well (these have not been shown since the data points get too cluttered). It is interesting to observe that Runs 9 and 10 give data over a very large range of shear rate, and one could as well use just one or both of these set-ups for a routine laboratory experiment.

It should be emphasized that Eq. (3) is applicable only over small ranges of shear rate (and so over a small range of t, as the meniscus falls). A log-log plot of this equation does not show straight lines for some cases, and one must exercise some judgment to fit the points. Moreover, the viscosity of CMC (a polyelectrolyte) solutions in deionized water is very sensitive to the concentration of small amounts of salts that may be present.[1] The addition of small quantities of NaCl to the solution could help improve the reproducibility of the results substantially, and would help if one were to compare the results obtained by different groups of students taken over several weeks.

Figure 4 shows one set of data (Run 9, Table I) that has been analyzed using both the power law assumption for the solution as well as the more accurate Schummer technique. The results superpose quite well, but a shift in the curves is quite evident, as discussed in Ref. 10.

CONCLUSIONS

A simple experimental set-up was developed to study the decrease of the apparent viscosity of a 0.07% (by weight) aqueous solution of Na-CMC with increasing shear rate. Two experimental units were found that covered a reasonably large range of shear rates of 500 to 6000 s⁻¹. The primary advantage of the present study is that analysis of the raw data can be performed using equations that are easily understood by juniors in chemical engineering, and standard computer packages (e.g., Excel®, etc.) can be used for this purpose.

Additional experimental data can easily be taken after adding sodium chloride to the CMC solution, to study the effect of molecular contraction of the polyelectrolyte.[1] The results obtained using the power law assumption are compared to more elaborate methods of analysis, and a few additional experiments have been suggested for the more enterprising student.

APPENDIX 1

Details of the Derivation of Eqs. (3) and (8)

The macroscopic mechanical energy balance[4] is applied
between points 1 and 2 (Figure 1a) with the following assumptions:

- The column is vertical
- The kinetic energies of the liquid at 1 and 2 are negligible
- Entrance or other losses are negligible, and the only losses are due to viscous effects in the capillary

This leads to

$$g(L+h) = \frac{\Delta P}{\rho} \frac{2 \tau_0}{r_0} \quad (A.1)$$

where \( \tau_0 \) is the shear stress at the capillary wall, \( r = r_0 \), and \( (\Delta P)_{\text{capillary}} \) is the pressure drop across the length, \( L \), of the capillary.

A force balance over a control volume of radius, \( r \), and having a differential length, \( dz \), gives

$$-\frac{dP}{dz} = \frac{2 \tau}{r} \quad (A.2)$$

or

$$-\frac{dP}{dz} = \left( \frac{\Delta P}{L} \right)_{\text{capillary}} \frac{2 \tau_0}{r_0} \quad (A.3)$$

Equations (A.2) and (A.3) give

$$\tau_0 = \tau \left( \frac{r_0}{r} \right) \quad (A.4)$$

Using the following variation of Eq. (1)

$$\tau = K \left( \frac{-du}{dr} \right)^n \quad (A.5)$$

where \( u \) is the axial velocity at location, \( r \), in Eq. (A.4), we obtain

$$\dot{\gamma}(r) = \left( \frac{-du}{dr} \right) \left( \frac{\tau_0}{r_0 K} \right)^{1/n} r^{1/n} \quad (A.6)$$

This can be integrated from \( r = r_0 \left( \tau = \tau_0 \right) \) to \( r = \tau \left( \tau = \tau \right) \) to give

$$u(r) = \left( \frac{\tau_0}{K r_0} \right)^{1/n} \left[ \frac{\left( \frac{1}{n} \right)^{1/n} - r^{1/n+1}}{1 + \frac{1}{n}} \right] \quad (A.7)$$

Equation (A.7) can easily be integrated over \( 0 \leq r \leq r_0 \) to give the mass average velocity, \( v \), as

$$v = r_0 \left( \frac{\tau_0}{K} \right)^{1/n} \left( \frac{1}{3} + \frac{1}{n} \right) \quad (A.8)$$

which can be rearranged (and Eq. A.1 used) to give

$$\tau_0 = \frac{K v^n}{r_0} \left( \frac{3n+1}{n} \right)^n = \frac{r_0 \left( \frac{\Delta P}{L} \right)_{\text{capillary}}}{2} \quad (A.9)$$

Equation (A.9) can be combined with Eq. (A.1.1) to give Eq. (3).

Equation (A.6) can be simplified to give

$$\dot{\gamma}(r) = \left( \frac{\tau_0}{K r_0} \right)^{1/n} \left( \frac{\rho g(L+h)}{2LK} \right)^{1/n} \quad (A.10)$$

which leads to Eq. (8) (with \( r = r_0 \)).

### APPENDIX 2

**Details of the Schummer Approximation**

The apparent shear rate \( \dot{\gamma}_{\text{ap}} \), and the apparent viscosity, \( \eta_{\text{ap}} \), are defined by

$$\dot{\gamma}_{\text{ap}} = \frac{4v}{\pi r_0^2} \quad (a)$$

$$\eta_{\text{ap}} = \frac{\dot{\gamma}_{\text{ap}}}{\gamma_{\text{ap}}} = \frac{\tau_0}{r_0 K} \rho g(L+h) \quad (b) \quad (A.2.1)$$

Schummer states that the "true" shear rate, \( \dot{\gamma} \), corresponding to \( \dot{\gamma}_{\text{ap}} \) (at which the viscosity is equal to \( \eta_{\text{ap}} \)) is given by

$$\dot{\gamma} = 0.83 \dot{\gamma}_{\text{ap}} = \frac{3.32v}{r_0} \quad (A.2.2)$$

The experimental data can be used to give the average velocity, \( v \), in the capillary, as a function of time. This can be used with Eqs. (A.2.1b) and (A.2.2) to evaluate \( \eta_{\text{ap}} \) and the "true" (or the corresponding) shear rate, \( \dot{\gamma} \), to give a more accurate plot of \( \eta \) vs \( \dot{\gamma} \).

### REFERENCES

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The Earth’s Carbon Cycle

Continued from page 303.

nario (i.e., the difference between the end points of curves of the lower strip chart of Figure 5) is the amount of carbon that would have to be replaced by an equivalent energy source. Follow-up questions for consideration and/or further simulations: What alternate sources of energy might fill the gap? Could it be filled by sequestering carbon in the terrestrial biota (reforestation activities)? ...in geologic storage? ...in the deep ocean waters? Would those possibilities lead to a permanent stabilization? What is the trend of the fabricated emissions curve in 2100? What is its ultimate fate if atmospheric CO₂ is to stay level at 572 ppmv?

Start from the beginning with an alternative model that presumably improves on this one (e.g., by adding layers to the ocean or atmosphere, a spatial variation to the terrestrial reservoirs). Calibrate, tune, and test the model against the results shown here.

CONCLUDING COMMENTS

Many of the Earth’s biogeochemical processes can be studied and modeled within the context of the usual chemical engineering curricular material. The carbon cycle, the focus of this article, is a particularly apt example because, though basically complex, it can be usefully described by a simple mathematical model. Additionally, it is being disturbed and altered by human activities, possibly to the extent of causing global warming and other climate changes, and is therefore a subject of current interest and concern.

Aside from students learning about this particular subject, important and timely as it is, in my view another worthwhile outcome is that they gain confidence in their ability to analyze physical situations that may not be on their usual bill-of-fare and to apply their chemical engineering tools to the formation of a mathematical description. Never mind that the description is soaked with simplifications and assumptions—such as perfectly mixed boxes for oceans, single-rate expressions for all of the Earth’s photosynthesis, and so on. A great deal is learned by pondering, investigating, and debating the bases for such simplifications and assumptions.

This article describes my coverage of the subject in a course devoted to topics on ecology and the environment. The coverage is scalable—downward to a brief treatment and selected homework assignments integrated into some of the usual core course offerings, or upward to the development of more sophisticated models and the application of more advanced descriptions of the rate processes, mathematical analysis, and computational methods. Whatever the scope, students benefit from the broadening experience of applying their chemical engineering tools in a quantitative way to an important subject outside the mainstream.

Readers who would like to have an electronic copy of this module, which consists of a slide show with links to spread-sheets, simulations, etc., including the LabVIEW simulator, should contact me at <schmitz.l@nd.edu>.

ACKNOWLEDGMENT

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As defined by Feuer and Fulton, \[1\] performance-based assessment refers to assessment techniques that require students to create a final product, such as a written report, oral presentation, or portfolio of their work, as opposed to the more conventional assessment techniques of written quizzes or exams. Performance assessment can also be defined as an assessment method that evaluates a student's ability to perform a specific procedure or task; \[2\] in this context, the assessment must contain a performance task, a student-response format, and a scoring system. Examples would include judging a student's ability to manipulate laboratory equipment or respond to an open-ended problem. \[3\] Slater suggests designing a performance task that is "somewhat undefined, complex, and has multiple entry and exit points," that is, a task that has more than one correct solution path. \[4\]

The advantages of performance-based assessment techniques have been documented by several studies in the educational literature. \[4\] Many studies emphasize the "real-world" nature of performance assessment; \[5\] student work is evaluated in a manner that is much closer to what will be encountered in the work environment. Perhaps most importantly, research has shown that alternative assessment helps in the evaluation of students with various learning styles and educational backgrounds, promoting excellence among a more diverse student population. \[6\]

These "alternative assessment" techniques \[7\] are not new to engineering education. Traditional performance-based assessment is often used (although not often acknowledged as such) in junior- and senior-level courses in the form of laboratory experiments, written lab reports, design projects, and oral presentations; and the ABET EC 2000 guidelines have brought increased attention to outcomes-based assessment. \[7\] But alternative assessment is not widely used in the freshman- and sophomore-level courses for a variety of reasons. Educators may worry that freshmen and sophomores do not have the depth and breadth of knowledge to complete a design project or written paper, or that there is simply not enough class time to have students give oral presentations...after all, there is barely enough class time to teach these students mass and energy balances and thermodynamics. There is another means of implementing performance-based assessment in these courses, however—one that has remained largely under-used in engineering education: student portfolios.

**WHAT IS A PORTFOLIO?**

Portfolios are collections of student work, typically selected according to guidelines set forth by the instructor. \[3\] These guidelines may have a one-to-one correspondence with the course objectives, or an instructor may choose to highlight particular course objectives. An example of required items from the freshman chemical engineering course at UMass, which I will discuss in more detail below, is given in Table 1. Along with each item, students are asked to submit a statement of why the item was chosen. This element of self-analysis or self-reflection is crucial if portfolios are to be more than just "student folders." \[9\] For comparison, the course ob-

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At the end of this course, students should

1. A problem with a “nonroutine” solution, where students had to employ new strategies or methods of solution
2. A homework problem that involved teamwork or group work
3. A problem that gave the student a good sense of real-world applications
4. A problem involving data analysis or data fitting
5. A problem involving the use of MathCAD
6. A problem involving the use of Microsoft Excel
7. A self-analysis of the student’s strengths and weaknesses with regards to concepts learned in class
8. Reflections on chemical engineering, this class, and any thoughts on career choices

### TABLE 1
Required Portfolio Entries for Freshman Course in Chemical Engineering Fundamentals

<table>
<thead>
<tr>
<th>Objective</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. A problem with a “nonroutine” solution</td>
<td>Where students had to employ new strategies or methods of solution.</td>
</tr>
<tr>
<td>2. A homework problem that involved teamwork or group work</td>
<td>Involving teamwork or group work.</td>
</tr>
<tr>
<td>3. A problem that gave the student a good sense of real-world applications</td>
<td>Providing a good sense of real-world applications.</td>
</tr>
<tr>
<td>4. A problem involving data analysis or data fitting</td>
<td>Data analysis or data fitting.</td>
</tr>
<tr>
<td>5. A problem involving the use of MathCAD</td>
<td>Using MathCAD.</td>
</tr>
<tr>
<td>6. A problem involving the use of Microsoft Excel</td>
<td>Using Microsoft Excel.</td>
</tr>
<tr>
<td>7. A self-analysis of the student’s strengths and weaknesses with regards to concepts learned in class</td>
<td>Self-analysis of strengths and weaknesses.</td>
</tr>
<tr>
<td>8. Reflections on chemical engineering, this class, and any thoughts on career choices</td>
<td>Reflecting on chemical engineering, the course, and thoughts on career choices.</td>
</tr>
</tbody>
</table>

### TABLE 2
Course Objectives for Freshman Course in Chemical Engineering Fundamentals

At the end of this course, students should

- Understand concepts of engineering calculations, including significant figures and dimensional analysis, and be able to perform unit conversions
- Understand process flowsheets, know how to draw and label a flowsheet, and be able to clearly define subsystems within processes to set up conservation equations
- Understand conservation of mass and be able to solve material balances on steady processes
- Understand thermodynamic quantities such as internal energy, enthalpy, and heat capacity
- Understand the concept behind distillation and be able to perform simple vapor-liquid equilibria calculations using Raoult’s Law and Henry’s Law
- Understand conservation of energy and be able to set up simple energy balances
- Be able to use software packages (for instance, Microsoft Excel or MathCAD) to set up and solve engineering calculations and aid in data analysis
- Be able to use the principles and tools learned in this course to solve problems not covered in detail as part of the course and to continue learning related material as needed in the future.

Many studies emphasize the “real-world” nature of performance assessment; student work is evaluated in a manner that is much closer to what will be encountered in the work environment.

A widely cited benefit of portfolio assessment is an improvement in communication skills and creative-thinking skills, particularly in mathematics and science, two disciplines where students often have difficulty communicating their results. Studies in college physics classes have shown that portfolios may serve to help students organize work and internalize concepts; however, preliminary studies of portfolio use in undergraduate chemistry courses indicate that there is a disconnect between student performance on exams and in portfolio entries with regard to specific course objectives.

Evaluators in chemical engineering may feel uncomfortable with the concept of “student self-reflection”; after all, we are here to teach students, not to ask them how they “feel” about engineering, right? We prefer hard numbers and are more accustomed to quantitative assessment methods. But the utility of portfolios has been demonstrated in several science, mathematics, and engineering courses. Many states require use of portfolios in all subject areas for grades four through twelve, and portfolios have been successfully used in undergraduate physics, chemistry, and geology courses.

The chemical engineering program at the Colorado School of Mines has relied heavily on portfolio assessment for over a decade, and Olds and Miller give an excellent description of the use of portfolios in the ChE curriculum. Both Alverno College and Rose-Hulman Institute of Technology have implemented an electronic portfolio system for all students. Preliminary results from the Rose-Hulman project indicate that students find the electronic portfolio system easy to use, and that use of a web-based system reduced some of the disadvantages of conventional portfolios, including storage, user access, and availability.

It is important to keep in mind the difficulties and limitations associated with portfolio assessment. Portfolios are not appropriate for assessing factual knowledge or recall abilities; thus, they should be used in conjunction with conventional, quantitative assessment techniques. Portfolios can be difficult to manage and time-consuming to grade, which
Perhaps most importantly, research has shown that alternative assessment helps in the evaluation of students with various learning styles and educational backgrounds, promoting excellence among a more diverse student population.

makes them easiest to implement in courses with small to medium enrollments. Slater\textsuperscript{[9]} and Wink\textsuperscript{[10]} have reported techniques to extend the use of portfolios to large lecture courses, however.

Although there has been an emphasis on the use of portfolios in upper-level "capstone" courses, such as senior design and the unit operations laboratory,\textsuperscript{[11]} I focus on their use in introductory chemical engineering courses. I believe portfolio assessment has unique benefits to beginning engineering students, as described further in the following paragraphs.

GRADING PORTFOLIOS

Implementing innovative assessment is all well and good, but how are we going to evaluate and grade student portfolios? Since the portfolio entries have presumably been graded as part of a homework assignment or exam earlier in the semester, it does not seem fair to me to place the students in "double jeopardy" by basing the portfolio grade on whether or not the problems are correct. I chose to grade portfolios by giving equal weight to three criteria:

- Completeness and organization
- Quality and style of writing
- Level of thought, analysis, and reflection in each entry

The first two criteria are easy to evaluate. The first refers to whether students have all the required items, including a table of contents and page numbers. The second criterion refers to writing style and grammar, again fairly straightforward to evaluate.

The third criterion is a little more subjective and requires some planning on the part of the instructor. I evaluated the level of thought and analysis by judging the extent to which each entry addressed two to three "thought questions," which are listed in Table 3. Students were given these questions at the start of the semester to help guide them through the self-analysis process.

Slater\textsuperscript{[9]} recommends developing a "scoring rubric," whereby the portfolio grade is based on the extent to which students demonstrate mastery of the required number of objectives. For example, you may require students to have at least eight entries, each of which is related to a specific course objective. A simple scoring rubric could then be an "A" grade for demonstrating adequate mastery in seven or more objectives (as evidenced by the portfolio entries), a "B" grade in five or more objectives, and so on. More detailed examples, developed for a unit operations course, are given by Olds and Miller;\textsuperscript{[12]} see also the examples given by Slater.\textsuperscript{[9]}

EXAMPLE

Portfolios in the Introductory ChE Course

In the spring of the freshman year, students at UMass take a course titled Chemical Engineering Fundamentals. The course content covers units and dimensions, mass balances, simple reactive systems (i.e., CSTRs and PFRs), and forms of energy. The typical enrollment is 40-50 students, most of whom are engineering majors with an interest in chemical engineering. After completing the freshman year requirements, students can apply for admission into the chemical engineering major. Thus, many students in the ChE Fundamentals course are still unsure of their choice of major.

I chose to implement portfolio assessment in this course as an optional assignment. The portfolio assignment could be used to replace a low grade on either of two midterm exams or a low homework grade, but not the final exam. Many instructors give students the option of "dropping" one low grade, so I did not feel that the use of portfolios would cause grade

<table>
<thead>
<tr>
<th>TABLE 3</th>
<th>Questions for Student Self-Analysis in Portfolio Entries</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>What concept or topic was involved with this problem? What skills did you use in solving it?</td>
</tr>
<tr>
<td>2.</td>
<td>How did this problem help you learn something new?</td>
</tr>
<tr>
<td>3.</td>
<td>Did you learn anything about yourself, your thought process, or your strengths and weaknesses as a result of this activity?</td>
</tr>
<tr>
<td>4.</td>
<td>What strategies did you use? What were you thinking as you worked the problem?</td>
</tr>
<tr>
<td>5.</td>
<td>Would you do anything differently if you had more time?</td>
</tr>
<tr>
<td>6.</td>
<td>Can you describe any connections between the activity and other concepts, subject areas, or real-life situations?</td>
</tr>
<tr>
<td>7.</td>
<td>Does the problem represent a special achievement for you, a sense of accomplishment at having learned a particular concept, or a sense of improvement over time?</td>
</tr>
</tbody>
</table>
Student Feedback and Assessment Survey

The class enrollment was 41 students. Forty-one percent of the students (17 students) completed the portfolio assignment. Grades on the portfolios were roughly in the low "C" to high "A" range. For most students, the portfolio grade was used to replace a low homework grade, but the difference in the final grade for the course with and without the portfolio was never more than a letter grade.

I was somewhat distressed to find that several students counted on the portfolio to bring up their low homework grade and thus did not spend as much time on the homework assignments throughout the semester as I would have liked. I have since altered the portfolio guidelines to allow students to replace a low midterm exam grade, but not the final exam or a low homework grade.

I found that grading of the portfolios was time consuming, but I did not feel that it took longer than grading exams. The time commitment is similar to that required for evaluating written reports, and I made comments on all portfolios regarding grammar and writing style.

Students were asked to complete a survey upon completion of the course, and the survey questions and student responses are given in Table 4 and Figure 1, respectively.
Portfolios can be particularly useful for beginning chemical engineering students, who often do not have class projects that require them to synthesize concepts and present their results in a written format.

These are preliminary results; obviously, data need to be taken on a larger sample size before conclusions can be drawn. The results also may be biased due to wording of the survey questions. This needs to be addressed before definitive conclusions can be reached, and I am currently updating and redesigning the survey questions for future classes.

On the whole, the response from students was quite positive. The strongest and most uniform response was to Questions 2 and 4; 86% of students who completed a portfolio strongly agreed or agreed that the portfolio helped them to learn more about themselves and their strengths and weaknesses in chemical engineering and problem solving, and 89% of all students felt that the use of both quantitative and qualitative assessment methods were appropriate in the course. It remains unclear whether or not the portfolio assignment helped students improve their written communication skills.

Several of the written comments that accompanied portfolio entries were quite encouraging, and I have listed some of the more memorable comments in Table 5. There were also comments both positive and negative, that were useful to me as an educator. Students were very honest about components of the class that they liked and disliked. Most of these comments were made in response to Item 8, Table 1, reflections on chemical engineering and the class. Examples of these comments are also given in Table 5.

CONCLUSIONS AND RECOMMENDATIONS

Portfolios can be particularly useful for beginning chemical engineering students, who often do not have class projects that require them to synthesize concepts and present their results in a written format. Interestingly, students did not feel as though the assignment improved their written communication skills, but the portfolio assignment did seem to give these incoming students an opportunity to reflect on their abilities and their choice of major. Portfolios can also be used to assess course objectives that are difficult to evaluate using traditional techniques.

Based on my experience, I have some guidelines and recommendations for implementation of portfolios:

► Be prepared to read up on assessment techniques. Several of the references listed contain excellent examples of student entries and grading schemes. I found the National Institute of Science Education Field-Tested Learning Assessment Guide website particularly useful. (Found at <http://www.wcer.wisc.edu/nise/cll/flag/default.asp>.)

► Be clear about expectations for portfolios at the start of the semester. You may want to give students sample entries.

► Remind students that they should be saving homework sets and collecting problems for entries in their portfolio. This is extremely important for freshman-level students who are still learning how to organize their coursework.

► If you allow students to use a portfolio grade as a replacement, make sure their expectations are realistic. One fabulous portfolio assignment will not pull a final “D” grade up to an “A”—as I mentioned above, the overall effect on the final grades in the course was never more than a letter grade.

It is worth noting that implementing portfolios as a “replacement” for a poor exam could allow a student to bring a failing grade up to a “D.” Instructors need to decide for themselves whether this is permissible and to develop their own guidelines accordingly.

For example, I specified that if students received a zero grade on an exam or homework due to academic dishonesty, this grade could not be “replaced” under any circumstances. One could imagine extending this rule to any failing grade to prevent the above scenario. Finally, I found that it was problematic to allow students to replace a low homework average with the portfolio grade.

► Create a grading scheme that places emphasis on what you think is most important, whether this is good writing, clear organization, self-reflection,
TABLE 5
Sample Comments from Student Portfolios

New Strategies of Problem Solving (Item 1) and Self-Analysis (Item 8)

- “I now have more confidence knowing that if I can’t solve a problem using the accepted method of solution, I will be able to come up with a new method, perhaps something nonroutine, in order to solve the problem.”
- “This problem showed me that I should have more confidence in my ability to find a solution when it doesn’t simply present itself after a series of steps.”
- “I could apply things I had learned in a completely different context to other situations. This is actually quite comforting, as I’ve always wondered if I’ll be able to use the things I learn now later on in life when I might actually need them.”
- “I’ve had trouble [with] time management, as I have usually been able to understand the problems but have not left myself enough time to gather it all in a presentable format.”
- “My weakness is that every time I hit a wall, I tend not to do anything about it. I can only blame myself for not attempting, [but] I already made my choice in staying in this major and it is all up to me in keeping that choice.”

Reflections on Chemical Engineering and The Fundamentals Course (Item 8)

- “All in all I enjoyed the class, I enjoy being a chemical engineering student, and I look forward to the day when I am employed as a fabulous chemical engineer.”
- “I dislike computers and I dreaded using them for this class. I probably would have stuck with this major if it were not for MathCAD and Excel. I do not think being taught [MathCAD] for one class period is enough class time.”
- “Since the class is almost over, I feel a real sense of accomplishment. I know that it is only a freshman level class, but I put a great deal of effort and time into the class...It makes me proud to say that I’m a chemical engineering major when people ask me.”
- “I feel like I’ve gotten a much better idea about what chemical engineers do through the various assignments and from the oral presentations of my peers.”
- “I feel that we did not [spend] much time on using the computer.”
- “Before taking this class I wasn’t positive that chemical engineering was the right major for me. I felt that perhaps I would not be able to handle the workload or grasp all of the material that I needed to know. However, I now feel that I am actually capable of becoming an engineer.”
- “I love going to my chemical engineering classes, they are the only ones that I don’t purposely skip.”
- “As a result of this class I am much more confident about my choice of major and the preparation it will give me to succeed in the career I want to pursue.”

or assessment of a specific course objective. Make sure your grading scheme is clear to the students at the start of the semester.

ACKNOWLEDGMENTS

I would like to acknowledge my Chemical Engineering Fundamentals students for participating in this work. Professor Donald Wink (Chemistry, University of Illinois at Chicago) provided me with a copy of his recent ACS presentation on portfolio assessment and suggested several of the works cited in this article, which was greatly appreciated. The manuscript reviewers, particularly Reviewer #3, made several useful and constructive comments. Mrs. Kanak Bhatia (Ed.D. candidate, University of Delaware) also suggested several helpful references and made comments on the manuscript.

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ASPECTS OF ENGINEERING PRACTICE
Examining Value and Behaviors in Organizations

RAMON L. ESPINO
University of Virginia • Charlottesville, VA 22904-4741

Since 1995, the School of Engineering and Applied Sciences at the University of Virginia has offered an elective course that examines human values and practices in engineering organizations. The course is available to all fourth-year engineering students and is taken by 40 to 50 students each year. It is taught by the Brenton S. Halsey Visiting Professor of Chemical Engineering, who is selected annually from individuals with high-level experience in industry. Support for the Chair comes from a generous endowment by The James River Corporation in honor of its founding CEO, Brenton Halsey. Previous Halsey Professors and their affiliations are given in Table 1.

The details of the course content and execution are left to the discretion of the Halsey Professor, but its core objective is to provide engineering students with significant insight into the professional and nontechnical aspects of engineering practice. The intention is to better prepare the University of Virginia engineering graduates to succeed in the business and technical world that they will be entering after graduation. This paper describes the course materials, assignments, and assessments for the spring semester of 2001, which is representative of recent offerings.

DEVELOPING THE COURSE

The teaching experiences of previous Halsey Professors contributed significantly to the current course content. Although the objectives have remained the same, there is now more emphasis on the students reading and analyzing information prior to class. This information is generally in the form of Harvard Business School (HBS) Cases and Notes. The result of this approach is more in-depth discussion in class.

I built the course syllabus around the HBS Cases and Notes. Harvard Business School Publishing(1) offers an Index of Cases and Notes available for purchase. I suggest one HBS Case and two HBS Notes per week, requiring about nine hours of homework (reading and writing a summary) per week. Lectures to reinforce and elaborate upon the major themes of the course are strongly recommended. We have found that many of these should be given by outside speakers from business and government in order to emphasize the broad applicability of the concepts being discussed. Finally, additional reading material can be used to round out the course.

COURSE STRATEGY AND TEACHING METHOD

I developed the syllabus to follow the chronological order of the professional and business career of an engineering graduate. Selecting the first employer is the starting point, followed by early career assignments and culminating with the complex organizational, personal, and business challenges of a senior manager. HBS Cases provide a well-written plat-

The objective of the course was to increase student awareness of the nontechnical competencies they should possess in order to succeed in the work world.

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Chemical Engineering Education
form that describes specific situations with no direct answers or outcomes.

The additional reading assignment consisted mainly of HBS Notes, which provided a conceptual framework for the students to analyze the cases with some knowledge of basic concepts on business practices, interpersonal behavior, and human values. The students were all expected to read two books: *Getting to Yes* and *The Seven Habits of Highly Effective People.*

The classes were designed to be highly interactive, with the bulk of the time spent discussing the HBS Cases and Notes. In addition, there were lectures on

- Styles of communicating and interacting
- Individual competencies

### TABLE 1
Halsey Professors at the University of Virginia

<table>
<thead>
<tr>
<th>Year</th>
<th>Name</th>
<th>Company/Position</th>
</tr>
</thead>
<tbody>
<tr>
<td>1995</td>
<td>N.H. Prater</td>
<td>Mobay/CEO</td>
</tr>
<tr>
<td>1996</td>
<td>J.M. Trice, Jr.</td>
<td>Monsanto/Director-HR</td>
</tr>
<tr>
<td>1997</td>
<td>R.A. Moore, Jr.</td>
<td>International Paper/VP</td>
</tr>
<tr>
<td>1998</td>
<td>D.L. Ashcraft</td>
<td>Temple-Island/VP</td>
</tr>
<tr>
<td>1999</td>
<td>J.D. Stein</td>
<td>BASF/CEO</td>
</tr>
<tr>
<td>2000</td>
<td>V.A. Russo</td>
<td>Scott Paper/VP</td>
</tr>
<tr>
<td>2001</td>
<td>R.L. Espino</td>
<td>Exxon/R&amp;D Manager</td>
</tr>
<tr>
<td>2002</td>
<td>A.R. Hirsig</td>
<td>ARCO Chemical/CEO</td>
</tr>
</tbody>
</table>

### TABLE 2
HBS Cases

<table>
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<th>Title</th>
<th>Topic</th>
</tr>
</thead>
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<tr>
<td>Kevin Simpson</td>
<td>Interviewing and selecting your employer</td>
</tr>
<tr>
<td>Elizabeth Fisher</td>
<td>Dual career decisions</td>
</tr>
<tr>
<td>Lisa Benton</td>
<td>Conflicts in your first assignment</td>
</tr>
<tr>
<td>Amelia Rodgers</td>
<td>First group-leader assignment</td>
</tr>
<tr>
<td>Anne Livingston</td>
<td>Changing jobs and new leadership role</td>
</tr>
<tr>
<td>Tech Transfer at...</td>
<td>Conflict between development and production</td>
</tr>
<tr>
<td>Thurgood Marshall...</td>
<td>Leader of middle-level managers</td>
</tr>
<tr>
<td>Conflict in a diverse...</td>
<td>Harassment and social conflict</td>
</tr>
<tr>
<td>David Fletcher</td>
<td>Hiring your ideal business team</td>
</tr>
<tr>
<td>MOD IV Product...</td>
<td>Effective teamwork</td>
</tr>
<tr>
<td>PPG-Developing...</td>
<td>Risks and rewards of empowerment</td>
</tr>
<tr>
<td>John Smithers at Sigtek</td>
<td>Leading a quality process initiative</td>
</tr>
<tr>
<td>Jensen Shoes</td>
<td>Managing a diversity conflict</td>
</tr>
<tr>
<td>Corning Glass Works</td>
<td>Leadership during a business downturn</td>
</tr>
</tbody>
</table>

- Conflict management
- Teams and team performance
- Strategic planning
- Developing a personal career plan

Six outside speakers led discussions on various aspects of their business careers. These included

- Managing family and business life
- How to improve leadership skills
- Conflict management and negotiation
- Working with consulting companies
- Attending business school
- Reinforcing organizational values

A detailed outline of the course is presented in Table 3 (next page). The two 75-minute class periods each week allowed adequate time for discussion of the Case and the Notes, as well as for the lectures given by the Halsey Professor or by invited speakers.

**LEARNING THROUGH THE HBS CASES**

The “Case Method” is based on real-life situations that represent the kind of challenges that engineers and managers are likely to face during their work life. The cases helped students sharpen their analytical skills, their ability to communicate clearly and forcefully, and most importantly, helped them to develop their problem-solving abilities. Table 2 indicates the topic being discussed in each case.

The students were assigned the HBS Case a week in advance. They were required to write a 3-to-4-page summary of their assessment of the situation and their proposed solution(s). They were also asked to document the key learnings they had derived from the case. It was gratifying to observe their increasing sophistication in analysis and problem solving during the course of the semester.

There were a number of interesting observations that resulted from discussion of the HBS Cases. The students paid a lot of attention to the interpersonal style of the protagonists and were quite sensitive to antisocial behavior. They were, to my surprise, expecting to experience such behavior in the workplace. This applied even to harassment situations. Another class-wide attitude was to view most conflicts as rooted in poor communication, and it took a lot of discussion for them to see poor communication simply as the external manifestation of a more profound conflict.

**LEARNING KEY CONCEPTS THROUGH THE HBS NOTES**

The course provides an introduction to a number of critical competencies engineers need in order to succeed in organizations. These were provided mainly through reading and discussion of HBS Notes. The Notes were also given to the students a week in advance of the class discussion. There
was a close coupling between the teachings in the Notes and the Case being discussed in parallel. This worked well, as confirmed by the frequent references to concepts presented in the Notes in the students’ analyses of Cases. It is unrealistic to expect the students to fully master all the concepts, but it was clear that they became very aware of their importance. The hope is that when they are confronted with similar situations, they will refer to these Notes for guidance.

We discussed the differences between management and leadership and the many complex and ambiguous issues that most managers face. We spent very productive time on the influence of culture and history on subtle but important differences in managers’ behavior in the USA, Europe, Japan, India, China, and Latin America. Having some students from outside the USA gave immediacy to these discussions.

As expected, issues of business ethics grabbed the students’ attention and elicited strong and quite varied opinions. In fact, I was surprised at the diversity of viewpoints, how strongly they were held, and that there was no correlation with gender, race, or economic background.

| TABLE 3  |
| Course Outline |

| Week 1 | Homework/Class Discussion • HBS Notes on “Learning by the case method” and “How to choose a leadership pattern” |
| Lecture • Individual and team competencies |

| Week 2 | Homework/Class Discussion • HBS Notes on “Understanding context” and “Conflicting responsibilities” |
| HBS Case “Kevin Simpson” |
| Lecture • Styles of communicating and interacting |

| Week 3 | Homework/Class Discussion • HBS Notes on “Managing your career” |
| HBS Case “Elizabeth Fisher” |
| Lecture • Invited Speaker—Managing family and business life |

| Week 4 | Homework/Class Discussion • HBS Notes on “Power dynamics in organizations” |
| HBS Case “Lisa Benton” |
| Lecture • The seven habits of highly effective people |

| Week 5 | Homework/Class Discussion • HBS Notes on “Managing your boss” and “Exercising influence” |
| HBS Case “Amelia Rodgers” |
| Lecture • Invited Speaker—Improving your leadership skills |

| Week 6 | Homework/Class Discussion • HBS Notes on “Evaluating an action plan” and “Understanding communications in one-to-one relationships” |
| HBS Case “Ann Livingston and Power Max Systems” |
| Lecture • The seven habits of highly effective people |

| Week 7 | Homework/Class Discussion • HBS Notes on “Beyond the myth of a perfect mentor” and “Managing networks” |
| HBS Case “Technology transfer at a defense contractor” |
| Lecture • Invited Speaker—Conflict management and negotiation |

| Week 8 | Homework/Class Discussion • HBS Notes on “Power dependence and effective management” and “Influence tactics” |
| HBS case “Thurgood Marshall High School” |
| Lecture • Conflict management styles |

| Week 9 | Homework/Class Discussion • HBS Notes on “Integrity management” and “Managing a task-force” |
| HBS Case “Managing conflict in a diverse environment” |
| Lecture • Invited Speaker—Working in a consulting company |

| Week 10 | Homework/Class Discussion • HBS Notes on “Barriers and gateways to communications” and “On good communications” |
| HBS Case “David Fletcher” |
| Lecture • Invited Speaker—Should you get an MBA? |

| Week 11 | Homework/Class Discussion • HBS Notes on “The power of talk” and “The discipline of teams” |
| HBS case “Mod IV product development team” |
| Lecture • Getting to Yes |

| Week 12 | Homework/Class Discussion • HBS Notes on “The challenge of commitment” and “A note on high-commitment work systems” |
| HBS Case “PPG—Developing a self-directed workforce” |
| Lecture • Strategic planning |

| Week 13 | Homework/Class Discussion • HBS Notes on “Organization structure,” “Organization effectiveness,” and “The challenge of change” |
| HBS Case “John Smithers at Sigtek” |
| Lecture • Invited Speaker—Reinforcing organizational values |

| Week 14 | Homework/Class Discussion • HBS Notes on “Business ethics: the view from the trenches,” “Ethics without a sermon,” and “Ways of thinking about and across differences” |
| HBS Case “Jenssen Shoes” |
| Lecture • Developing a personal career plan |

| Week 15 | Final Homework: |
| • A personal career plan |
| • Analysis of the “Most admired company...” |
| • Group report of HBS Case “Corning Glass Works” |
I was disappointed in the students' lack of interest in learning about team building, task-force management, and building commitment in the workplace. The students felt that they knew about these topics and that they were already proficient. I do not believe I ever convinced them there was a lot for them to learn and that success in these areas requires skills they actually did not possess.

OTHER FEATURES OF THE COURSE

The students were given a three-part final homework assignment. One element was a personal mission statement with an associated five-year career development plan. The plan could also include other facets of their life, such as family, health, religion, community involvement, etc. For each of the elements they were encouraged to follow a disciplined approach that included short-term (6 months), midterm (2-3 years), and long-term (5 years) plans. For each time period, they were asked to state goals and specific objectives and to define strategies and action steps. They were initially unenthusiastic about this task, but the final product indicates that they thought hard about it and put together a realistic and credible plan.

The second element of the final homework was a team project. Groups of four students were asked to analyze a fairly complex HBS Case of a Corning Glass Works Division undergoing a change in management during a business downturn. They were asked to devise strategies and specific action plans for the division as well as a self-assessment of their team performance. The reports indicated a wide range of team performance, with the key problems being an inability to agree on an action plan, finding time to work together, and uneven participation by team members. This assignment came at the very end of the semester, which was too late to refute their earlier assertions that “teamwork was something they knew how to handle.”

The third element of the final homework was an analysis of a company’s performance during the last four years. Each student selected a company from those reviewed by Fortune Magazine in its annual publication of “America’s Most Admired Companies.” They were asked to analyze the performance of the company they chose, to identify reasons for any change in rankings during the four-year period, and to forecast future trends.

The objective of this exercise was to allow the students to apply to a specific company-wide situation what they had learned about effective management, leadership, and managing change. The companies chosen reflected the students’ wide range of career interests and included, among others, entertainment, communications, financial, computer technology, oil and chemicals, consumer products. They were asked to suggest the future direction the company needed to take to improve performance. A majority suggested expanding global reach and more technology investment, while only a few focused on improving cost competitiveness.

STUDENT ASSESSMENT AND FEEDBACK

During the semester, the students were asked to provide feedback on course content and to assess its effectiveness. The data are summarized in Table 4 and show that the majority of the class found the course very useful. They rated the discussions of HBS Cases and Notes, my work experiences and personal stories, and the outside speakers the highest. They were less enthusiastic about the other reading material, perhaps because they were not used to this amount of reading in an engineering course.

SUMMARY

The objective of the course was to increase student awareness of the nontechnical competencies they should possess in order to succeed in the work world. It is unrealistic to expect that at the end of a semester they would have mastered all these competencies, but it was evident that they were much more sensitive to the importance of such skills and had grasped the essentials. Also, they were left with an excellent collection of HBS Cases and Notes that could serve them well when confronted with similar situations. As I frequently indicated to them, I wished that I had such a learning experience in my engineering schooling and early career.

The main reason for writing this article is to encourage other colleges and universities to consider offering a course along the general outline that I have described. I also encourage experienced business practitioners to teach such a course. The Halsey Professors are unanimous: it was an exciting and gratifying experience to share what you have learned with the next generation of engineering and business leaders.

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S. Tom Picraux, Ph.D. Caltech. Nanostructured materials, epitaxy, and thin-film electronic materials

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Faculty

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Roger B. Boulton, Professor • Ph.D., University of Melbourne, 1976 • Fermentation and reaction kinetics, crystallization

Stephanie R. Dungan, Associate Professor • Ph.D., Massachusetts Institute of Technology, 1992 • Micelle transport, colloidal and interfacial science in food processing

Roland Faller, Assistant Professor • Ph.D., Max-Planck Institute for Polymer Research, 2000 • Molecular modeling of soft condensed matter

Bruce C. Gates, Professor • Ph.D., University of Washington, Seattle, 1966 • Catalysis, solid superacid catalysis, zeolite catalysts, bimetallic catalysts, catalysis by metal clusters

Jeffery C. Gibeling, Professor • Ph.D., Stanford University, 1979 • Deformation, fracture and fatigue of metals, layered composites and bone

Jonna R. Groza, Professor • Ph.D., Rensselaer Polytechnic Institute, 1984 • Biomaterials, membrane interactions, intermolecular and interfacial forces in complex fluid systems

Enrique J. Lavernia, Professor • Ph.D., Massachusetts Institute of Technology, 1986 • Synthesis of structural materials and composites; nanostructured materials and composites, thermal spray processing

Jörg F. Löffler, Assistant Professor • Ph.D., Swiss Federal Institute of Technology (ETH), Zurich, 1997 • Nanostructured and amorphous materials; magnetic, structural, and thermophysical properties, neutron and x-ray scattering

Karen A. McDonald, Professor • Ph.D., University of California, Santa Barbara, 1985 • Plant cell culture bioprocessing algal cell cultures

Amiya K. Mukherjee, Professor • Ph.D., University of Maryland, College Park, 1985 • Plant cell culture bioprocessing algal cell cultures

Zahair A. Munir, Professor • Ph.D., University of California, Berkeley, 1963 • Combustion synthesis, multilayer combustion systems, functionally graded materials

Alexandra Narrosky, Professor • Ph.D., University of Chicago, 1967 • Thermodynamics and solid state chemistry; high temperature calorimetry

Ahmet N. Palazoglu, Professor • Ph.D., Rensselaer Polytechnic Institute, 1984 • Process control and process design of environmentally benign processes

Ronald J. Phillips, Professor • Ph.D., Massachusetts Institute of Technology, 1989 • Transport processes in bioseparations, Newtonian and non-Newtonian suspension mechanics

Robert L. Powell, Professor • Ph.D., Johns Hopkins University, 1978 • Rheology, suspension mechanics, magnetic resonance imaging of suspensions

Sohshu K. Rishin, Professor and Chair • Ph.D., University of California, Berkeley, 1976 • Semiconductor quantum dots, high Tc superconducting ceramics, polymer composites for optics

Dewey D.Y. Ryu, Professor • Ph.D., Massachusetts Institute of Technology, 1967 • Biomolecular process engineering and recombinant bioprocess technology

Julie M. Schennumer, Associate Professor • Ph.D., Massachusetts Institute of Technology, 1987 • Materials systems analysis; pollution prevention and waste minimization; process economics

James F. Shackelford, Professor • Ph.D., University of California, Berkeley, 1971 • Structure of materials, biomaterials, nondestructive testing of engineering materials

J.M. Smith, Professor Emeritus • Sc.D., Massachusetts Institute of Technology, 1943 • Chemical kinetics and reactor design

Pieter Stroeve, Professor • Sc.D., Massachusetts Institute of Technology, 1973 • Membrane separations, Langmuir Blodgett films, colloid and surface science

Stephen Whitaker, Professor • Ph.D., University of Delaware, 1959 • Multiphase transport phenomena

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Atmospheric Chemistry and Physics  Fluid Mechanics
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Biomaterials  Microelectronics Processing
Biomedical Engineering  Microstructured Fluids
Bioseparations  Polymer Science
Catalysis  Protein Engineering
Chemical Vapor Deposition  Statistical Mechanics

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Faculty

John Angus
Harihara Baskaran
Robert Edwards
Donald Feke
Jeffrey Glass
Uziel Landau
Chung-Chiun Liu
J. Adin Mann
Heidi Martin
Philip Morrison
Peter Pintauro
Syed Qutubuddin
Robert Savinell
Thomas Zawodzinski

For more information on Graduate Research, Admission, and Financial Aid, contact:

Graduate Coordinator
Department of Chemical Engineering
E-mail: grad@cheme.cwru.edu
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William Krantz
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Chemical Engineering
PO Box 210171
University of Cincinnati
Cincinnati, Ohio 45221-0171

E-mail: mcarden@alpha.che.uc.edu
or jlin@alpha.che.uc.edu

The faculty and students in the Department of Chemical Engineering are engaged in a diverse range of exciting research topics. Assistantships and tuition scholarships are available to highly qualified applicants to the MS and PhD degree programs.

- **Advanced Materials**
  Inorganic membranes, nanostructured materials, microporous and mesoporous materials, advanced materials processing, thin film technology, fuel cell and sensor materials, self-assembly

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- **Environmental Research**
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- **Membrane Technology**
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- **Polymers**
  Thermodynamics, polymer blends and composites, high-temperature polymers, hydrogels, polymer rheology, computational polymer science, polymerization technology

- **Separation Technologies**
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Andreas Acrivos: Rheology of concentrated suspensions; Dielectrophoresis in flowing suspensions; Dynamical systems theory and chaotic particle motions

Alexander Couzis: Polymorph selective templated crystallization; Molecularly thin organic barrier layers; Surfactant facilitated wetting of hydrophobic surfaces; soft materials

Morton Denn: Polymer science and rheology; non-Newtonian fluid mechanics

Lane Gilchrist: Bioengineering with cellular materials; Spectroscopy-guided molecular engineering; Structural studies of self-assembling proteins; Bioprocessing

Robert Graff: Coal liquefaction; Pollution prevention; Remediation

Leslie Isaacs: Preparation and characterization of novel optical materials; Recycling of pavement materials; Application of thermo-analytic techniques in materials research

Jae Lee: Theory of reactive distillation; Process design and control; Separations; Bioprocessing

Charles Maidarelli: Interfacial fluid mechanics and stability; Surface tension driven flows and microfluidic applications; Surfactant adsorption, phase behavior and nanostructuring at interfaces

Irven Rinard: Process design methodology; Dynamic process simulation; Micro-reaction technology; Process control; Bioprocessing

David Rumschitzki: Transport and reaction aspects of arterial disease;

Interfacial fluid mechanics and stability; Catalyst deactivation and reaction engineering

Reuel Shinnar: Advanced process design methods; Chemical reactor control; Spinodal decomposition of binary solvent mixtures; Process economics; Energy and environment systems

Carol Stein: Polymer solutions and hydrogels; Soft biomaterials, Controlled release technology

Gabriel Tardos: Powder technology; Granulation; Fluid particle systems; Electrostatic effects; Air pollution

Sheldon Weinbaum: Fluid mechanics, Biotransport in living tissue; Modeling of cellular mechanism of bone growth; bioheat transfer; kidney function

Herbert Weinstein: Fluidization and multiphase flows: multiphase chemical reactor analysis and design, Multiphase reactor analysis and design

ASSOCIATED FACULTY:

Jimmy Feng: (Mechanical Eng.) Liquid crystals
Joel Koplik: (Physics) Fluid mechanics; Molecular modeling: Transport in random media

Hernan Makse: (Physics) Granular mechanics
Mark Shattuck: (Physics) Experimental granular rheology; Computational granular fluid dynamics; Experimental spatio-temporal control of patterns

CONTACT INFORMATION:

Department of Chemical Engineering
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New York, NY 10031
www-che.engr.cuny.cuny.edu
che.hr@aol.com
Engineering Degrees

M. Sc. Chemical Engineering
D. Eng. Applied Biomedical Engineering
D. Eng. Chemical Engineering

CSU Faculty
A. Annapragada (University of Michigan)
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G. Chatzimavroudis (Georgia Institute of Technology)
G.A. Coulman (Case Western Reserve University)
J.E. Gatica (State University of New York at Buffalo)
B. Ghorashi (Ohio State University)
E.S. Godleski (Cornell University)
R. Lustig (Institute of Thermo- and Fluiddynamics of the Ruhr-University Bochum, Germany)
D.B. Shah (Michigan State University)
O. Talu (Arizona State University)
S.N. Tewari (Purdue University)
S. Unigara (Michigan Technological University)

CCF Collaborating Faculty
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B. Davis (Pennsylvania State University)
K. Derwin (University of Michigan)
A. Fleischman (Case Western Reserve University)
M. Grabiner (University of Illinois)
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C. McDevitt (University of London, U.K.)
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W. Smith (Cleveland State University)
A. van den Bogert (University of Utrecht, The Netherlands)
I. Vesely (University of Western Ontario, Canada)
G. Yue (University of Iowa)

For more information, write to:
Graduate Program Coordinator • Department of Chemical Engineering
Cleveland State University • Cleveland, OH 44115
Telephone: 216-687-2569 • E-mail: ChE@csvax.egr.csuohio.edu
http://www.csuohio.edu/chemical_engineering/

Fenn College has more than 75 years of experience in providing outstanding engineering education.

Graduate Studies in Chemical and Applied Biomedical Engineering at Cleveland State University's (CSU's) Fenn College of Engineering offers a wealth of opportunity in a stimulating environment.

Research opportunities are available in collaboration with the Biomedical Engineering Department of the renowned Cleveland Clinic Foundation (CCF), Cleveland’s Advanced Manufacturing Center, local and national industry, and Federal agencies, to name a few. Assistantships and Tuition Fee Waivers are available on a competitive basis for qualified students.

Cleveland State University has 16,000 students enrolled in its academic programs. It is located in the center of the city of Cleveland, with many outstanding cultural and recreational opportunities nearby.

RESEARCH AREAS
Adsorption Processes
Agile Manufacturing
Artificial Heart Valves
Biomechanics
Bioreactor Design
Bioseparations
Blood Flow
Combustion
Computational Fluid Dynamics
Drug Delivery Systems
Environmental Pollution Control
Materials Synthesis and Processing
Medical Imaging
MEMS Technology
Orthopedic Devices
Process Modeling and Control
Reaction Engineering
Statistical Mechanics
Surface Phenomena and Mass Transfer
Thermodynamics and Fluid Phase Equilibrium
Tissue Engineering
Tribology
Ventricular Assist Devices
Zeolites: Synthesis, Adsorption, and Diffusion

Assistantships and Tuition/Fee Waivers are available on a competitive basis for qualified students.
The Boulder campus has a controlled enrollment of about 22,000 undergraduates and 5,000 graduate students. The beautiful campus has 200 buildings of rough-cut sandstone with red-tile roofs. The excellent educational opportunities and beautiful location attract outstanding students from every part of the United States and 85 countries.

The University of Colorado has its main campus located in Boulder, an attractive community of 90,000 people located at the base of the Rocky Mountains. Boulder has over 300 days of sunshine per year, with relatively mild and dry seasons. The city is an active and innovative town that provides a rich array of recreational and cultural activities.

### Department of Chemical Engineering Faculty and Research Interests

<table>
<thead>
<tr>
<th>Faculty Name</th>
<th>Research Interests</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kristi S. Anseth</td>
<td>Polymers, Biomaterials, Tissue Engineering</td>
</tr>
<tr>
<td>Christopher N. Bowman</td>
<td>Polymers, Membrane Materials</td>
</tr>
<tr>
<td>David E. Clough</td>
<td>Process Control, Applied Statistics</td>
</tr>
<tr>
<td>Robert H. Davis</td>
<td>Fluid Mechanics, Biotechnology, Membranes</td>
</tr>
<tr>
<td>John L. Falconer</td>
<td>Catalysis, Zeolite Membranes</td>
</tr>
<tr>
<td>R. Igor Gamow</td>
<td>Biophysics, High Altitude Physiology, Human Performance, Diving Physiology</td>
</tr>
<tr>
<td>Steven M. George</td>
<td>Surface Chemistry, Thin Films, Nanoengineering</td>
</tr>
<tr>
<td>Doug Gin</td>
<td>Polymers</td>
</tr>
<tr>
<td>Ryan Gill</td>
<td>Biotechnology</td>
</tr>
<tr>
<td>Christine M. Hrenya</td>
<td>Fluidization, Granular Systems, Fluid Mechanics</td>
</tr>
<tr>
<td>Dhinakar S. Kompala</td>
<td>Biotechnology, Animal Cell Cultures, Metabolic Engineering</td>
</tr>
<tr>
<td>J. Will Medlin</td>
<td>Heterogeneous Catalysis, Solid-State Sensors, Computational Chemistry</td>
</tr>
<tr>
<td>Richard D. Noble</td>
<td>Membranes, Separations</td>
</tr>
<tr>
<td>W. Fred Ramirez</td>
<td>Process Control, Biotechnology</td>
</tr>
<tr>
<td>Theodore W. Randolph</td>
<td>Biotechnology, Supercritical Fluids</td>
</tr>
<tr>
<td>Robert L. Sani</td>
<td>Transport Phenomena, Applied Mathematics</td>
</tr>
<tr>
<td>Daniel K. Schwartz</td>
<td>Interfacial and Colloid Science</td>
</tr>
<tr>
<td>Alan W. Weimer</td>
<td>Ceramics, Energy, Reaction Engineering</td>
</tr>
</tbody>
</table>

Graduate students may participate in the interdisciplinary Biotechnology Training Program and the interdisciplinary NSF Industry/University Cooperative Research Center for Membrane Applied Science and Technology and the Center for Fundamentals and Applications of Photopolymerizations.

For information and application
Graduate Admissions Committee • Department of Chemical Engineering
University of Colorado • Boulder, CO 80309-0424
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http://www.Colorado.EDU/che/
Evolving from its origins as a school of mining founded in 1873, CSM is a unique, highly-focused University dedicated to scholarship and research in materials, energy, and the environment.

The Chemical Engineering Department at CSM maintains a high quality, active, and well-funded graduate research program. According to the NSF annual survey of research expenditures, our department has placed in the top 25 nationally each of the last 5 years. Research areas within the department include:

Materials Science and Engineering
- Organic and inorganic membranes (Way, Baldwin)
- Polymeric materials (Dorgan, McCabe, Wu)
- Colloids and complex fluids (Marr, Wu)
- Electronic materials (Wolden)
- Fuel cell membranes (Way)

Theoretical and Applied Thermodynamics
- Natural gas hydrates (Sloan)
- Molecular simulation and modelling (Ely, McCabe)

Transport Properties and Processes
- Dermal absorption (Bunge)
- Microfluidics (Marr)

Space and Microgravity Research
- Membranes on Mars (Way, Baldwin)
- Water mist flame suppression (McKinnon)

Reacting Flows
- Flame kinetics (McKinnon, Dean)
- Reaction mechanisms (Dean, McKinnon)
- High-T fuel cell kinetics (Dean)

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- Magnetic Resonance Imaging
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- Polymeric Materials
- Porous Media Phenomena
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FACULTY

Brian C. Batt, Ph.D.
University of Colorado

Laurence A. Belfiore, Ph.D.
University of Wisconsin

David S. Dandy, Ph.D.
California Institute of Technology

M. Nazmul Karim, Ph.D.
University of Manchester

James C. Linden, Ph.D.
Iowa State University

Vincent G. Murphy, Ph.D.
University of Massachusetts

Kenneth F. Reardon, Ph.D.
California Institute of Technology

Kristina D. Rinker, Ph.D.
North Carolina State University

A. Ted Watson, Ph.D.
California Institute of Technology

Ranil Wickramasinghe, Ph.D.
University of Minnesota
Biochemical Engineering and Biotechnology

James D. Bryers, Ph.D., Rice University (Joint Appointment)
  Biochemical Engineering, Biofilm Processes, Biomaterials

Robert W. Coughlin, Ph.D., Cornell University
  Biotechnology, Biochemical and Environmental Engineering Catalysis, Kinetics, Separations, Surface Science

Ranjan Srivastava, Ph.D., University of Maryland
  Experimental and Computational Biology, Biomolecular Network Analysis, Stochastic Biological Phenomena, Evolutionary Kinetics

Thomas K. Wood, Ph.D., North Carolina State University
  Microbiological Engineering, Bioremediation with Genetically-Engineered Bacteria, Enzymatic Green Chemistry, Biochemical Engineering, Biocorrosion

Polymer Science

Patrick T. Mather, Ph.D., University of California, Santa Barbara
  Polymers, Microstructure and Rheology, Liquid Crystalinity, Inorganic-Organic Hybrids

Richard Parnas, Ph.D., University of California, Los Angeles
  Composites, Biomaterials

Montgomery T. Shaw, Ph.D., Princeton University
  Polymer Rheology and Processing, Polymer-Solution Thermodynamics

Robert A. Weiss, Ph.D., University of Massachusetts
  Polymer Structure-Property Relationships, Ion-Containing and Liquid Crystal Polymers, Polymer Blends

Lei Zhu, Ph.D., University of Akron
  Polymer Phase Transitions, Structures of Morphologies of Block Copolymers, Polymeric Nanocomposites, Biodegradable Block Copolymers for Drug Delivery

Computer Aided Modeling

  Modeling and Optimization, Molecular Design, Artificial Intelligence, Flexibility Analysis

Thomas F. Anderson, Ph.D., University of California at Berkeley
  Modeling of Separation Processes, Fluid-Phase Equilibria

Douglas J. Cooper, Ph.D., University of Colorado
  Process Modeling, Monitoring and Control

Michael B. Cutlip, Ph.D., University of Colorado
  Kinetics and Catalysis, Electrochemical Reaction Engineering, Numerical Methods

Suzanne Schadel Fenton, Ph.D., University of Illinois, Urbana-Champaign
  Computational Fluid Dynamics, Turbulence, Two-Phase Flow

Environmental and Energy Engineering

Can Erkey, Ph.D., Texas A&M University
  Supercritical Fluids, Catalysis, Nanotechnology

James M. Fenton, Ph.D., University of Illinois, Urbana-Champaign

Joseph J. Heible, Ph.D., Massachusetts Institute of Technology
  Air Pollution, Aerosol Science, Nanoscale Materials Synthesis and Characterization, Combustion

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- Biochemical and Biomedical Engineering
- Fluid Dynamics, Stability, and Rheology
- Molecular Thermodynamics and Computer Simulation
- Polymer Science and Engineering
- Reaction Engineering: Surface Science, Kinetics, and Reactor Design

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For further information, write:

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e-mail: DGS@CHEME.CORNELL.EDU, or "visit" our World Wide Web server at: http://www.cheme.cornell.edu
Graduate Study & Research in Chemical Engineering

at

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- Biotechnology and biocommodity engineering
- Environmental science and engineering
- Fluid mechanics
- Materials science and engineering
- Process design and evaluation

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---

### Faculty & Research Areas

- **Ian Baker** (Oxford) \> Structure/property relationships of materials, electron microscopy
- **John Collier** (Dartmouth) \> Orthopaedic prostheses, implant/host interfaces
- **Alvin Converse** (Delaware) \> Kinetics & reactor design, enzymatic hydrolysis of cellulose
- **Benoit Cushman-Roisin** (Florida State) \> Numerical modeling of environmental fluid dynamics
- **Harold Frost** (Harvard) \> Microstructural evolution, deformation, and fracture of materials
- **Tillman Gerngross** (Technical University of Vienna) \> Engineering of glycoproteins, fermentation technology
- **Ursula Gibson** (Cornell) \> Thin film deposition, optical materials
- **Francis Kennedy** (RPI) \> Tribology, surface mechanics
- **Daniel R. Lynch** (Princeton) \> Computational methods, oceanography, and water resources
- **Lee Lynd** (Dartmouth) \> Biomass processing, pathway engineering, reactor & process design
- **Victor Petrenko** (USSR Academy of Science) \> Physical chemistry of ice
- **Horst Richter** (Stuttgart) \> Thermodynamics, multiphase flow, energy conversion, process design
- **Erland Schulson** (British Columbia) \> Physical metallurgy of metals and alloys
- **Charles E. Wyman** (Princeton) \> Biomass pretreatment & hydrolysis, cellulase synthesis & kinetics, process design

---

For further information, please contact:

Chemical Engineering Graduate Advisor • Thayer School of Engineering • Dartmouth College • Hanover, NH 03755

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Chemical Engineering Education
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RESEARCH AREAS

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Biomaterials
Biomedical Engineering
Colloids and Interfacial Engineering
Molecular Dynamics Simulations
Plasma Processing
Polymer Science and Engineering
Process Control and Dynamics
Rheology and Fluid Mechanics
Safety Engineering
Systems Analysis and Optimization
Tissue Engineering
Transport Phenomena

FACULTY

Charles Weinberger, Head (University of Michigan)
Cameron Abrams (University of California)
Richard Cairncross (University of Minnesota)
Donald Coughanowr (University of Illinois)
Nily Dan (University of Minnesota)
Elihu Grossmann (University of Pennsylvania)
Cato Laurencin (Massachusetts Institute of Technology)
Young Lee (Purdue University)
Anthony Lowman (Purdue University)
Stephen Meyer (Clemson University)
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Computational Engineering and Transport Processes

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Biointerfacial and Biomedical Engineering
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M.E. Pozo de Fernandez, Ph.D.
R.G. Barile, Ph.D.
M.M. Tomadakis, Ph.D.
J.E. Whitlow, Ph.D.

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- Florida Solar Energy Center
- Florida Institute of Phosphate Research
- Department of Energy
- Florida Space Grant

Graduate Student Assistantships and Tuition Remission Available

Research Interests

- Spacecraft Technology
- Alternative Energy Sources
- Materials Science
- Environmental Engineering
- Expert Systems

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Georgia Institute of Technology
School of Chemical Engineering

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Atlanta, Georgia 30332-0100
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Faculty and Their Research

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V. BALAKOTAIAH
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A. T. CAPITANO
Tissue Engineering; In Vitro Toxicology

V. M. DONNELLY
Plasma Processing; Electronic Materials

M. J. ECONOMIDES
Petroleum engineering; Energy

D. J. ECONOMOU (JOHN & REBECCA MOORES PROFESSOR)
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R. KRISHNA MOORTI
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K. K. MOHANTY
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M. NIKOLAOU
Computer-aided process engineering

J. T. RICHARDSON
Catalysis & reaction engineering; Superconductivity; Fuel cells

F. M. TILLER (EMERITUS)
Fluid/particle separation

P. G. VEKILOV
Phase transitions in protein solutions

R. C. WILLSON
Biomolecular recognition; Nucleic acid technology

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For more information

www.chee.uh.edu
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Graduate Office
Chemical Engineering
University of Houston
Houston, TX 77204-4004
Chemical Engineering at

Howard University

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Faculty and Research Interests

Mobolaji E. Aluko, Professor and Chair
PhD, University of California, Santa Barbara
Reactor modeling • crystallization • microelectronic and ceramic materials processing • process control • reaction engineering analysis

Joseph N. Cannon, Professor • PhD, University of Colorado
Transport phenomena in environmental systems • computational fluid mechanics • heat transfer

Ramesh C. Chawla, Professor • PhD, Wayne State University
Mass transfer and kinetics in environmental systems • bioremediation • incineration • air and water pollution control

William E. Collins, Associate Professor • PhD, University of Wisconsin-Madison
Polymer deformation, rheology, and surface science • biomaterials • bioseparations • materials science

M. Gopala Rao, Professor • PhD, University of Washington, Seattle
Adsorption and ion exchange • process energy systems • radioactive waste management • remediation of contaminated soils and groundwater

John P. Tharakan, Associate Professor • PhD University of California, San Diego
Bioprocess engineering • protein separations • biological hazardous waste treatment • bio-environmental engineering

Robert J. Lutz, Visiting Professor • PhD, University of Pennsylvania
Biomedical engineering • hemodynamics • drug delivery • pharmacokinetics

Herbert M. Katz, Professor Emeritus • PhD, University of Cincinnati
Environmental engineering

For further information and applications, write to

M.S. Program

Director, Graduate Studies • Chemical Engineering Department
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Phone 202-806-6624 Fax 202-806-4635

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The University of Illinois at Chicago
Department of Chemical Engineering

• MS and PhD Graduate Program •

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Lewis E. Wedgewood, Associate Professor
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RESEARCH AREAS

Transport Phenomena: Transport properties of fluids, slurry transport, and multiphase fluid flow. Fluid mechanics of polymers and other viscoelastic media.

Thermodynamics: Molecular simulation and statistical mechanics of liquid mixtures. Superficial fluid extraction/retrograde condensation, asphaltene characterization.


Materials: Microelectronic materials and processing, heteroepitaxy in group IV materials, and in situ surface spectroscopies at interfaces. Combustion synthesis of ceramics and synthesis in supercritical fluids.

Product and Process Development and design, computer-aided modeling and simulation, pollution prevention.

For more information, write to
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URL: http://www.uic.edu/depts/chme/
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Richard D. Braatz  Advanced Process Control
Steve Granick  Polymers and Biopolymers, Nanorheology/Tribology, and Surface Spectroscopies
Vinay K. Gupta  Interfacial Phenomena: Structure and Dynamics in Thin Films
Jonathan J. L. Higdon  Fluid Mechanics and Computational Algorithms
Paul J. A. Kenis  Microreactors, Microfluidic Tools, and Microfabrication
Sangtae Kim  Bioinformatics, Microfluidics/Nanofluidics
Mark J. Kushner  Plasma Chemistry and Plasma Materials Processing
Deborah E. Leckband  Bioengineering and Biophysics
Jennifer A. Lewis  Colloidal Assembly, Complex Fluids, and Mesoscale Fabrication
Richard I. Masel  Kinetics, Catalysis, Microfuel Cells, and Microchemical Systems
Anthony J. McHugh  Polymer Science and Engineering
Daniel W. Pack  Biomolecular Engineering and Biotechnology
Nikolaos V. Sahinidis  Optimization and Process Systems Engineering
Kenneth S. Schweizer  Macromolecular, Colloidal, and Complex Fluid Theory
Edmund G. Seebauer  Microelectronics Processing and Nanotechnology
Michael S. Strano  Nanofabricated Materials, Molecular Electronics, and Fullerene Nanotechnology
Huimin Zhao  Molecular Bioengineering and Biotechnology
Charles F. Zukoski  Colloid and Interfacial Science

For information and application forms write:
Department of Chemical and Biomolecular Engineering
University of Illinois at Urbana-Champaign
114 Roger Adams Lab, Box C-3
600 S. Mathews Ave.
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http://www.chemeng.illinois.edu

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http://www.chee.iit.edu/ • e-mail: chee@iit.edu

FACULTY AND RESEARCH AREAS

Chairman • Hamid Arastoopour
Associate Chair for Undergraduate Affairs • Fouad Teymour
Associate Chair for Graduate Affairs • Satish Parulekar

Javad Abbasaki; separation processes, gas cleaning, air pollution
Nader Aderangi; unit operations, chemical processes
Paul R. Anderson; precipitation kinetics, evaluation of oxide adsorbents for water and wastewater treatment
Hamid Arastoopour; computational multiphase flow, fluidization, material processing, particle technology, fluid-particle flow
Barry Bernstein; computational fluid mechanics, material properties, polymer rheology
Donald J. Chmielewski; process control, pollution prevention
Ali Cinar; chemical and food process control, nonlinear input-output modeling, statistical process monitoring
Dimitri Gidaspow; hydrodynamics of fluidization using kinetic theory, gas-solid transport
Henry R. Linden; fossil fuel technologies, energy and resource economics, energy and environmental policy
Demetrios J. Moschandreas; ambient and indoor air pollution, statistical analysis, environmental impact assessment
Allan S. Myerson; crystallization from solution, nucleation, molecular modeling
Kenneth E. Noll; air resources engineering, air pollution meteorology, hazardous waste treatment
Krishna R. Pagilla; water and wastewater engineering, environmental microbiology, soil remediation, sludge treatment
Satish Parulekar; biochemical engineering, chemical reaction engineering
Victor H. Pérez-Luna; biomedical and tissue engineering
Jai Prakash; solid state chemistry, materials synthesis and characterization for energy conversion and storage applications
Jay D. Schieber; kinetic theory, polymer rheology predictions, transport phenomena, non-Newtonian fluid mechanics
J. Robert Selman; applied electrochemistry and electrochemical engineering, battery and fuel cell design
Eugene S. Smotkin; FTIR spectroscopy of electrode surfaces, electrochemical mass spectrometry, fuel cells, combinatorial catalyst screening
Fouad A. Teymour; polymer reaction engineering, mathematical modeling, nonlinear dynamics
David C. Venerus; polymer rheology and processing, transport phenomena in polymeric systems
Darsh T. Wasan; thin liquid films; interfacial rheology; foams, emulsion and dispersion, environmental technologies

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Ted Knowlton • Harold Lindahl • Robert Lyczkowski • Zoltan Nagy
Alex Nikolov • Ali Oskouie • Giselle Sandi • Charles Sizer • Hwa-Chi Wang
Graduate program for M.S. and Ph.D. degrees in Chemical and Biochemical Engineering

FACULTY

Gary A. Aurand
North Carolina State U. 1996
Supercritical fluids/
High pressure
biochemical reactors

Audrey Butler
U. of Iowa 1989
Chemical precipitation
processes

Greg Carmichael
U. of Kentucky 1979
Global change/
Supercomputing/
Air pollution modeling

Vicki H. Grassian
U. of California-Berkeley 1987
Surface chemistry/
Heterogeneous processes

C. Allan Guymon
U. of Colorado 1997
Polymer reaction engineering/UV curable coatings/
Polymer liquid crystal composites

Stephen K. Hunter
U. of Utah 1989
Bioartificial organs/
Microencapsulation technologies

Julie L.P. Jessop
Michigan State U. 1999
Polymers/
Microlithography/
Spectroscopy

Robert Linhardt
Johns Hopkins 1979
Biopolymers and
pharmaceutical applications

David Murhammer
U. of Houston 1989
Insect cell culture/
Bioreactor monitoring

Tonya L. Peeples
Johns Hopkins 1994
Bioremediation/
Extremophile physiology and biocatalysis

David Rethwisch
U. of Wisconsin 1985
Membrane science/
Polymer science/
Catalysis

V.G.J. Rodgers
Washington U. 1989
Transport phenomena in bioseparations/
Membrane separations

Alec B. Scranton
Purdue U. 1990
Photopolymerization/
Reversible emulsifiers/
Polymerization kinetics

Ramaswamy Subramanian
Indian Institute of Science 1992
Structural enzymology/Structure function relationship in proteins

John M. Wieneck
Case Western Reserve 1989
Protein crystallization/
Surfactant technology

For information and application:
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Chemical and Biochemical Engineering
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Robert C. Brown
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Graduate Study and Research in Chemical Engineering at Johns Hopkins

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Michael J. Betenbaugh, PhD • University of Delaware

**Recombinant DNA Technology**

**Protein Folding and Aggregation**
Michael J. Betenbaugh, PhD • University of Delaware

**Equations of State • Statistical Thermodynamics**
Marc D. Donohue, PhD • University of California, Berkeley

**Solvent Replacement**

**Nanostructured Materials**

**Colloid/Protein Adsorption**

**Rheology of Suspensions**
Jeffrey J. Gray, PhD • University of Texas at Austin

**Biomaterials Synthesis**

**Controlled/Targeted Drug Delivery**
Justin S. Hanes, PhD • Massachusetts Institute of Technology

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**Phase Transitions and Critical Phenomena**

**Polymer Systems Far from Equilibrium**

**Particle-Tracking Microrheology**

**Denis Wirtz, PhD • Stanford University**

**For further information contact:**

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Kyle V. Camarda (Ph.D., Illinois)
John C. Davis (Ph.D., Wyoming)
Don W. Green, (Ph.D., Oklahoma)
Colin S. Howat (Ph.D., Kansas)
Carl E. Locke, Jr., (Ph.D., Texas)
Trung V. Nguyen (Ph.D., Texas A&M)
Karen J. Nordheden (Ph.D., Illinois)
Russell D. Osterman (Ph.D., Kansas)
Marylee Z. Southard (Ph.D., Kansas)
Susan M. Williams (Ph.D., Oklahoma)
Bala Subramaniam, Chair (Ph.D., Notre Dame)
Shapour Vossoughi (Ph.D., Alberta, Canada)
G. Paul Willhite (Ph.D., Northwestern)

Research

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Catalytic Materials and Membrane Processing
Controlled Drug Delivery
Corrosion, Fuel Cells, Batteries
Electrochemical Reactors and Processes
Electronic Materials Processing
Enhanced Oil Recovery Processes
Fluid Phase Equilibria and Process Design
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Contacts

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Graduate Program
Chemical and Petroleum Engineering
University of Kansas—Learned Hall
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Environmental Pollution Control
Hazardous Waste Treatment
Membrane Separations
Multiphase Flow
Polymeric Materials Properties
Process Systems Engineering and Artificial Intelligence
Separative Reactors
University of Kentucky
Department of Chemical & Materials Engineering

- Catalysis
- Environmental Engineering
- Biopharmaceutical & Biocellular Engineering
- Materials Synthesis
- Advanced Separation & Supercritical Fluids Processing
- Membranes & Polymers
- Aerosols

The Chemical Engineering Faculty
Donn Hancher, Interim Chair • Purdue University
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E. Grulke • Ohio State University
C. Hamrin (Professor Emeritus) • Northwestern University
D. Kalika • University of California, Berkeley
M. Keane • National University of Ireland
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B. Knutson • Georgia Institute of Technology
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A. Ray • Clarkson University
J.T. Schrodt • University of Louisville
T. Tsang • University of Texas

Paducah, KY, Program
P. Dunbar • University of Tennessee
R. Lee-Desautels • Ohio State University
D. Silverstein • Vanderbilt University
J. Smart • University of Texas

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• virus and protein production

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• process modeling

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• catalytic membranes and fuel cells
• industrial catalysis

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• thermo-electrical simulation

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• polymeric foams

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• polymeric foams

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• vapor phase membranes
• industrial process engineering

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Québec (QC) Canada G1K 7P4
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Marvin Charles (Polytechnic Institute of Brooklyn) • bioprocess design • cGMP R&D
Manoj K. Chaudhry (SUNY-Buffalo) • adhesion • thin films • surface chemistry
John C. Chen (University of Michigan) • two-phase vapor-liquid flow • fluidization • radiative heat transfer • environmental technology
Mohamed S. El-Aasser (McGill University) • polymer colloids and films • emulsion copolymerization • polymer synthesis and characterization
James T. Hsu (Northwestern University) • bioseparations • applied recombinant DNA technology
Andrew Klein (North Carolina State University) • emulsion polymerization • colloidal and surface effects in polymerization
Mayuresh V. Kothare (California Institute of Technology) • model predictive control • constrained control • microchemical systems
William L. Luyben (University of Delaware) • process design and control • distillation
William E. Schiesser (Princeton University) • numerical algorithms and software in chemical engineering
Arup K. Sengupta (University of Houston) • use of adsorbents, ion exchange, reactive polymers, membranes in environmental pollution
Cesar A. Silebi (Lehigh University) • separation of colloidal particles • electrophoresis • mass transfer
Leslie H. Sperling (Duke University) • mechanical and morphological properties of polymers • interpenetrating polymer networks
Fred P. Stein, Emeritus (University of Michigan) • thermodynamic properties of mixtures
Harvey G. Stenger, Jr. (Massachusetts Institute of Technology) • reactor engineering
Israel E. Wachs (Stanford University) • materials characterization • surface chemistry • heterogeneous catalysis • environmental catalysis
Leonard A. Wenzel, Emeritus (University of Michigan) • thermodynamics • cryogenics and mixed-gas adsorption

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Additional information and applications may be obtained by writing to:

Dr. James T. Hsu, Chairman • Graduate Committee
Department of Chemical Engineering • Lehigh University • 111 Research Drive • Iacocca Hall • Bethlehem, PA 18015
FAX: (610) 758-5057 • E-MAIL: inchegs@lehigh.edu • WEBSITE: www.lehigh.edu/~inchm/index.html
Faculty

C.S. Fang, PhD, University of Houston, TX (1968)
F.F. Farshad, PhD, University of Oklahoma, OK (1975)
J.D. Garber (Head), PhD, Georgia Institute of Technology, GA (1971)
A.G. Hill, PhD, Louisiana Technical University, LA (1980)
J.N. Linsley, PhD, Rice University, TX (1970)
A.B. Ponter, DSc, Birmingham University, UK (1986) PhD, Manchester (1966)
J.R. Reinhardt, PhD, University of Arkansas, AR (1977)

Research Centers

Corrosion Research Center • Dr. J.D. Garber, Director
Center for Metals, Polymers and Composites Research • Dr. R.D.K. Misra, Director

Research Areas

• Corrosion
  Gas and Oil Well Modeling
  Pipeline Steels
  Hydrogen-Induced Cracking

• Materials: Structure/Processing/Performance
  Irradiation of Polymers with UV/Ozone
  Deformation Behavior of Polymers and Composites
  Formability and Fracture Toughness of High-Strength Steels
  Cold Work Embrittlement of Interstitial-Free Steels
  Casting of Precious Metals and Alloys

• Fluid Flow and Transport Phenomena
  Phase Inversion
  Drop Coalescence
  Liquid Spreading
  Multiphase Flow
  Surface Roughness

• Thermodynamics and Process Engineering
  Phase Equilibria in Multiphase Systems
  Chemical Reactor Design, Stability and Dynamics
  Process Simulation and Design

Department of Chemical Engineering
University of Louisiana at Lafayette
PO Box 44130
Lafayette, LA 70504-4130

For more information:
www.louisiana. engr.edu/chee/ or e-mail: dmisra@louisiana.edu (Graduate Coordinator)

Fall 2002
THE CITY

Baton Rouge is the state capitol and home of the major state institution for higher education — LSU. Situated in the Acadian region, Baton Rouge blends the Old South and Cajun Cultures. Baton Rouge is one of the nation's busiest ports and the city's economy rests heavily on the chemical, oil, plastics, and agricultural industries. The great outdoors provide excellent recreational activities year-round, especially fishing, hunting, and water sports. The proximity of New Orleans provides for superb nightlife, especially during Mardi Gras. The city is also only two hours away from the Mississippi Gulf Coast, and four hours from either Gulf Shores or Houston.

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TO APPLY, CONTACT

DIRECTOR OF GRADUATE INSTRUCTION
Gordon A. and Mary Cain Department of Chemical Engineering
Louisiana State University
Baton Rouge, LA 70803
Telephone: (1800) 256-2084  FAX: (225) 578-1476
e-mail: gradcoor@che.lsu.edu

FACULTY

T.J. CLEIJ (Ph.D., Utrecht University)
Polymeric Materials, Science and Engineering

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Biochemical Reaction Engineering, Applied Math

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Supercritical Fluid Extraction, Ultrasound Kinetics

B.J. McCLOY (Ph.D., University of Minnesota)
Separation, Transport, Reaction Engineering

R.W. PIKE (Ph.D., Georgia Institute of Technology)
Fluid Dynamics, Reaction Engineering, Optimization

E.J. PODLHA (Ph.D., Columbia University)
Electrical Phenomena, Alloy and Composite Materials

D.D. REIBLE (Ph.D., California Institute of Technology)
Environmental Transport, Transport Modeling

A.M. STERLING (Ph.D., University of Washington)
Transport Phenomena, Combustion

J.J. SPIVEY (Ph.D., Louisiana State University)
Catalysis

L.J. THIBODEAUX (Ph.D., Louisiana State University)
Chemodynamics, Hazardous Waste Transport

K.E. THOMPSON (Ph.D., University of Michigan)
Transport and Reaction in Porous Media

K.T. VALSARAJ (Ph.D., Vanderbilt University)
Environmental Transport, Separations

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Chemical Engineering Department
Manhattan College
Riverdale, NY 10471

chmldept@manhattan.edu
http://www.engineering.manhattan.edu/graduate/application/create_account.aspx

Manhattan College is located in Riverdale, an attractive area in the northwest section of New York City.
Faculty and Research Areas

Raymond A. Adomaitis (IIT) • Systems modeling and simulation methodologies; semiconductor manufacturing
Mikhail A. Anisimov (Moscow) • Critical phenomena and phase transitions in fluids and fluid mixtures
Timothy A. Barbari (Texas-Austin) • Membrane science, polymer science, biomaterials
William E. Bentley (Colorado) • Biochemical/metabolic engineering, applications of molecular biology
Richard V. Calabrese (Massachusetts) • Multiphase flow, turbulence and mixing
Kyu Yong Choi (Wisconsin) • Polymer reaction engineering
Panagiotis Dimitrakopoulos (Illinois-Urbana) • Biofluid mechanics, biophysics and microrheology
Sheryl H. Ehrman (UCLA) • Aerosol and nanoparticle technology
John P. Fisher (Rice) • Tissue engineering, biomaterials
James W. Gentry (Texas-Austin) • Aerosol science and engineering
Sandra C. Greer (Chicago) • Physical chemistry, polymer science, biomacromolecules, phase equilibria
Maria I. Klapa (MIT) • Metabolic engineering, bioinformatics, modeling of biological networks
Peter Kofinas (MIT) • Polymer science and engineering
Thomas J. McAvoys (Princeton) • Process control, fault detection
Tracey R. Pulliam Holoman (Maryland) • Biochemical engineering and bioremediation
Jan V. Sengers (U. Amsterdam) • Critical phenomena, thermophysical properties of fluids and fluid mixtures
Srinivasa R. Raghavan (N.C. State) • Polymers, colloids, complex fluids, self-assembly
Nam Sun Wang (Caltech) • Biochemical engineering
William A. Weigand (IIT) • Biochemical engineering, bioprocess control and optimization
Evanghelos Zafiriou (Caltech) • Process control, identification and optimization

Location: The University of Maryland is located in close proximity to the nation’s capital, Washington, D.C., and a number of government laboratories, including NIST, NIH, NRL, ARL, USDA, and FDA.

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FOR FURTHER INFORMATION
CONTACT:
Graduate Program Coordinator
Department of Chemical and Biochemical Engineering
University of Maryland Baltimore County
1000 Hilltop Circle
Baltimore, Maryland 21250
Phone: (410) 455-3400
FAX: (410) 455-1049

FACULTY

D. D. FREY, Ph.D. California-Berkeley
Separation and transport processes in biotechnology; protein purification; chromatography.

T. GOOD, Ph.D. University of Wisconsin-Madison
Cellular Engineering; Protein Aggregation: In Vitro Models of Disease

M. R. MARTEN, Ph.D. Purdue
Bioprocess engineering; Fermentation; Cell biology and protein secretion; Proteomics

A. R. MOREIRA, Ph.D. Pennsylvania
rDNA fermentation; Regulatory issues; Scale-up; Downstream processing

G. F. PAYNE, Ph.D.* Michigan
Plant cell tissue culture; *Streptomyces* bioprocessing; Adsorptive separation; Toxic waste treatment

G. RAO, Ph.D. Drexel
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J. M. ROSS, Ph.D. Rice
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J.M. Douglas, Emeritus (Delaware)
N.S. Forbes (Berkeley)
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H.H. Winter (Stuttgart)

Current Areas of MS and PhD Research
• Process design:
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• Materials:
  - Polymers and inorganics, multiscale modeling
• Kinetics and reaction engineering:
  - Catalytic, biological, noncatalytic
• Molecularly based modeling:
  - Statistical mechanics, quantum chemistry, molecular
    simulations
• Fluid mechanics and polymer rheology
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Fall 2002
# Chemical Engineering

## Faculty

**M.H.I. Baird Emeritus** • PhD (Cambridge) • Mass Transfer • Solvent Extraction

**J.L. Brash Emeritus** • PhD (Glasgow) • Biomedical Engineering • Bio Materials • Polymers

**J.M. Dickson** • PhD (Virginia) • Membrane Transport Phenomena • Reverse Osmosis

**C. Filipe** • PhD (Clemson) • Environmental Biotechnology • Environmental Engineering

**R. Ghosh** • DPhil (Oxford) • Bioseparation • Membrane Technology

**A.E. Hamielec Emeritus** • PhD (Toronto) • Polymer Reaction Engineering

**A.N. Hrymak** • PhD (Carnegie Mellon) • Computer Aided Design • Polymer Processing

**J.F. MacGregor** • PhD (Wisconsin) • Computer Process Control • Polymer Reaction Engineering

**T.E. Marlin** • PhD (Massachusetts) • Computer Process Control

**R.H. Pelton** • PhD (Bristol) • Water Soluble Polymers • Colloid Polymer Systems

**Y. Samyudia** • PhD (Queensland) • Computer Process Control

**C.L.E. Swartz** • PhD (Wisconsin) • Computer Process Control • Optimization

**H. Sheardown** • PhD (Toronto) • Biomaterials • Tissue Engineering

**L.W. Shemilt Emeritus** • PhD (Toronto) • Radioactive Waste Management

**P.A. Taylor** • PhD (Wales) • Computer Process Control

**M. Thompson** • PhD (Waterloo) • Polymer Processing • Extrusion and Reactive Extrusion

**J. Vlachopoulos** • DSc (Washington University) • Polymer Processing • Rheology • Numerical Methods

**P.E. Wood** • PhD (Caltech) • Experimental and Computational Fluid Mechanics • Heat Transfer

**S. Zhu** • PhD (McMaster) • Polymer Reaction Engineering • Polymer Synthesis • Polymerization Process Modeling

## Adjunct Faculty

**T. Kourti** • PhD (McMaster) • Computer Process Control

**K. Kostanski** • PhD (Tech U. Szczecin) • Polymerization and Polymer Characterization

**S.L. Quinn** • PhD (Queens) • Statistical Process Control

**J.D. Wright** • PhD (Cambridge) • Pulp and Paper • Computer Process Control • Process Dynamics and Modeling

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Chemical Engineering Education
Faculty

1. Ronald Larson  Chair, Polymers, DNA, complex fluids, fluid mechanics
2. Stacy G. Bike  Colloids, polymers, complex fluids
3. Mark A. Burns  Microfabricated analytical systems, biochemical separations
4. H. Scott Fogler  Fused reactions, colloids, gelation kinetics
5. John L. Gland  Surface science
6. Sharon Glotzer  Soft materials and complex fluids
7. Erdogan Gulari  Catalysis, electronic materials, combinatorial chemistry
8. Jennifer J. Linderman  Engineering approaches to cell biology
9. Susan Montgomery  Undergraduate program advisor
10. David J. Mooney  Cellular and tissue engineering
11. Chester Ni  Bioinformatics, pharmaceutics
12. Phillip E. Savage  Reactions in supercritical water, "green" chemistry
13. Johannes Schwank  Heterogeneous catalysis, surface science, gas sensors
14. Christina Smolke  Biomolecular and metabolic engineering
15. Michael Solomon  Light scattering and rheology of complex fluids
16. Levi T. Thompson, Jr.  Catalysis, electrocatalysis, materials processing
17. Henry Y. Wang  Pharmaceutical engineering, bioprocessing
18. Walter Weber  Environmental processes and sustainability
19. Ralph T. Yang  Separations, adsorption, catalysis
20. Robert M. Ziff  Percolation, catalysis, statistical thermodynamics

For More Information, Contact:
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Web: http://www.engin.umich.edu/dept/cheme/
Graduate Study in Chemical Engineering and Materials Science

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FELLOWSHIPS

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Biomaterials, Ceramic Bone Substitutes, Bone Tissue Engineering, Colloidal Processing of Ceramics and Ceramic Composites

K. A. BERGLUND • Ph.D., 1981, Iowa State University
Applied Spectroscopy, Food and Biochemical Engineering, Crystallization from Solution, New Uses of Agricultural Crops

T.R. BIELER • Ph.D., 1989, University of California
High Temperature Creep, Superplasticity; Texture of Metals, Intermetallics, and Composites; Solder and Electronic Heat Sink Materials; Metal Matrix Composite Fabrication; High Strain Rate Deformation

D.M. BRIEDE • Ph.D., 1981, Iowa State University
Biochemical Engineering, Biobased Industrial Products, Biomass Conversion, Life Cycle Analysis

E.D. CASE • Ph.D., 1980, Iowa State University
Microcracking in Ceramics, Thermal Fatigue, Ceramic/Ceramic Joining, Bioceramics, Microwave Processing of Ceramics and Ceramic Composites

C. CHAN • Ph.D., 1990, University of Pennsylvania
Metabolism and Diabetes, Alzheimer and Parkinson's disease, Metabolic Engineering, Tissue Engineering, Bioinformatics and Multivariate Analysis

M.A. CRIMP • Ph.D., 1987, Case Western Reserve University

R. DRZAL • Ph.D., 1974, Case Western Reserve University
Surface and Interfacial Phenomena, Adhesion, Polymer Composite Materials, Surface Characterization, Surface Modification of Polymers, Polymer Composite Processing, Adhesive Bonding

D.S. GRUMMON • Ph.D., 1986, University of Michigan
Superelasticity and Shape-Memory in Titanium-Nickel Thin Films, Microactuators, Thermoelectric Martensite Transformations, Ion Beam Surface Modification of Materials, Surface Effects in Fatigue Crack Initiation, Mechanical Metallurgy

M.C. HAWLEY • Ph.D., 1964, Michigan State University
Kinetics, Catalysis, Reactions in Plasmas, Polymerization Reactions, Composite Processing, Biomass Conversion, Reaction Engineering

R. JAYARAMAN • Ph.D., 1975, Princeton University
Polymer Rheology, Processing of Polymer Blends and Composites, Computational Methods

A. LEE • Ph.D., 1987, University of Illinois at Urbana-Champaign
Inorganic-Organic Hybrid Polymers, Physical and Mechanical Characterization, Dynamics of Polymeric Glasses

C.T. LIRA • Ph.D., 1985, University of Illinois at Urbana-Champaign
Thermodynamics and Phase Equilibria of Complex Systems, Adsorption, Supercritical Fluid Studies

J.P. LUCAS • Ph.D., 1981, University of Minnesota
Microstructure Evolution/Characterization of Pb-Free Solders, Alloys, and their Composites; Nonoxidation Characterization of Deformation in Small-Volumes and Thin Films; Moisture Effects in Resin Matrix Composites; Metal Matrix Composite

M.E. MACKAY • Ph.D., 1985, University of Illinois at Urbana-Champaign
Polymer Rheology and Thermodynamics, Nanotechnology, Dendrimers, Hyperbranched Polymers, Surface Properties

D.J. MILLER • Ph.D., 1982, University of Florida
Kinetics and Catalysis, Reaction Engineering, Catalytic Conversion of Biomass-Based Materials

R. NARAYAN • Ph.D., 1975, University of Bombay
Polymer Blends and Alloys, Biodegradable Plastics, Biofiber Composites, Extrusion Polymerization and Reactive Compounding, Biodegradation and Composting Studies

J. NOGAMI • Ph.D., 1986, Stanford University
Electronic Materials, Scanned Probe Microscopy, Surface Characterization, Growth and Nanostructured Materials

R.Y. OFOLI • Ph.D., 1994, Carnegie Mellon University
Colloid and Interfacial Science: Colloid Stability, Adsorption of Proteins, Receptor-Ligand Interactions at the Liquid-Liquid Interface, Micellar Solubilization

C.A. PETTY • Ph.D., 1970, University of Florida
Fluid Mechanics, Turbulent Transport Phenomena, Solid-Fluid and Liquid-Liquid Separations, Hydrocyclones

K.N. SUBRAMANIAN • Ph.D., 1966, Michigan State University
Mechanical Properties of Metals and Ceramics, Crystalization of Glasses, Erosion, Composite Materials, Lead-Free Electronic Solders

R.M. WORDEN • Ph.D., 1986, University of Tennessee
Biochemical Engineering, Microbial Transport Processes, Synthesis Gas Fermentations, Metabolic Engineering, Microbial Ecology

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Thermodynamics and dynamics of polymers and polymer mixtures

Robert W. Carr
Chemical kinetics, reaction engineering

C. Barry Carter
Electron microscopy of semiconductors and ceramics, solid-state reactions and growth of thin films

James R. Chelikowsky
Structural/electronic properties of complex systems

Robert F. Cook
Mechanical behavior of materials, microelectronic device fabrication and packaging

Edward L. Cussler
Mass transfer, novel separation processes

John S. Dahler (Emeritus)
Nonequilibrium statistical mechanics

Prodromos Daoutidis
Nonlinear process control, process analysis and design

H. Ted Davis
Colloid and interface science, statistical mechanics

Jeffrey J. Derby
Materials processing, high performance computing

Lorraine Falter Francis
Ceramic processing, electrical and mechanical properties of ceramics

Arnold G. Fredrickson (Emeritus)
Biochemical engineering, microbial populations

C. Daniel Frisbie
Molecular materials and interfaces, molecular electronics

William W. Gerberich
Fracture micromechanics, interfacial defects

Wei-Shou Hu
Biochemical engineering

Satish Kumar
Transport processes in complex fluids, stability, dynamics, and manipulation of interfaces, transport processes in microscale systems

Chris Leighton
Magnetic and electronic properties of thin film magnetic materials and heterostructures

Timothy P. Lodge
Polymer structure and dynamics, polymer characterization

Christopher W. Macosko
Polymer processing, rheology, polymer networks and blends

Richard B. McClurg
Thermodynamics and kinetics of phase changes

Alon V. McCormick
Reaction engineering of materials synthesis, spectroscopy, molecular simulation

David C. Morse
Statistical mechanics, polymeric and complex fluids

David J. Norris
Nanomaterials, photonic crystals, molecular spintronics

Richard A. Oriani (Emeritus)
Corrosion, thermodynamics of solids, cold fusion

Christopher Palmström
Epitaxial growth processes and heterostructure formation, properties of thin film

Lanny D. Schmidt
Surface chemistry, heterogeneous catalysis, reaction engineering

L. E. Scriven
Fluid mechanics and rheology, transport, reaction and stress phenomena, materials processing

David A. Shores
High temperature corrosion, fuel cells

John M. Sivertsen (Emeritus)
Magnetic, microelectronic, and tribological materials

William H. Smyrl
Electrochemical engineering, modeling electrochemical systems, microvisualization of reactive surfaces

Friedrich Srienc
Biochemical engineering, cell cycle and growth models, biopolymers

Robert T. Tranquillo
Cell and tissue engineering

Michael D. Ward
Molecular materials, crystal growth, electrochemistry

Renata M. M. Wentzcovitch
Electronic and structural properties of condensed matter systems; first principles molecular dynamics

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Environmental Remediation, Electrokinetics, Chemical Extraction, Stabilization/Solidification, Waste Treatment, Heavy Metal Soils

W. Todd French, Assistant Research Professor
Applied Microbiology, Bioremediation, Industrial Microbiology, Microbial Enhanced Oil Recovery

Clifford E. George, Professor
Industrial Biotechnology, Industrial Applications of Microwave Power/Heating and Electrochemistry, Process Control, Chemical Plant/Oil Refinery Operations and Safety

Priscilla J. Hill, Assistant Professor
Crystallization, Process Design, Solids Processing

Irvin A. Jefcoat, Professor and Henry Chair
Pollution Prevention/Waste Minimization

Rudy E. Rogers, Professor
Natural Gas Storage and Transport, Formation Rates in Ocean Sediments, CO₂ Sequestration, Natural Gas Production from Seabed Hydrates

Kirk H. Schulz, Director and Deavenport Chair
Surface Science, Catalysis, Electronic Materials

Hossein Toghiani, Associate Professor
Composite Materials, Catalysis, Fuel Cells, Thermodynamics of Liquid Mixtures

Rebecca K. Toghiani, Associate Professor
Thermodynamics, Separations

Mark E. Zappi, Professor
Waste Treatment, Industrial Biotechnology, Chemical Oxidation, Biotreatment, Hyphenated Remediation Techniques

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University of Nebraska

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Jennifer Brand • University of California, San Diego
Supercritical Fluid Processing; Natural Product Processing; Environmental Remediation

L. Davis Clements • University of Oklahoma
Computer-Aided Process Design; Process Synthesis; Fuels and Chemicals from Biomass

James Eakman • University of Minnesota
Computer-Aided Process Engineering; Solids Properties & Processing; Reaction Engineering

James Hendrix • University of Nebraska
Remediation of Mine Tailings Waste; Novel Analytical Chemistry; Non-Ideal Reactors

Gustavo Larsen • Yale University
Heterogeneous Catalysis: Spectroscopic Characterization of Catalysts

Lee Lauderback • Purdue University
Surface Analysis; Heterogeneous Catalysis

Michael Meagher • Iowa State University
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tion; Downstream Process, Purification, and Process Development; Butanol Recovery by Pervaporation
Chair, Graduate Studies

Hossein Noureddini • University of Nebraska
Production of Chemicals from Agricultural Products; Mathematical Modeling of Polymerization Kinetics

Delmar Timm • Iowa State University
Polymer Composites; Step-Wise Polymerization Kinetics; Kinetic Analysis Using GPC

Hendrik Viljoen • University of Pretoria
Plasma-Enhanced CVD; Detonation & Combustion; Ceramics

For further information, write

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D. Hahn; Agri. Univ. of Wageningen (Netherlands)
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M. Huang; University of Massachusetts
K. Hyun; University of Missouri-Columbia
H. Kimmel; City University of New York
D. Knox; Rensselaer Polytechnic Institute
G. Lewandowski; Columbia University
N. Loney; New Jersey Institute of Technology
A. Perna; University of Connecticut
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L. Simon; Colorado State University
K. Sirkar; University of Illinois-Urbana
S. Sofer; University of Texas
R. Tomkins; University of London (UK)
J. Wu; University of Delaware
M. Xanthos; University of Toronto (Canada)

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- C. Jeffrey Brinker
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- John G. Curro
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- Sang M. Han
- David Kauffman
- Ronald E. Loehman
- Gabriel P. López
- Richard W. Mead
- H. Eric Nuttall
- Jonathan Phillips
- Timothy L. Ward
- Ebtisam S. Wilkins

**Research Areas**

- Electroanalytical Chemistry, Biomedical Engineering
- Plasma Processing, Plasma Diagnostics
- Ceramics, Sol-Gel Processing, Self-Assembled Nanostructures
- Semiconductor Manufacturing Technology, Plasma Etching and Deposition
- Polymer Theory, Computational Modeling
- Catalysis, Interfaces, Advanced Materials
- Surface Characterization, 3-D Materials Characterization
- Semiconductor Manufacturing Technology, Plasma Etching and Deposition
- Plant Design, Environmental Engineering
- Glass-Metal and Ceramic-Metal Bonding and Interfacial Reactions
- Chemical Sensors, Hybrid Materials, Biotechnology, Interfacial Phenomena
- Unit Operations, Resource Extraction
- Environmental Science, Waste Transport Management, Colloid Science
- Materials Science, Catalysis, Plasma Physics and Chemistry
- Aerosol Materials Synthesis, Inorganic Membranes
- Biomedical Sensors and Waste Treatment

For more information, contact:

Jeffrey Brinker, Graduate Advisor
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  Transport Phenomena, Electrochemistry, Environmental Engineering
- **Ron K. Bhada**, Professor Emeritus, *University of Michigan*
- **Joe L. Creed**, Assistant Dean, *New Mexico State University*
  Engineering Design
- **Francisco R. Del Valle**, College Professor, *Massachusetts Institute of Technology*
  Food Engineering
- **Charles L. Johnson**, Professor and Head, *Washington University-St. Louis*
- **Richard L. Long**, Professor and Associate Head *Rice University*
  Transport Phenomena, Biomedical Engineering, Separations
- **Martha C. Mitchell**, Associate Professor, *University of Minnesota*
  Advanced Materials, Statistical Mechanics, Molecular Modeling
- **Stuart H. Munson-McGee**, Professor, *University of Delaware*
  Advanced Materials, Separations
- **John T. Patton**, Professor Emeritus, *Oklahoma State University*
- **David A. Rockstraw**, Associate Professor, *University of Oklahoma*
  Separations, Environmental Engineering, Kinetics
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Areas of Research
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- Statistical Mechanics & Molecular Simulations
- Environmental Science
- Electronic Materials
- Kinetics & Reaction Engineering
- Interfacial Science
- Polymer Science
- Nanotechnology
- Bio Catalysis
- Supercritical Fluids

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Fedkiw  Ollis
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Sickle Cell Adhesion
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Research Areas

Biomaterials
Biological Photonic Devices
Blood Rheology
Catalysis and Reaction Engineering
Combinatorial Materials Synthesis
Combustion Synthesis
Drug Delivery
Electrochemical Processes
Environmentally Conscious Design
Enzyme Encapsulation

Inorganic Membranes
Ionic Liquids
Molecular Modeling
Multiphase Flows
Nanostructured Materials
Nonlinear Dynamics
Parallel Computing
Polymeric Materials
Superconducting Materials
Tissue Engineering

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The Department

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Chemical Engineering

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Aerosol Science and Technology
Process Control
Separations
Energy and Environmental Engineering
Thin Film Materials
Chemical Reaction Engineering
Bioreactor Analysis
Downstream Processing of Proteins
Biomedical Engineering

Financial Aid
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The Faculty
Gerardine G. Botte (Ph.D., South Carolina, 2000)
W. J. Russell Chen (Ph.D., Syracuse, 1974)
Nicholas Dinos, Emeritus (Ph.D., Lehigh, 1967)
Douglas J. Goetz (Ph.D., Cornell, 1995)
Tingyue Gu (Ph.D., Purdue, 1990)
Daniel A. Gulino (Ph.D., Illinois, 1983)
Srdjan Nesic (Ph.D., Saskatchewan, 1991)
Michael E. Prudich, Chair (Ph.D., West Virginia, 1979)
Darin Ridgway, P.E. (Ph.D., Florida State, 1990)
Kendree J. Sampson (Ph.D., Purdue, 1981)
Valerie L. Young (Ph.D., Virginia Tech., 1992)

For More Information Contact:
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- Brian P. Grady, Associate Professor • multiphase & block copolymers • ion-containing polymers • polymer-matrix composites • biodegradable and bioabsorbable polymers • nanotechnology at interfaces
- Roger G. Harrison, Jr., Associate Professor • production of proteins & peptides using recombinant DNA technology • separation & purification of biochemicals • protein engineering for biomedical and environmental application • protein engineering
- Jeffrey H. Harwell, Conoco/DuPont Professor, Executive Associate Dean for the College of Engineering • tertiary oil recovery • unconventional low energy separation processes • mass transfer • dynamics of multicomponent mass transfer processes • surface phenomena • adsorption kinetics • subsurface remediation
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- Lance L. Lobban, Winn Chair & Director • catalytic reaction rate mechanisms & modeling • partial oxidation of hydrocarbons • photocatalysis
- Richard G. Mallinson, Professor • chemical reaction engineering • energy project valuation • synthetic and alternative fuels • natural gas utilization • methane conversion
- Peter S. McFetridge, Research Assistant Professor, Director of Cell & Tissue Culture Facility • vascular tissue engineering • biomedical design, development and application • vascular perfusion reactor engineering
- Matthias U. Nollert, Associate Professor • biomedical engineering • cellular metabolism and transport • platelet and leukocyte adhesion • fluid mechanics
- Edgar A. O'Rear, III, Winn Professor • drug delivery • surface chemistry & physics • kinetics • blood trauma associated with medical devices • biorheology • organic chemistry
- Dimitrios Papavassiliou, Assistant Professor • integrated process simulations • transport phenomena in biological systems • small scale transport at the interface between statistical mechanics and classical mechanics
- Daniel E. Resasco, S.A. Wilson Professor • heterogeneous catalysis, reaction engineering & kinetics • design of catalysts for pollutant abatement • carbon nanotubes • physical chemistry of surfaces
- Melissa M. Rieger, Assistant Professor • electrochemical phenomena and electrochemical engineering • carbon nanotube electro-chemistry • material systems and electrochemical processes in microelectronic processing • electrochemical behavior of polymeric materials
- John F. Scamehorn, Asahi Glass Chair • surface & colloid science • tertiary oil recovery • detergency • membrane separations • adsorption • pollution control • polymers • paper & plastics deinking
- David W. Schmidtke, Assistant Professor • design & development of new analytical devices & technologies for medical therapy • biosensors • cell adhesion • high speed/high resolution video microscopy of fluid mechanics in the blood stream
- Robert L. Shambaugh, Professor • polymerization chemistry • polymer • processing technology • fiber spinning, texturing & extrusion • wastewater • engineering • physicochemical treatment • ozonation • gas-liquid reactions
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Sundarajan V. Madihally (Ph.D., Wayne State University)
R. Russell Rhinehart (Ph.D., North Carolina State University)
James E. Smay (Ph.D., University of Illinois)
D. Alan Tree (Ph.D., University of Illinois)
Jan Wagner (Ph.D., University of Kansas)
James R. Whiteley (Ph.D., Ohio State University)

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Biochemical Processes
Biomaterials
Colloids/Ceramics
Environmental Engineering
Fluid Flow/CFD
Gas Processing
Hazardous Wastes
Ion Exchange
Molecular Design
Nanomaterials
Phase Equilibria
Polymers
Process Control
Process Simulation
Solid Freeform Fabrication
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- C. McConica
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- J. McGuire
  Biointerfacial Phenomena, Biomaterials
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R. Gross
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K. Levon
Conductive polymers, biosensors

J. Mijovic
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Y. Shnidman
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L. Stiel
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I. Teraoka
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A. Ullman
Surface science and engineering, nanotechnology

E. Ziegler
Air pollution control engineering

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Chromatin structure and dynamics

W. Zurawsky
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Princeton University

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Jay B. Benziger
Jeffrey D. Carbeck
Pablo G. Debedetti (Chair)
Christodoulos A. Floudas
Yannis G. Kevrekidis
Morton D. Kostin
Athanassios Z. Panagiotopoulos
Robert K. Prud’homme
Richard A. Register
William B. Russell
Lynn M. Russell
Dudley A. Saville
George W. Scherer
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David W. Wood

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Chemical Engineering
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or email: chegrad@princeton.edu

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FACULTY

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David S. Corti
W. Nicholas Delgass
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Michael T. Harris
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Gil U. Lee
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Joseph F. Pekny
Nicholas A. Peppas
Doraiswami Ramkrishna
Gintaras V. Reklaitis
Jennifer L. Sinclair
Kendall Thomson
George T. Tsao
Venkat Venkatasubramanian
Nien-Hua L. Wang
Phillip C. Wankat

RESEARCH AREAS

Biomedical Engineering
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Catalysis and Reaction Engineering
Fluid Mechanics and Transport Phenomena
Interfacial Engineering and Colloid Science
Molecular Modeling and Statistical Mechanics
Nanofabrication and Nanomaterials
Particle Technology
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Surface Science

For More Information
Graduate Studies
Purdue University
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West Lafayette, Indiana 47907-1283
Phone: (765) 494-4057
www.che.purdue.edu
Chemical Engineering at Rensselaer Polytechnic Institute

The Chemical Engineering Department at Rensselaer has long been recognized for its excellence in teaching and research. Its graduate programs lead to research-based M.S. and Ph.D. degrees and to a course-based M.E. degree. Programs are also offered in cooperation with the School of Management and Technology which lead to an M.E. in Chemical Engineering and to an MBA or the M.S. in Management. Owing to funding, consulting, and previous faculty experience, the department maintains close ties with industry. Department web site: http://www.eng.rpi.edu/dept/chem-eng/

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e-mail: grad-admissions@rpi.edu
http://www.rpi.edu/dept/grad-services/

Faculty and Research Interests

Michael M. Abbott, abbotm2@rpi.edu  
Thermodynamics; equations of state; phase equilibria

Elmar R. Altwicker, altwie@rpi.edu  
Professor Emeritus
Spouted-bed combustion; incineration; trace-pollutant kinetics

Georges Belfort, belfog@rpi.edu  
Membrane separations; adsorption; biocatalysis; MRI; interfacial phenomena

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Process modeling, control, design, and optimization

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Wastewater treatment; biochemical engineering

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Semiconductor materials processing; transport and reaction analyses

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Displacement, membrane, and preparative chromatography; environmental research

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Biochemical engineering; biocatalysis, polymer science, bioseparations

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Combustion; high-temperature kinetics; gas-phase reactions

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Macromolecular self-assembly, computer simulations, statistical thermodynamics of liquids, hydration phenomena

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Microelectronics; reverse osmosis; crystal growth; ceramic composites

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Polymer nanostructures, nanocomposites, dynamics of glasses and gels, thermodynamics of complex fluids

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Heat transfer; interfacial phenomena; porous materials
RICE
Chemical Engineering at Rice University

FACULTY

• William W. Akers* (Michigan, 1950)
• Constantine D. Armeniades (Case Western Reserve, 1969)
• Walter G. Chapman (Cornell, 1988)
• Sam H. Davis, Jr.* (MIT, 1957)
• Jacqueline L. Goveas (Princeton, 1996)
• J. David Hellums* (Michigan, 1961)
• Joe W. Hightower* (Johns Hopkins, 1963)
• George J. Hirasaki (Rice, 1967)
• Riki Kobayashi* (Michigan, 1951)
• Paul E. Laibinis (Harvard University, 1991)
• Nikolaos V. Mantzaris (Minnesota, 2000)
• Clarence A. Miller (Minnesota, 1966)
• Matteo Pasquarello (Minnesota, 2000)
• Mark A. Robert (Swiss Fed. Inst. Tech., 1980)
• Michael S. Wong (MIT, 2000)
• Kyriacos Zygourakis (Minnesota, 1981)

Joint with Bioengineering

• Lary V. McIntire (Princeton, 1970)
• Antonios G. Mikos (Purdue, 1988)
• Ka-Yiu San (Caltech, 1984)
• Jennifer L. West (Texas, 1996)

*Emeritus Faculty

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• Fluid Mechanics
• Interfacial Phenomena
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• Nanotechnology
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• Petroleum Engineering
• Polymer Science
• Reaction Engineering
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S. H. CHEN, Ph.D. 1981, Minnesota
Polymer Science and Engineering • Organic Materials for Optics and Photonics • Molecular Dynamics Simulation

E. H. CHIMOWITZ, Ph.D. 1982, Connecticut
Critical Phenomena • Statistical Mechanics of Fluids • Computer-Aided Design

D. R. HARDING, Ph.D. 1986, Cambridge (England)
Chemical Vapor Deposition • Mechanical and Transport Properties • Advanced Aerospace Materials

S. D. JACOBS, Ph.D. 1975, Rochester
Optics, Photonics, and Optoelectronics • Magnetorheology • Optics Manufacturing

J. JORNE, Ph.D. 1972, California (Berkeley)
Electrochemical Engineering • Microelectronics Processing • Theoretical Biology

Biomedical Engineering • Lung Surfactant • Molecular Biophysics

L. J. ROTHBERG, Ph.D. 1984, Harvard
Organic Materials and Device Sciences • Light-Emitting Diodes • Thin Film Transistors

Y. SHAPIR, Ph.D. 1981, Tel Aviv (Israel)
Critical Phenomena • Transport in Disordered Media • Scaling Behavior of Growing Surfaces

S. V. SOTIRCHOS, Ph.D. 1982, Houston
Reaction Engineering • Transport and Reaction in Porous Media • Processing of Ceramic Materials and Composites

J. H. D. WU, Ph.D. 1987, M.I.T.
Biocatalysis • Bone marrow Tissue Engineering • Genetic and Protein Engineering

H. YANG, Ph.D. 1998, Toronto
Nanomaterials • Meso- and Nanofabrication • Materials and Structures for Photonics and Biophotonics

M. YATES, Ph.D. 1999, Texas (Austin)
Colloids and Interfaces • Materials Synthesis in Microemulsions • Nanoparticle/Polymer Composites • Supercritical Fluids • Microencapsulation

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Faculty

C. Stewart Slater, Chair • Rutgers University
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Stephanie Farrell • New Jersey Institute of Technology
Zenaida Gephardt • University of Delaware
Robert P. Hesketh • University of Delaware
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James Newell • Clemson University
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Research Areas

Membrane Separations • Reaction Engineering • Mammalian & Insect Cell Culture • Pharmaceutical and Food Processing Technology • Biochemical Engineering • Green Engineering • Controlled Release • Novel Separation Processes • High-Performance Polymer Processing • Process Design and Optimization • Particle Technology • Supercritical Fluids • Environmental Engineering

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Research Areas

Biotechnology • Reaction Engineering • Process Systems Engineering • Pharmaceutical Engineering • Polymers

Faculty

► Helen M. Buettner, Associate Professor, Ph.D., University of Pennsylvania, 1987 • Applied neurobiology, cell motility, cell-substrate interactions, crystallization of pharmaceuticals

► Yee C. Chiew, Professor; Ph.D., University of Pennsylvania, 1984 • Statistical thermodynamics, microscopic structures of fluids and particle systems, interfacial phenomena

► Alkis Constantinides, Professor; D.E.Sc., Columbia University, 1970 • Biochemical engineering, optimization and control of fermentation processes, applied numerical analysis, artificial intelligence

► Peter Couchman, Professor; Ph.D., University of Virginia, 1976 • Thermodynamics, transition, and equation of state behavior of single and multicomponent systems, particularly polymers, surface phenomena

► Burton Z. Davidson, Professor; Ph.D., P.E., Northeastern University, 1963 • Systems simulation and optimization, environmental engineering, health and safety engineering management

► Panos G. Georgopoulos, Associate Professor; Ph.D., California Institute of Technology, 1986 • Atmospheric/environmental chemical engineering, turbulent transport, biochemodynamic modeling

► Benjamin J. Glasser, Assistant Professor; Ph.D., Princeton, 1995 • Multiphase flows and reactors, granular materials and particulate suspensions, nonlinear dynamics of transport processes

► Masaonori Hara, Professor; Ph.D., Kyoto University, 1981 • Polymer physics, polymer chemistry, polymer blends and composites, ionic polymers

► Marianne G. Ierapetritou, Assistant Professor; Ph.D., Imperial College, 1995 • Process systems engineering, process design, planning, and scheduling, uncertainty and environmental considerations, nonlinear and mixed integer optimization

► Johannes G. Khinast, Assistant Professor; Ph.D., Graz, 1995 • Reactors and environmental engineering, reactive flows, numerical analysis of large dynamical systems

► Michael T. Klein, Dean and Board of Governors Professor of Engineering; Sc.D., MIT, 1981 • Kinetics, catalysis and reaction engineering, automated kinetic modeling, hydrocarbon conversion, reactions in supercritical fluids

► Prabhas V. Moghe, Associate Professor; Ph.D., University of Minnesota, 1993 • Cell and tissue engineering, cell-biomaterial interactions, biomimetic materials

► Fernando Muzzio, Professor; Ph.D., University of Massachusetts, 1991 • Transport phenomena, mixing, chaotic flows, powder technology

► Henrik Pedersen, Professor; Ph.D., Yale University, 1978 • Biochemical engineering, immobilized enzymes, plant cell biotechnology, fiber-optic sensors

► Charles M. Roth, Assistant Professor; Ph.D., University of Delaware, 1994 • Nuclear acid biotechnology, molecular biology, and biochemical engineering, bioseparations

► Jerry I. Scheinbein, Professor; Ph.D., University of Pittsburgh, 1975 • Polymer electroprocessing, structure-electroactive properties of polymeric materials, ferroelectric, piezoelectric, pyroelectric, dielectric and electroactive properties of polymers

► M. Silvina Tomassone, Assistant Professor; Ph.D., Northeastern University, 1998 • Molecular dynamics, interfacial analysis, phase transitions

► Shaw S. Wang, Professor; Ph.D., Rutgers University, 1970 • Kinetics and thermodynamics of food-process engineering, and studies of biochemical and biological processes

► Martin L. Yarmush, Professor; Ph.D., Rockefeller University, 1979; M.D., Yale University, 1984 • Applied immunology, artificial organs, bioseparations, protein engineering, biotechnology

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Research Programs
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Rheology
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Sol-Gel Processing
Solvent Extraction
Surface Science
Supercritical Fluids
Thermodynamics
Waste Management
Waste Processing
Faculty
Paschalis Alexandridis (MIT) • amphiphilic polymers, self-assembly, complex fluids, nanomaterials, interfacial phenomena
Stelios T. Andreadis (Michigan) • bioengineering, gene therapy, tissue engineering of genetically modified skin
Jeffrey R. Errington (Cornell) • molecular simulation, statistical thermodynamics, biopreservation
Vladimir Hlavacek (ICT -Prague) • reaction engineering, nanopowders, explosives and detonations, analysis of chemical plants
Matthaeos Koffas (MIT) • metabolic engineering, bioinformatics
David A. Kofke (Pennsylvania) • molecular modeling and simulation, solid phase equilibria
Carl R. F. Lund (Wisconsin) • heterogeneous catalysis, chemical kinetics, reaction engineering
T. J. (Lakis) Mountziaris (Princeton) • electronic and photonic materials, nanoparticles, biosensors, multiphase flows
Sriram Neelamegham (Rice) • biomedical engineering, cell biomechanics, vascular engineering
Johannes M. Nitsche (MIT) • fluid mechanics, transport phenomena, bioactive surfaces, biological pores, transdermal transport
Eli Ruckenstein (Bucharest) • catalysis, surface phenomena, colloids and emulsions, biocompatible surfaces and materials
Michael E. Ryan (McGill) • polymer and ceramics processing, rheology, non-Newtonian fluid mechanics
Mark T. Swihart (Minnesota) • chemical kinetics, modeling of reactive flows, computational chemistry, nanoparticle formation
E. (Manolis) S. Tzanakakis (Minnesota) • cell and tissue engineering, biochemical engineering

Adjunct Faculty
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William M. Mihalko (School of Medicine) • orthopaedics
Bruce Nicholson (Biological Sciences) • gap junctions and connexins
Athos Petrou (Physics) • spectroscopy, semiconductor nanostructures
Carel Jan van Oss (Microbiology) • colloid and interface science
Yaoqi Zhou (Biophysics) • protein folding, simulation of biomolecules

Emeritus Faculty in Residence
Robert J. Good (Michigan) • adhesion and interface science, philosophy of science
Thomas W. Weber (Cornell) • process control
Sol W. Weller (Chicago) • catalysis, coal liquefaction, history of chemical engineering

Chemical engineering faculty participate in many interdisciplinary centers and initiatives, including The Center for Advanced Molecular Biology and Immunology, The Center for Computational Research, The Center for Advanced Photonic and Electronic Materials, The Institute for Lasers, Photonics, and Biophotonics, The Institute for Bioinformatics, and The Center for Advanced Technology for Biomedical Devices

For more information and an application, write to: Director of Graduate Studies, Department of Chemical Engineering, University at Buffalo (SUNY), Buffalo, New York, 14260-4200, or go to http://www.cheme.buffalo.edu

All Ph.D. students are supported as research or teaching assistants. Additional fellowships sponsored by Praxair, Inc., The National Science Foundation IGERT program, and the State University of New York are available to exceptionally well-qualified applicants.
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H. Du (PhD, Penn State University)
T.E. Fischer (ScD, Federal Inst. of Technology, Zurich)
B. Gallois (PhD, Carnegie-Mellon University)
D.M. Kalyon (PhD, McGill University)
S. Kovenklioglu (PhD, Stevens Institute of Technology)
A. Lawal (PhD, McGill University)
W.Y. Lee (PhD, Georgia Institute of Technology)
M. Libera (ScD, Massachusetts Inst. of Technology)
G. Rothberg (PhD, Columbia University)
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Research in

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Processing of Electronic and Photonic Materials
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The Next Step
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Bioprocessing, Thermodynamics
Duane D. Bruns (Ph.D., Houston, 1974)
Process Control, Modeling
John R. Collier (Ph.D., Case Institute, 1966)
Polymer Processing and Properties
Robert M. Counce (Ph.D., Tennessee, 1980)
Separations and Transport, Environmental
Peter T. Cummings (Ph.D., Melbourne, 1980)
Molecular Thermodynamics, Design, Environmental
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Non-Newtonian Fluid Dynamics
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Biochemical Engineering, Biosensors
David J. Keffer (Ph.D., Minnesota, 1996)
Molecular Modeling of Adsorption, Diffusion and Reaction in Zeolites
Charles F. Moore (Ph.D., Louisiana State, 1969)
Process Control
John W. Prados (Ph.D., Tennessee, 1957)
Safety and Risk Assessment
Tsewei Wang (Ph.D., M.I.T., 1977)
Process Control, Bioprocessing
Frederick E. Weber (Ph.D., Minnesota, 1982)
Computer-Aided Design, Radiation Chemistry

Adjunct and Part-Time Faculty from Oak Ridge National Laboratory
Hank D. Cochran (Ph.D., M.I.T.): Thermodynamics, Statistical Mechanics
Brian H. Davison (Ph.D., Caltech): Biochemical Engineering
Jack S. Watson (Ph.D., Tennessee): Separations and Transport, Nuclear Fusion
The University of Texas at Austin

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Faculty and their research

David T. Allen, Ph.D., Caltech, 1983 • environmental modeling, reaction engineering
Angela M. Belcher, Ph.D., U. of C. Santa Barbara, 1997 • organic/inorganic, biomolecular & biological-electronic hybrid materials
Roger T. Bonnecaze, Ph.D., Caltech, 1991 • suspension rheology, transport phenomena, electrical impedance tomography
Thomas F. Edgar, Ph.D., Princeton U., 1971 • process modeling, control, optimization
John G. Ekerdt, Ph.D., U. of C. Berkeley • electronic materials chemistry, surface science
R. Bruce Eldridge, Ph.D., U. of Texas, 1986 • separations research
Benny Freeman, Ph.D., U. of C. Berkeley, 1988 • polymer structures, processing and properties
Venkat Ganesan, Ph.D., MIT, 1999 • statistical mechanics, simulations of self-assembly in complex fluids
George Georgiou, Ph.D., Cornell U., 1987 • microbial, protein biotechnology
Peter F. Green, Ph.D., Cornell U., 1985 • materials science, polymer melts
Adam Heller, Ph.D., Hebrew U., 1961 • electrochemical biosensing, environmental photoelectrochemistry
Gyeong S. Hwang, Ph.D., Caltech, 1999 • multiscale modeling & simulation, semiconductors, nanotechnology
Keith P. Johnston, Ph.D., U. of Illinois, 1981 • polymer and surface thermodynamics, supercritical fluids
Miguel José-Yacaman, Ph.D., National University of Mexico, 1973 • materials science, electron microscopy, nanoparticles
Brian A. Korgel, Ph.D., U. of C. Los Angeles, 1997 • complex fluids, nanostructured materials
Douglas R. Lloyd, Ph.D., U. of Waterloo, 1977 • polymeric membrane formation, liquid separations
Yueh-Lin Loo, Ph.D., Princeton U., 2001 • polymer physics & chemistry, micro- & nanostructured materials
C. Buddie Mullins, Ph.D., Caltech, 1990 • surface science, molecular beams, semiconductor thin-film growth
S. Joseph Qin, Ph.D., U. of Maryland, 1992 • process modeling and control
Gary T. Rochelle, Ph.D., U. of C. Berkeley, 1977 • air pollution control, reactive mass transfer
Peter J. Rossky, Ph.D., Harvard U., 1978 • theoretical chemistry, liquids, condensed phase quantum dynamics
Isaac C. Sanchez, Ph.D., U. of Delaware, 1969 • statistical thermodynamics of polymer liquids and solutions
Christine E. Schmidt, Ph.D., University of Illinois, 1995 • cell and tissue engineering
Makul M. Sharma, Ph.D., U. of Southern California, 1985 • surface and colloid chemistry
Thomas M. Truskett, Ph.D., Princeton U., 2001 • statistical mechanics, molecular modeling
J. Michael White, Ph.D., U. of Illinois, 1966 • chemical reactions on surfaces
C. Grant Willson, Ph.D., U. of C. Berkeley, 1973 • polymer synthesis, photochemical processing

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**Faculty**

R.G. Anthony, Head • Ph.D., University of Texas, 1966
  - C.D. Holland Professor
  - Catalysis, reaction engineering ion exchange

A. Akgerman • Ph.D., U. of Virginia, 1971
  - Chevron II Professor
  - Reaction engineering, waste treatment

J.T. Baldwin, Ph.D. • Texas A&M University, 1968
  - Process design

M.A. Bevan, Ph.D. • Carnegie Mellon University, 1999
  - Colloidal Science

D.B. Bukur, Associate Head • Ph.D., U. of Minnesota, 1974
  - Reaction engineering, math methods

J.A. Bullin, Ph.D. • U. of Houston, 1972, Professor Emeritus
  - Gas sweetening, asphalt characterizations

R. Darby, Ph.D. • Rice University, 1972, Professor Emeritus
  - Rheology, polymers

R.R. Davison, Ph.D. • Texas A&M U., 1962, Professor Emeritus
  - Asphalt characterization

L.D. Durbin, Ph.D. • Rice University, 1961, Professor Emeritus
  - Process control

M. El-Halwagi, Ph.D. • University of California, 1990
  - McFerrin Professor
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P.T. Eubank, Ph.D. • Northwestern University, 1961
  - Joe M. Nesbitt Professor
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D.M. Ford, Ph.D. • University of Pennsylvania, 1996
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G. Froment, Ph.D. • University of Gent, Belgium, 1957
  - Reaction engineering

C.J. Glover, Ph.D. • Rice University, 1974
  - Director, Center for Asphalt & Materials Chemistry
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K.R. Hall, Ph.D. • University of Oklahoma, 1967
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D.T. Hanson, Ph.D. • University of Minnesota, 1968
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Y. Kuo, Ph.D., Dow Professor • Columbia University, 1979
  - Microelectronics

S. Mannan, Ph.D. • University of Oklahoma, 1986
  - Director, Mary Kay O'Connor Process Safety Center

E. Sevick-Muraca, Ph.D. • Carnegie Mellon University, 1989
  - Biomedical/Biochemical

D.F. Shantz, Ph.D. • University of Delaware, 2000
  - Structure-property relationships of porous materials, synthesis of new materials

V. Ugaz, Ph.D. • Northwestern University, 1999
  - Microfabricated Bioseparation Systems
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FULL-TIME PROFESSORS

Assoc. Prof. Eliana DeBernardez Clark, Ph.D. (U.N.L. Argentina)
(on leave)
Biocatalysis, protein folding, protein aggregation

Prof. Gregory D. Botsaris, Ph.D. (M.I.T.)
Crystallization, nucleation, applied surface science

Prof. Maria Flytzani-Stephanopoulos, Ph.D. (Univ. of Minnesota)
Environmental catalysis, pollution prevention, clean energy, and transportation technologies

Prof. David L. Kaplan, Ph.D. (Syracuse University)
Bioengineered polymers related to self-assembly, biomaterials and tissue engineering

Asst. Prof. Kyongbum Lee, Ph.D. (M.I.T.)
Biotechnology, metabolic engineering, bioinformatics

Assoc. Prof. Jerry H. Meldon, Ph.D. (M.I.T.)
Membrane science and technology, mass transfer with chemical reaction including mathematical modeling

Assoc. Prof. Daniel F. Ryder, Ph.D. (Worcester Polytechnic Institute)
Advanced process control applications

Prof. Nak-Ho Sung, Ph.D. (M.I.T.)
Polymers and composites, interface science, polymer diffusion, surface modification

Optimization, nucleation, reaction kinetics, VLSI fabrication

RESEARCH PROFESSORS

Asst. Prof. Aurelie Edwards, Ph.D. (M.I.T.)
Transport across biological membranes, role of microcirculation in the renal medulla

Asst. Prof. Regina Valuzzi, Ph.D. (Univ. of Massachusetts, Amherst)
Ordering of highly structured patterned polymers into complex nanostructured materials

Assoc. Prof. Vladimir Volloch, Ph.D. (Moscow University)
Cellular and molecular biology

ADJUNCT PROFESSORS

Asst. Prof. Dale Gyure, Ph.D. (University of Colorado)
Prof. Walter Juda, Ph.D. (University of Lyons)
Electrochemistry and chemical reaction engineering

Asst. Prof. Brian Kelley, Ph.D. (M.I.T.)
Novel methods for protein purification, large-scale purifications, high-density bacterial fermentation

Prof. Gordana Vunjak-Novakovic, Ph.D. (University of Belgrade)
Transport phenomena, tissue engineering, bioreactors

Asst. Prof. Stefan Winkler, Ph.D. (Tufts University)
Protein assembly
Faculty and Research Areas

Daniel C.R. DeKee • Rheology of Natural and Synthetic Polymers • Constitutive Equations • Transport Phenomena and Applied Mathematics

Richard D. Gonzalez • Synthesis and Characterization of Supported Metal Catalysts • Fundamental Studies in Reactor Design • In-situ Spectroscopic Methods • Reactions in Organized Media

Vijay T. John • Biomimetic and Nanostructured Materials • Interfacial Phenomena • Polymer-Ceramic Composites • Surfactant Science

Daniel J. Lacks • Molecular Simulation • Thermodynamics of Condensed Phases • Dynamical Processes in Solids • Physical Properties of Polymer Materials • Density Functional Theory

Victor J. Law • Modeling Environmental Systems • Nonlinear Optimization and Regression • Transport Phenomena • Numerical Methods

Yunfeng Lu • Nanostructured and Microelectronic Materials, Sol-Gel Processes and Organic/Inorganic Hybrid Materials, Membrane Separations and Catalysts, Chemical Sensors and Biosensors

Brian S. Mitchell • Fiber Technology • Materials Processing • Composites

Kim C. O’Connor • Animal-Cell Technology • Organ/Tissue Regeneration • Recombinant Protein Expression

Kyriakos D. Papadopoulos • Colloid Stability • Coagulation • Transport of Multi-Phase Systems Through Porous Media • Colloidal Interactions

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Tulane is located in a quiet, residential area of New Orleans, approximately six miles from the world-famous French Quarter. The chemical engineering department currently enrolls approximately 40 full-time graduate students. Graduate fellowships include a tuition waiver plus stipend.
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The Faculty

L.P. Ford • Kinetics of dry etching of metals, surface science
K.D. Luks • Thermodynamics, phase equilibria
F.S. Manning • Industrial pollution control, surface processing of petroleum
C.L. Patton • Thermodynamics, applied mathematics
G.L. Price • Zeolites, heterogeneous catalysis
C.M. Sheppard • Refining reaction processes, process design, process hazard reduction
K.L. Sublette • Bioremediation, biological waste treatment, ecological risk assessment
K.D. Wisecarver • Multiphase reactors, multiphase flows

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R. Robert Balcarcel (Ph.D., Massachusetts Institute of Technology)
Biotechnology and bioengineering; mammalian cell cultures; cell life cycles; pharmaceutical production.

Robert J. Bayuzick (Ph.D., Vanderbilt University)
Solidification, nucleation; evolution of microstructure; microgravity science; physical metallurgy; containerless processing; oxide superconductor processing.

Frank M. Bowman (Ph.D., California Institute of Technology)
Air pollution; atmospheric chemistry mechanisms; gas-aerosol transport; modeling complex chemical reaction systems.

Peter T. Cummings (Ph.D., University of Melbourne)
Computational nanoscience and nanoengineering; molecular modeling of fluid and amorphous systems; parallel computing; computer-aided process design and optimization; bacterial migration in situ bioremediation.

Kenneth A. Debelak (Ph.D., University of Kentucky)
Development of plant-wide control algorithms; intelligent process control; activity modeling; effect of changing particle structures in gas-solid reactions; environmentally benign chemical processes; mixing in bioreactors.

Tomlinson Fort (Emeritus, Ph.D., University of Tennessee)
Capillarity; insoluble monolayers/L-B films; adsorption; contact angles and wetting; polymer interfaces; spreading on liquid surfaces; fine particles; flow in porous media.

G. Kane Jennings (Ph.D., Massachusetts Institute of Technology)
Surface modification; experimental molecular engineering; corrosion inhibition; microelectronics processing.

M. Douglas LeVan (Ph.D., University of California, Berkeley)
Fixed-bed adsorption; adsorption equilibria; adsorption processes (pressure-swing adsorption, temperature-swing adsorption, adsorptive refrigeration); process design.

Bridget R. Rogers (Ph.D., Arizona State University)
Nucleation and microstructure evolution of thin films; fundamentals of thin film processing for microelectronic applications (mass transport, kinetics, and effects of substrate topography on CVD, sputter deposition and etch processes).

John A. Roth (Ph.D., University of Louisville)
Chemical reactor design; industrial waste water treatment; sorption processes; chemical oxidation for waste treatment; hazardous waste management; electrochemistry.

Karl B. Schnelle, Jr. (Ph.D., Carnegie Mellon University)
Turbulent transport in the environment, control of toxic emissions and SO₂ and NOₓ from coal fired boilers, solution thermodynamics, applications of process simulation to microcomputers, supercritical extraction applied to soil remediation.

Robert D. Tanner (Ph.D., Case Western Reserve University)
In situ bubble fractionation of excreted proteins from growing baker’s yeast; selective protein recovery from a semi-solid air fluidized bed fermentation process; bubble and foam fractionation of proteins.
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Giorgio Carta, PhD, University of Delaware
Adsorption, ion exchange, biocatalysis, environmentally benign processing

Robert J. Davis, PhD, Stanford University
Heterogeneous catalysis, characterization of metal clusters, reaction kinetics

Erik J. Fernandez, PhD, University of California, Berkeley
Purification of biological molecules, protein structure, magnetic resonance imaging and spectroscopy

Roseanne M. Ford, PhD, University of Pennsylvania
Environmental remediation, microbial transport in porous media

John L. Gainer, PhD, University of Delaware
Biochemical engineering, biomedical applications, environmentally benign solvents

Andrew C. Hillier, PhD, University of Minnesota
Interfacial engineering, electrochemistry, scanning probe microscopy

John L. Hudson, PhD, Northwestern University
Reaction system dynamics, chaos and pattern formation, electrochemistry

Donald J. Kirwan, PhD, University of Delaware
Mass transfer and separations, crystallization, biochemical engineering

Matthew Neurock, PhD, University of Delaware
Molecular modeling, computational heterogeneous catalysis, kinetics of complex reaction systems

James P. Oberhauser, PhD, Univ. of California, Santa Barbara
Polymer solution flow and microstructure

John P. O’Connell, PhD, University of California, Berkeley
Molecular theory and simulation with applications to physical and biological systems
Chemical Engineering at Virginia Tech

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Research Centers and Focus Areas

Polymer Materials and Interface Laboratory
Center for Composite Materials and Structures
Center for Adhesives and Sealant Science
Center for Biomedical Engineering
Center for Self-Assembled Nanostructures and Devices
Biotechnology and Tissue Engineering
Surface Chemistry and Catalysis
Colloid and Surface Science
Computer-aided Design
Nanotechnology and Biomedical Devices
Supercritical Fluids and High Pressure Processing

Faculty . . .

Donald G. Baird (Wisconsin)
Polymer processing, non-Newtonian fluid mechanics

David F. Cox (Florida)
Catalysis, ultrahigh vacuum surface science

Richey M. Davis (Princeton)
Colloids and polymer chemistry, nanostructured materials

Kimberly E. Forsten-Williams (Illinois)
Computational bioengineering and cell and tissue engineering

Aaron S. Goldstein (Carnegie Mellon)
Tissue engineering, interfacial phenomena in bioengineering

Erdogan Kiran [Department Head] (Princeton)
Supercritical fluids, polymer science, high pressure techniques

Y. A. Liu (Princeton)
Pollution prevention and computer-aided design

Eva Marand (Massachusetts)
Transport through polymer membranes, advanced materials for separations

S. Ted Oyama (Stanford)
Heterogeneous catalysis and new materials

Len Peters [Vice Provost for Research] (Pittsburgh)
Atmospheric transport

Peter R. Rony (U.C. Berkeley)
Chemical microengineering

Ravi Saraf (Massachusetts)
Nanotechnology and biomedical devices, polymers

Joseph T. Sullivan (Minnesota)
Marketing and chemical distribution

Kevin E. Van Cott (Virginia Tech)
Biotechnology, nanotechnology

William H. Velander (Penn State)
Transgenic livestock bioreactors, biosensors

Garth L. Wilkes (Massachusetts)
Structure-property processing behavior of polymeric materials

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Web Page: http://depts.washington.edu/chemeng/

Chemical Engineering Faculty • Research Areas

Materials and Interfacial Phenomena
Stuart Adler, Ph.D., California (Berkeley)  •  Electrochemical Engineering; Solid-State Electrochemistry
G. Graham Allan (Joint), Ph.D., D.Sc., Glasgow  •  Fiber and Polymer Science
John C. Berg, Ph.D., California (Berkeley)  •  Interfacial Phenomena; Surface and Colloid Science
Samson A. Jeneke, Ph.D., Minnesota  •  Polymer Science & Engineering; Optoelectronic/Photonic Materials
Shaoyi Jiang, Ph.D., Cornell  •  Interfacial Phenomena and Nanotechnology
René M. Overney, Ph.D., Basel, Switzerland  •  Nanoscale Surface Science and Polymer Physics
Daniel T. Schwartz, Ph.D., California (Davis)  •  Electrochemical Engineering; Electrolytic Thin-Film Science
James C. Seferis, Ph.D., Delaware  •  Polymeric Composites; Manufacturing and Teaming
Eric M. Stuve, Ph.D., Stanford  •  Electrochemical Surface Science; Fuel Cell Electrocatalysis

Biochemical Engineering and Bioengineering
François Baneyx, Ph.D., Texas (Austin)  •  Biotechnology; Protein Technology; Biochemical Engineering
David G. Castner, Ph.D., California (Berkeley)  •  Biomaterial and Biomolecule Surface Analysis, Self-Assembled Monolayers
Thomas A. Horbett (Joint), Ph.D., Washington  •  Biomaterials; Peptide Drug Delivery
Mary E. Lidstrom, Ph.D., Wisconsin  •  Environmental Biotechnology; Molecular Bioengineering
Buddy D. Ratner (Joint), Ph.D., Brooklyn Polytechnic  •  Biomaterials; Polymers; Surface Characterization

Information and Process Technology
Bruce A. Finlayson, Ph.D., Minnesota  •  Mathematical Modeling
Bradley R. Holt, Ph.D., Wisconsin  •  Process Design and Control
N. Lawrence Ricker, Ph.D., California (Berkeley)  •  Process Control and Optimization

Environmental Technology
E. James Davis, Ph.D., Washington  •  Colloid Science; Aerosol Chemistry and Physics; Electrokinetcs
Barbara Krieger-Brockett, Ph.D., Wayne State  •  Reaction Engineering

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Graduate Programs in Chemical Engineering

Master's and doctoral programs in WSU's Department of Chemical Engineering are closely aligned with industry and government interests that often lead to professional opportunities. Our emphases in bioengineering, environmental restoration, and hydrocarbon processing involve you in such projects as biotreatment of hazardous contamination, diagnostic medical devices, and converting natural gas to useful products. Our Center for Multiphase Environmental Research provides interdisciplinary opportunities to solve complex problems at the interface of air, water, and earth.

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Financial Assistance

All full-time ChemE graduate students at WSU receive financial support to help cover costs of education, living, and insurance.

Student Life

Pullman's residential campus offers single and family housing for graduate students. Families with children have access to highly rated K-12 schools. Outdoor and recreational activities abound in the nearby mountains, rivers, and forests. Students may belong to the Graduate and Professional Student Association and numerous other student societies.

About WSU

Washington State University is a land-grant research university founded in Pullman in 1890. It enrolls more than 20,000 students at four campuses, and numerous Learning Centers throughout the state. As many as 100 advanced degrees are offered from 70 graduate programs within its eight colleges.

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WSU Graduate School
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Graduate Study in Chemical Engineering at Washington University

Master’s and Doctoral Programs

M. Al-Dahhan  ▶ Chemical Reaction Engineering, Multiphase Reactors, Mass Transfer, Process Engineering
L. Angenent  ▶ Biological Waste Conversion, Bioaerosol Control, Environmental Engineering
P. Biswas  ▶ Aerosol Dynamics, Environmental Engineering
M. P. Dudukovic  ▶ Multiphase Reaction Engineering, Tracer Methods, Environmental Engineering
J. T. Gleaves  ▶ Heterogeneous Catalysis, Surface Science, Microstructured Materials
J. L. Kardos  ▶ Composite Materials and Polymer Engineering
B. Khomami  ▶ Rheology, Polymer and Composite Materials Processing
P. A. Ramachandran  ▶ Chemical Reaction Engineering, Boundary Element Methods
R. Sureshkumar  ▶ Applications of transport processes involving complex polymeric and colloidal fluids
J. Turner  ▶ Environmental Reaction Engineering, Air Quality Policy and Analysis, Air Pollution Control

For Information Contact

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Washington University encourages and gives full consideration to application for admission and financial aid without respect to sex, race, handicap, color, creed or national origin.
Sandro R.P. da Rocha, Ph.D., UT Austin, 2000
Nanostructured materials from self-assembled amphiphiles in conventional and compressible media • Drug delivery and sensing devices • Molecular modeling and computer simulations

Esin Gulari, Ph.D., Caltech, 1973
Thermodynamics and transport properties of polymer solutions and melts • Processing of polymers with supercritical fluids • Light scattering based particle and drop sizing techniques

Yinlun Huang, Ph.D., Kansas State, 1992
Pollution prevention and waste minimization • Process design and synthesis

Rangaramanujam Kannan, Ph.D., Caltech, 1994 — Dynamics of polymeric systems and interfaces • Rheo-optical spectroscopy and scattering techniques

Ralph Kummler, Ph.D., John Hopkins, 1966 — Modeling of combined sewer overflows and sediments • Chemical kinetics • Computer simulation

Joseph F. Louvar, Ph.D., Wayne State, 1983 — Process design and safety • Risk analysis

Charles Manke, Ph.D., California, Berkeley, 1983 — Polymer processing and rheology • Molecular dynamics and kinetic theory of polymeric liquids

Guang-Zhao Mao, Ph.D., Minnesota, 1994 — Optoelectronic properties of thin films and crystals • Self-assembly of polymers and surfactants • Colloidal stability of waterborne paints • Real time imaging of surface phenomena at the molecular level

Howard Matthew, Ph.D., Wayne State, 1992 — Tissue engineering and biomaterials • Artificial organ substitutes

Simon Ng, Ph.D., Michigan, 1985 — Heterogeneous catalysis • Spectroscopic and thermal analysis of material surfaces

Jeffrey Potoff, Ph.D., Cornell, 1999 — Molecular simulation • Phase behavior • Complex systems

Susil Putatunda, Ph.D., IIT Bombay, 1983 — Effects of microstructure on fatigue • Fracture toughness • Creep in metals and alloys

Erhard Rothe, Ph.D., Michigan, 1959 — Applications of high-powered UV lasers • Machining of electronic chips • Diagnostics of internal combustion

Steven Salley, Ph.D., Detroit, 1976 — Biochemical/medical engineering • Design of artificial organs • Immobilized enzyme reactors

Gina Shreve, Ph.D., Michigan, 1991 — Environmental and biochemical applications • Microbially mediated biotransformations

Paul VanTassel, Ph.D., Minnesota, 1993 — Shape selective catalysis • Protein adsorption and bioseparations

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Nicholas L. Abbott
Biotechnology, interfacial phenomena, colloid chemistry, soft materials, nanotechnology

Juan de Pablo
Molecular thermodynamics, statistical mechanics, polymer physics

James A. Dumesic
Kinetics and catalysis, surface chemistry

Michael D. Graham
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Immobilized enzyme technology, photocatalysis, kinetics and catalysis, membrane separations

Daniel J. Klingenberg
Colloid science, complex fluids, suspension rheology

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David M. Lynn
Polymer synthesis, biomaterials, functional materials, gene and drug delivery, controlled release, high-throughput synthesis/screening

Manos Mavrikakis
Thermodynamics, kinetics and catalysis, surface science, computational chemistry, electronic materials, fuel cells

Regina M. Murphy
Biomedical engineering, protein-protein interactions, targeted drug delivery

Paul F. Nealey
Polymers, thin films, nanofabrication, cell-substrate interactions

Sean P. Palecek
Cellular engineering, biosensors, biochemical reaction kinetics

James B. Rawlings (Chairman)
Process modeling, dynamics and control, particle technology, crystallization

W. Harmon Ray
Reaction engineering, polymerization processes, process dynamics and control

Thatcher W. Root
Surface chemistry, catalysis, solid-state NMR, and protein chromatography

Eric V. Shusta
Drug delivery, protein engineering, biopharmaceutical design

Ross E. Swaney
Process design, synthesis, modeling, and optimization

John Yin
Molecular virology, bio-informatics, pre-biotic chemistry, systems biology
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- Bioseparations
- Bacterial Adhesion to Surfaces

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- Surface Science of Catalysis
- Supported Molten Metal Catalysis
- Zeolite Catalysis
- Computational Fluid Dynamics
- Catalytic Microkinetics

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- Neutron Scattering from Aerosols
- Nucleation and Phase Transitions
- Environmental Catalysis
- Fuel Cells/Catalytic Reforming
- Renewable Fuels and Chemicals

**Process Analysis and Control**
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- Process Condition Monitoring, Fault Detection and Diagnosis

**Faculty**

**Terri A. Camesano** • Ph.D., Penn State

**William M. Clark** • Ph.D., Rice

**Ravindra Datta** • Ph.D., U.C. Santa Barbara

**David DiBiasio** • Ph.D., Purdue

**Anthony G. Dixon** • Ph.D., Edinburgh

**Nikolaos K. Kazantzis** • Ph.D., Michigan

**Yi Hua Ma** • Sc.D., MIT

**Steven L. Matson** • Ph.D., U. Pennsylvania

**Fabio H. Ribeiro** • Ph.D., Stanford University

**Robert W. Thompson** • Ph.D., Iowa State

**Barbara E. Wyslouzil** • Ph.D., Caltech

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Menachem Elimelech, Ph.D. Johns Hopkins
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Gary L. Haller, Ph.D. Northwestern
Csaba G. Horváth, Ph.D. Frankfurt
Michael Loewenberg, Ph.D. Cal Tech
Lisa D. Pfefferle, Ph.D. Pennsylvania
Daniel E. Rosner, Ph.D. Princeton
Mark Saltzman, Ph.D. MIT
John Y. Walz, Ph.D. Carnegie Mellon

Adjunct Professors
• F. Peter Boer
• Donald M. Crothers
• William S. Hancock
• Joseph J. Pignatello
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Joint Appointments
• Thomas Graedel (School of Forestry & Environmental Studies)
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M.S. and Ph.D. Degree Programs

Faculty and Research Interests

Calvin H. Bartholomew (Stanford) • kinetics and catalysis
Larry L. Baxter (BYU) • combustion of fossil and renewable fuels
Merrill W. Beckstead (Utah) • propellant combustion, modeling
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John H. Harb (Illinois) • coal combustion, electrochemical engineering
William C. Hecker (UC Berkeley) • kinetics and catalysis
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Process and plant design  
Bruce A. Barna: Professor • PhD, New Mexico State, 1985

Demixing-polymerization, polymer materials  
Gerard T. Caneba: Associate Professor • PhD, California-Berkeley, 1985

Process control, neural networks, fuzzy logic control  
Tomas B. Co: Associate Professor • PhD, Massachusetts-Amherst, 1988

Chemical process safety  
Daniel A. Crowl: Professor • PhD, Illinois, 1975;  
Herbert Henry Dow Chair of Chemical Process Safety

Excited state chemistry and transport processes  
Edward R. Fisher: Professor • PhD, Johns Hopkins, 1965

Environmental reaction engineering  
Jason M. Keith: Assistant Professor • PhD, University of Notre Dame, 2000

Process control, energy systems  
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Polymer rheology, flow instabilities, complex fluids  
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Joseph H. Holles: Assistant Professor • PhD, University of Virginia, 2000

Environmental thermodynamics  
Tony N. Rogers: Associate Professor • PhD, Michigan Tech, 1994

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