ONTOLOGY-BASED APPROACH TO SIMULATION WITH APPLICATION TO CITRUS WATER AND NUTRIENT MANAGEMENT

By

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To my advisor, my parents and my girl friend

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After beginning a study at graduate school level, it was not easy to get an academic result. I always liked pursuing new topics and learning new technologies for the future. I would like to thank my advisor, Dr. Howard Beck. It was lucky for me to meet and collaborate with him. His ideas and advice stimulated me to achieve my research objectives. His passion for research and intellectual insights were motivating factors in my work. I would also like to extend my appreciation to my cochair, Dr. Kelly Morgan, and committee member, Dr. James Jones for their encouragement and guidance. Finally, I take this opportunity to thank my parents and my girl friend, Kyungmi.

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Abstract of Thesis Presented to the Graduate School
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Simulation in agriculture and natural resource management is a popular methodology for studying environmental and agricultural system problems. Traditionally, building a simulation is treated as a software engineering problem, and simulations are implemented through manual coding in a particular programming language. Problems of implementing a model and developing a simulation system include difficulties in managing and reusing existing models and simulation system because it is hard to understand the detailed specification of the system model when it is written in a specific program language. Also, model specification may be lost during the programming process, and it is difficult to maintain documentation describing the system because documents are external to the programming process. Visual simulation environments reduce the burden of programming, but there are still problems related to sharing knowledge about the system.

An ontology is an explicit specification of a conceptualization, which can be used to create a formal representation describing and categorizing concepts and relationships among the concepts in a particular domain. Ontologies enable sharing through a common understanding of

the structure of information in a domain, enhance reuse of domain knowledge, and make domain assumptions explicit by separating domain knowledge from operational knowledge. While ontologies have been used in many domains as a way to represent generic domain knowledge, an ontology-based approach to modeling and simulation in the domain of agriculture and natural resources has not been well explored.

In this thesis, ontology-based modeling and simulation methodologies and tools are developed which can be used by modeler and researcher to build mathematical models and simulations, and in the process provide a better way of representing knowledge about models, improve sharing and reusability, and provide a new basis for analysis of models and model elements. These tools are applied to develop CWMS (Citrus Water Management System) model as a way of evaluating the effectiveness of the proposed approach. An ontology for CWMS was developed using the Lyra ontology management system. Tools that were developed for building ontology-based models and simulations include the SimulationEditor, which is a high level modeling environment for designing a system structure based on a graphic interface, and the EquationEditor, which is a tool for designing a model in equation form and representing knowledge of each equation and symbol by using the underlying ontology.

The main contribution of this thesis is the application of ontology-based techniques to modeling and simulation in agriculture and natural resource domains through the development of these tools and their application to a particular problem.

CHAPTER 1
INTRODUCTION

Simulation in agriculture and natural resource management is a popular methodology for studying environmental and agricultural system problems. There has been much works on modeling crop, soil, water and nutrients in specific research domains (Peart and Curry, 1998), and recently interests in modeling and simulation methodology have moved to a reuse of existing models and simulation systems for building a large system (Leon et al., 2002). This will require better communication of model structure and components to the community of model builders who collaborate on an international level.

Traditionally, modeling and simulation are tasks based on programming to implement the processes necessary for operating or solving a model to mimic real system behavior within a particular domain. General processes include developing computer logic and flow diagrams, writing computer code, and implementing code on a computer to produce desired outputs (Peart and Curry, 1998). While visual simulation, an approach to modeling and simulating based on building diagrams of system components, is an intuitive and simple way to do this, programming languages are still used for developing more complicated simulating system because there are limitations on representing ability.

Classical problems of implementing a model and developing a simulation system include difficulties in managing and reusing existing models and system that are written in a particular programming language. Understanding a program written in a specific program language is difficult because it is too hard to get information about the detailed specification of the system. Usually this information is lost during the transformation to the program code (Furmento et al., 2001) and documents describing the model are physically separated from the implementation. Although documentations such as a paper or a manual and descriptions in program code partially

cover the gap in understanding, often documentation contain inaccurate information, the document description does not adequately explain the entire system in detail, and it is difficult to maintain both the system implementation and supporting documents.

Some simulation programs, such as Stella (Steed, 1992) and Simile (Muetzelfeldt and Massheder, 2003), solve many of these problems by providing a visual modeling environment and supporting embedded simulation and reporting tools. Visual environments eliminate or greatly simplify the process of programming and make models much easier to design and develop compared to hand coding of models in a traditional programming language, but sharing of modeling products is still restricted because these tools use proprietary model representation formats. Program source code is assumed to be an easily reusable, executable, flexible and expandable way of sharing models, so that even visual programs provide the functionality for generating program source code in a specific programming language from the models. However, the problem is that different symbols and mathematical expressions are used for the same concepts at the different viewpoints of modeller, so that there are enormous overlaps of concept and interaction in models. These issues motivate research on ways to explicitly represent the knowledge in a model (Lacy and Gerber, 2004; Cuske et al., 2005).

An ontology is an explicit specification of a conceptualization (Gruber, 1995), which has been applied to create a formal representation describing and categorizing concepts and the relationships among concepts in a particular domain. Classes are main elements of an ontology, which describes concepts in the domain, and properties represent various features and attributes of the concept. There is no single correct ontology of a particular domain, and several different ontologies might exist depending on the task or role of ontology in that domain (Guarino, 1997).

Ontologies are based on object-oriented design, and thus appear to be similar to object-oriented programming (Rumbaugh et al., 1991) and Unified Modeling Language (UML) (Booch et al., 1997), but they are different in several important aspects (Noy and McGuinness, 2001). In object-oriented programming, classes are regarded as types for instance, and each instance has one class as its type, whereas, ontologies declare that classes are regarded as sets of individuals, and each individual can belong to multiple classes. Also, in object-oriented programming classes have behavior defined through functions and methods. Ontologies are not programming languages, and classes in ontologies make their meaning explicit without any methods (Knublauch et al., 2006). This is an important distinction, because methods are coded using a programming language and thus behavior is not explicitly represented and is largely unknown except through manual analysis or processing of the program code.

Ontologies enable sharing of a common understanding of the structure of domain knowledge, reuse of domain knowledge, making domain assumptions explicit, separating domain knowledge from operational knowledge, and analysis of domain knowledge (Noy and McGuinness, 2001). These capabilities can be applied to the modeling and simulation domain. In recent studies, it has been determined that ontologies increase the potential for interoperability, integration, and reusability of simulation models (Miller et al., 2004). Also, ontologies can be a useful for the description, development, and composition of simulation models, and for mapping of input/output data.

In the domain of agriculture and natural resources, an ontology-based approach to simulation, which represents a model with ontology concepts, can address several problems with current methodology used to develop simulations. Whereas ontologies have been used as a way to build generic domain knowledge, only recently have attempts been made to develop an

ontology-based approach to modeling and simulation. There have been many well-studied physical processes in agriculture and natural resources, and different perspectives on the problems led to development of many similar but varied models. Also, as the problems in the agricultural domain has been diversified and widened to the environmental and natural resource domain, requirements increase for modeling and simulation to solve multi-scale problems and to integrate existing models rather than to develop new models for specific problems (Ewert et al., 2006). Therefore, a comprehensive management system to manage these diverse models is needed.

The objectives of the research presented in this thesis are twofold; 1) to develop ontology-based methodologies and tools to be used by modeler and researcher for building mathematical models and simulation in the agricultural and natural resource domain and 2) to apply the methodology and tools to develop a sophisticated soil water and nutrient model for evaluating the efficiency of the proposed ontology-based simulation approach.

Several software components were developed as a part of this research. The SimulationEditor is a high-level modeling environment for specifying a system structure based on a graphical interface. The EquationEditor is a tool for describing a model in equation form and for representing knowledge of the equations and symbols used in the model. The Citrus Water Management System (CWMS) is an application program applying the ontology-based simulation methodologies. CWMS provides growers with site-specific optimal nutrient and irrigation recommendations by simulating models based on soil characteristics, nutrient uptake patterns and weather conditions. The motivations behind this research are 1) to create methodologies based on ontology techniques to explicitly represent models and related mathematical expressions of parameters, 2) to create an environment for building reusable and

sharable model knowledge, 3) to provide the core representational facilities of structure diagrams, symbols/equations and descriptions, 4) to use the ontology as a database for systematically storing models and model elements, and 5) to assess the value of ontology-based simulation approach by applying it to modeling and simulation of CWMS.

The main contribution of this research includes the development of a methodology of ontology-based simulation, which provide two main software tools; the SimulationEditor and EquationEditor. These tools were used successfully to design and build a model and simulation for citrus water and nutrient management.

CHAPTER 2
LITERATURE REVIEW

Ontology Based Simulation

Recently, ontologies have received much attention for implementing mathematical models and building simulation systems. The aim of adapting ontologies for simulation systems is similar across various projects, but the design and implementation of an ontology is different depending on the problem domain (Benjamin et al., 2006).

Miller et al. (2004) noted that for modeling and simulation an ontology provides standard terminology which increases the potential for application interoperability and reuse of simulation artifacts. Furthermore, semantics represented in an ontology can be used for discovery of simulation components, composition of simulation components, implementation assistance, verification, and automated testing. He proposed a web-accessible ontology for discrete-event modeling (DEMO), which defines a taxonomy of models by describing structural characterization (State-oriented, Event-oriented, Activity-oriented, and Process-oriented models) and a model mechanism explaining how to run the model.

Although Miller focused on the creation of an ontology for general stochastic models such as Markov Processes or Petri Nets, Fishwick and Miller (2004) placed emphasis on capturing mostly object or instance-based knowledge. He presented a software framework, RUBE, which provides an integration method for the phenomenon of model and model object, and multiple visual modes of display to provide interfaces for developing dynamic model. 3D visualization (Park and Fishwick, 2005) is used to animate the responses of models. An ontology is used to define a schema of simulation model types and models, and a sample air reconnaissance scene is represented with the Web Ontology Language, OWL.

Some studies (Raubel and Kuhn, 2004; Cuske et al., 2005) addressed the use of a static ontology (Jurisica et al., 2004), which describes static aspect of the world focusing on entities, and in a simulation focusing on the data and the rules governing the simulation. They understood that data used by a model is a key characteristic of semantics, which an ontology of an information system should define, rather than building an ontology which is independent from simulation form or contents. For example, ontology-based task simulation (Raubel and Kuhn, 2004) uses an ontology for evaluating the usability and utility of a task or data for the decision-making process. JOntoRisk (Cuske et al., 2005), which is an ontology-based simulation platform in risk management domain, proposed a three level ontology hierarchy, consisting of a meta risk ontology, a domain risk model, an a risk knowledge base. Especially, a meta risk ontology defines the common characteristics of risk management simulation with world elements which are affected by risk, functional dependencies between world elements, random elements which are input parameters, and stochastic dependencies between random elements. Models refined from a meta risk ontology at a domain risk model have a strength on validating or reviewing the meta structure of simulation system.

SEAMLESS (Ittersum et al., 2007) is a component-based framework for agricultural systems which is used to assess agricultural and environmental policies and technologies from the field-farm level to the regional level in the European Union. For SEAMLESS, an ontology is designed to relate different concepts from models, indicators, and source data at different level, and to structure domain knowledge and semantic meta-information about components for retrieving and linking knowledge in components. It also is used to check the linkage between components through input and output variables in the system. An ontology, the Model Interface Ontology, encapsulates knowledge of biophysical agricultural models. Static and dynamic

models are included, and the system dynamics approach which describes a system with stocks and flows are applied to conceptualize models. This approach to model ontologies provides advantages which include the simplicity of model representation by using states, inputs, and outputs, but it has limits on representing mathematical expressions of models and manipulating models to build complex system. SEAMLESS does not attempt to represent models based on their mathematical equation form in the ontology.

A web-based simulation using an ontology in the hydrodynamic domain (Islam and Piasecki, 2004) is used to solve the governing equations for a two dimensional hydrodynamic model. A model ontology is created to describe a numerical model by defining a specific metadata set that describes hydrodynamic model data, which is used to search and retrieve metadata information. This approach gives an advantage in prescribing geospatial data and model data at model level. However, there is a limitation on building and describing model equation, and model should be provided in a specific form required by the system.

The Modelling Support Tool, MoST (Scholten et al., 2007), a software framework for supporting the full modeling process, used an ontological knowledge base (KB). The KB is a collection of knowledge on modeling for various domains of water management, which is developed by domain experts. They adopt ontological approaches to develop a knowledge structure, store the knowledge to the KB following an ontological structure, and build software applications to use the KB.

Model-Based Approach to Ontology

A model base is a massive collection of models and model components. As the number and scale of models grow, the conceptualization and role of models within a problem domain becomes wider and more complex. Some models may be considered as an integration of related unit process models, while previously a single-process model itself was enough to make a

simulation. As various concepts are applied to develop an ontology to build a model, it becomes a challenge to develop an ontology which contains different categorical views and which can be used to manage models (Ewert et al., 2006).

As there are diverse aspects to understanding and describing models in a specific domain, it is not easy to reuse existing model with other models or to replace a model with other models which satisfies the same requirements of input data and parameters. In large-scale problem domains, the need increases for comparing and evaluating models in order to locate an adequate model for a given environment. Lu et al. (2004) compared different models for estimating leaf area, and Eitzinger et al. (2004) performed a evaluation and comparison of water balance components in different models. To provide a model base, there is an effort to develop a set of crop models for a various crops and integrating models with farm decision support system (Reddy and Anbumozhi, 2004).

A modular approach to model development (Jones et al., 2001) introduced by categorizing and organizing crop model with biological, environmental and management module as a form of software component, which is an executable unit of independent production, in the agro-ecological domain (Donatelli et al., 2006a,b). Although they offer useful ideas on categorizing and reusing the existing components, they cannot fully address the difficulties of model management because they are developed for a specific program environment such as a FORTRAN and C++.

These difficulties make it important to organize a model base that can compare similar yet different models and components. It will be useful to categorize and organize models into a well designed framework for the purpose of locating and reusing models. There have been many

efforts to construct model bases, and recently ontologies are being applied to this purpose because of their strength in categorizing and organizing knowledge.

Watershed modeling is considered as aggregating a complex system of unit hydrology and chemical processes, which includes precipitation, infiltration, evapotraspiration and erosion. Haan et al. (1982) presented a collection of generic processes and practical models which have been used to study the hydrologic cycle in watersheds. MoST (Scholten et al., 2007) developed a model ontology following the structure of components in the simulation system to manage models, and it made it possible to switch one model with other models in the same process level for seeking appropriate model composition resulting in an adaptable conclusion. But, the complexity of the representation is not enough to describe detailed processes, and the large scale of the system makes it difficult to manage models. Although it enables model switching, it is limited to simple models.

Some research to support a decision making process over a farm or water management area provides a library of models that allows a user to build up a simulation system easily with unit process models (Athanasiadis et al., 2006; Scholten et al., 2007). The libraries contain ontologies for storing the farm management model knowledge which is gathered from references or experts. Usually, in those cases, models can be repeatedly used for building up a system, but there are limitations in modifying or creating another model from known models, even models which the system provides. A simple case is that an ontology is not designed originally to allow any manipulation, and this problem is usually found at the multi-scale simulation model.

To solve the difficulties of managing models in ontologies, the SEAMLESS built a model ontology which contains multi-scaled categories over an agricultural domain, and provided an interface for managing model knowledge, which is an authoring tool supporting to create and

categorize models and to modify model knowledge (Rizzoli et al., 2004; Athanasiadis et al., 2006). Model knowledge appearing in the interface includes a model description, creator, a components list using selected model, and model elements. Model elements describe model input, output, and state variables which can be used to select models. Although input, output, and state variables can be dictated in the interface, it does not represent the detailed and complicated mathematical relations between them. A model ontology just contains knowledge of concepts related with a mode as input/output or state variables, and their mathematical relationship is coded or internally described in the system. To resolve these limitations, it is required to focus on designing a model ontology based on their mathematical representation and meaning explicitly.

CHAPTER 3
ONTOLOGY-BASED APPROACHES AND TOOLS FOR SIMULATION

This approach to ontology-based simulation focuses on model authoring facilities and simulation execution tools. In the following sections, supporting technologies which enable modelers to develop ontology-based simulations are described. The SimulationEditor and the EquationEditor are the two main tools for building a simulation system. Additionally, system validation tools, a symbol referencing flow diagram and a sensitivity analysis tool, which provide facilities for model analysis, are also described.

Background Technologies

Ontology

An ontology is a formal explicit representation of concepts in a specific domain (Gruber, 1995). Specifically, in computer science and information science ontology is considered to be a data model which represents a collection of concepts in a domain and relationships between those concepts. To form the representation of a data model, several elements are considered including class, individual, attribute, and relationship.

An instance (also known as an object or individual) is a concrete (e.g. people) or abstract (e.g. number) object in an ontology, and a class (concept) is an abstract group of similar objects in the domain, which may contain individuals, other more specific classes or combination of both. An attribute characterizes and describes a property of a class, and has at least a name and a value. Since an important use of attributes is to describe the relationships between objects, a relationship is an attribute whose value is another object in the ontology. The power of ontology comes from the flexibility in describing relationships. A common relationship is the subsumption relation such as ‘is-superclass-of’, ‘is-subclass-of’, which defines classes that are more general or specific than other classes of instances, and the relation part-of which represents how instances

combine together to form composite instances (Noy and McGuinness, 2001). The procedure of developing an ontology consists of defining classes and individuals, arranging the classes in a taxonomic (subclass-superclass) hierarchy, defining attributes and describing allowed values for these attributes, and filling in the values of attributes for instances (Guarino, 1997).

Ontology Management System (OMS)

The Lyra ontology management system (Beck, 2007) is used to build an ontology for modeling, to develop tools for entering symbols and equations into the ontology, and to implement the tools that execute simulation and show their results. Lyra is an object database management system for ontology data, which provides a data model of the linguistic and semantic concepts in an ontology based on a formally defined ontology language. It supports management of large collections of ontology objects, reasoning facilities that help in organizing and searching for concepts, visual ontology design tools, and application development tools. It is designed as a server/client system implemented with Java. Clients communicate remotely with a database located on a remote server through Java Remote Method Invocation (RMI) technology.

Model and Simulation Ontology

The model and simulation ontology is developed with Lyra for building conceptual diagrams graphically, representing mathematical models with symbols and equations, and describing information related to each symbol and equation. It consists of two parts, system design and model implementation (Figure 3-1).

In order to build a simulation system diagram, three classes (project, diagram, graphic elements) are created in the model ontology. System design is a process of building a conceptual or structural diagram of concepts and relations between them with graphic elements, and each diagram belongs to a specific project. A graphic element may represent a set of equations

describing a detail (or independent) process in a complete set of models or explain a structural relationship which means a physical part of a system.

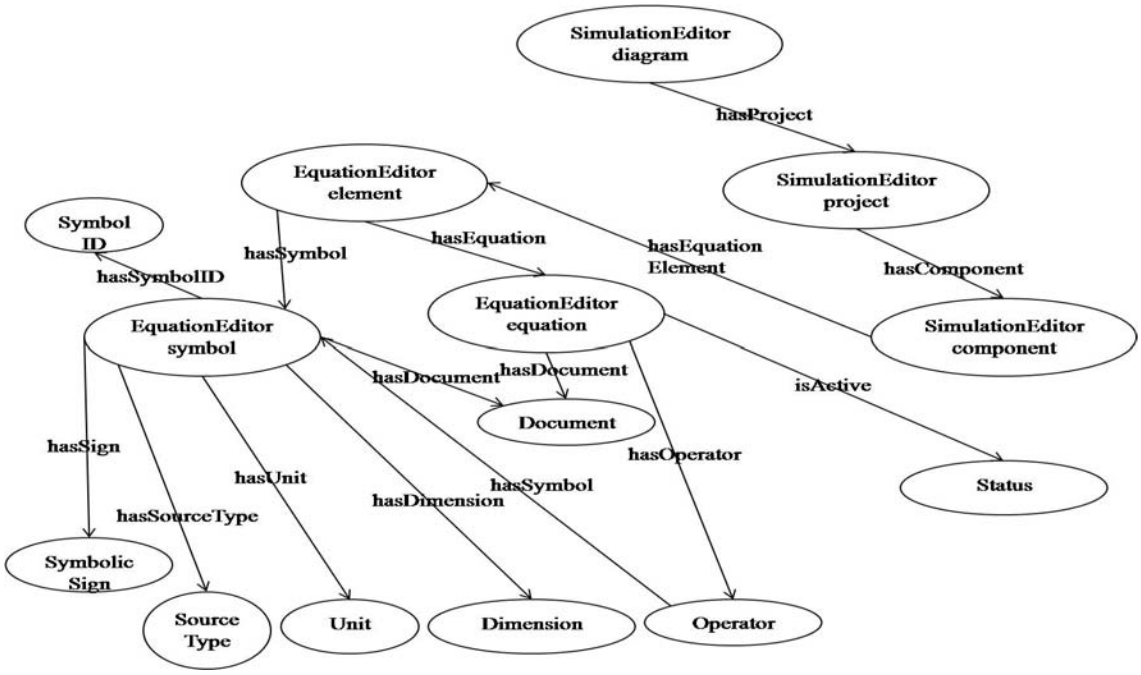


Figure 3-1. Concepts and relations in model ontology for simulation

Classes for representing a mathematical expression focus on symbols and equations. An equation includes knowledge about mathematic operators' hierarchical relations, symbols, and meaning. One challenge in describing a symbol is that a term for the symbol composing an equation may be used in other equations with the same or different meaning. A symbol (concept) is unique but having multiple names (terms) which are mapped to symbols, and enables reusability of the symbol in different models. A symbol may have one of three different sources for its value; constant, equation, and database.

EquationEditor

The EquationEditor is a tool for creating equations associated with a model, and properly defining symbols appearing in these equations. It provides a facility for creating, browsing, and inspecting all equations, symbols, and units appearing in the model. It uses an interface that resembles other equation editors such as Microsoft Office Equation Editor (Microsoft, 2003) and MatyType (MathType, 1996), but differs significantly because all the symbols in equations and equations are represented internally by using ontology objects. This provides a way to represent the meaning of equations and symbols that is not possible with other equation editors.

Equation Object Model (EOM)

The Equation Object Model (EOM) is an intermediate collection of basic objects that represents information describing a mathematical expression and communicates with the Lyra physical storage manage to retrieve and store equations and symbols (Figure 3-2). The main purpose of EOM is to represent the elements of mathematical expressions. Operators and other symbols of an equation are objects of the two main classes, MathTemplate and MathPrimitive. MathTemplate defines a type of operator and a collection of arguments. Character symbols and numerical symbols are subclasses of MathPrimitive. MathSymbol objects representing a symbol contain two properties; a linguistic-level property and a programmatic-level property. Symbol (in multiple terms), symbolID, and definition are linguistic-level properties. Programmatic-level contains three properties; source, matrixType, and matrixSymbolUsage. A property source represents the origin of the numerical value of the symbol (equationType, databaseType, or constant). If the symbol is a matrix, property matrixType gives the matrix dimensions. A flag, "constant" or "variable", is a value representing matrixSymbolUsage property. The value "constant" means that the value never changes, whereas "variable" means the value can change.

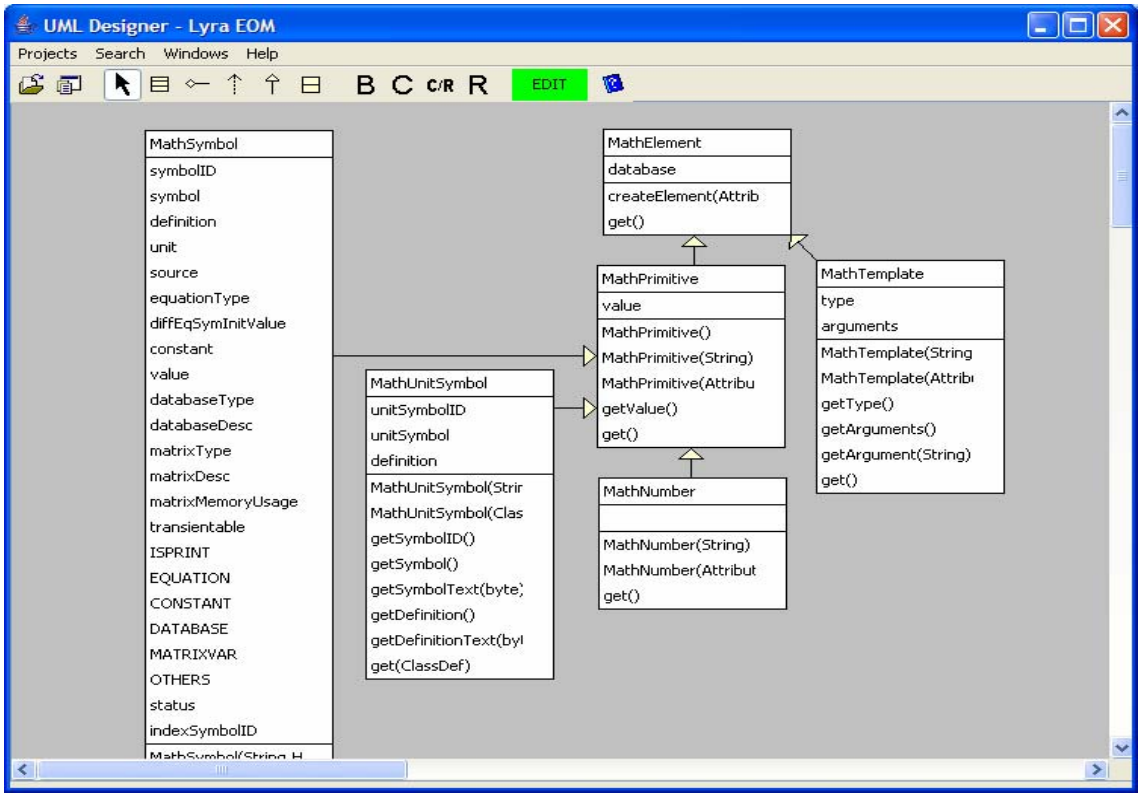


Figure 3-2. Class diagram of Lyra equation object model retrieving instances of model ontology

Components of the EquationEditor

The EquationEditor has three sub-editors, Symbol Editor, Mathematical Statement Editor, and Unit Editor, to create and maintain symbols, equations and symbol units.

Symbol Editor (Figure 3-3) is an editor for individual symbols appearing in equations and includes a symbolic expression of a symbol, a quantity of measurement, and a description of the linguistic and programmatic properties of the symbol. A symbol is implemented as a class in the ontology, which has a unique meaning within a specific domain. Often, the same symbolic character (term for the symbol) is used over different domains, but is used in different ways and has different meaning. Since a symbol has a distinguishing identifier representing a specific

concept in the ontology, a use of the same term for different symbols is permitted, and the domain ontologies can be used to resolve their ambiguous meaning.

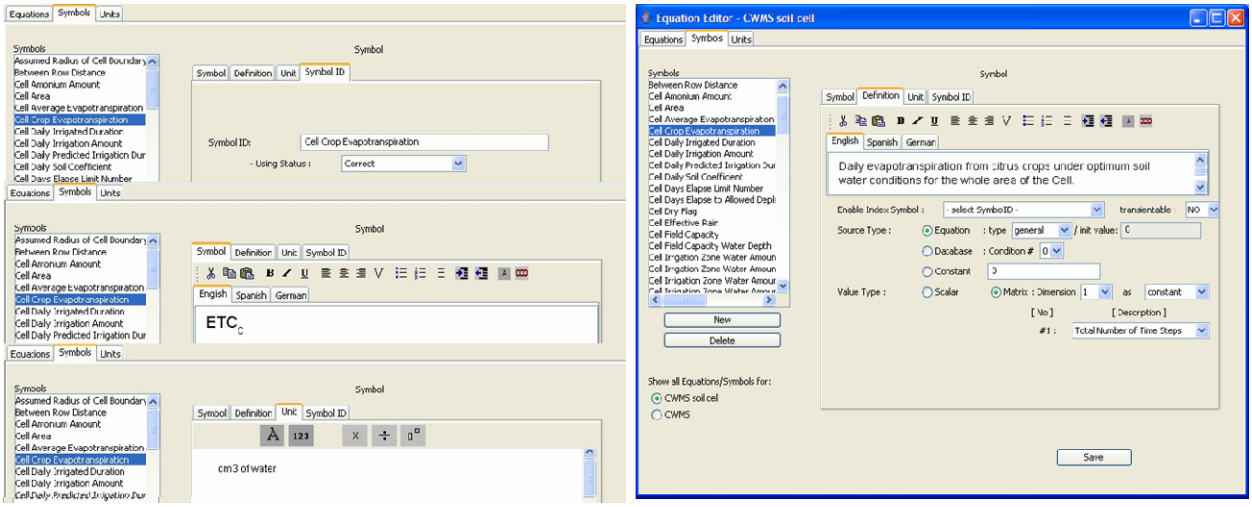


Figure 3-3. Features of the symbol editor in the EquationEditor: symbol ID, symbol, unit and description of Cell Crop Evapotranspiration

The value of a symbol is determined by one of three methods: from an equation, from a database, or from a constant which is directly assigned to the symbol. In the case where the symbol value is determined by an equation, there must be an equation in the database in which this symbol appears alone on the left side. To obtain the value from the database, some constraints may be required in order to locate and query a database to obtain the value (e.g. a current time and a soil layer number for querying a soil temperature at a specific date), and these constraints can be specified as a part of the symbol's properties (Figure 3-4).

Symbols can also be arrays, when a symbol can be used in different discrete intervals in space and time. For example, soil water content can be expressed in different soil layers which occur in different soil profiles, characterized by the depth from the soil surface, the soil profile number and time.

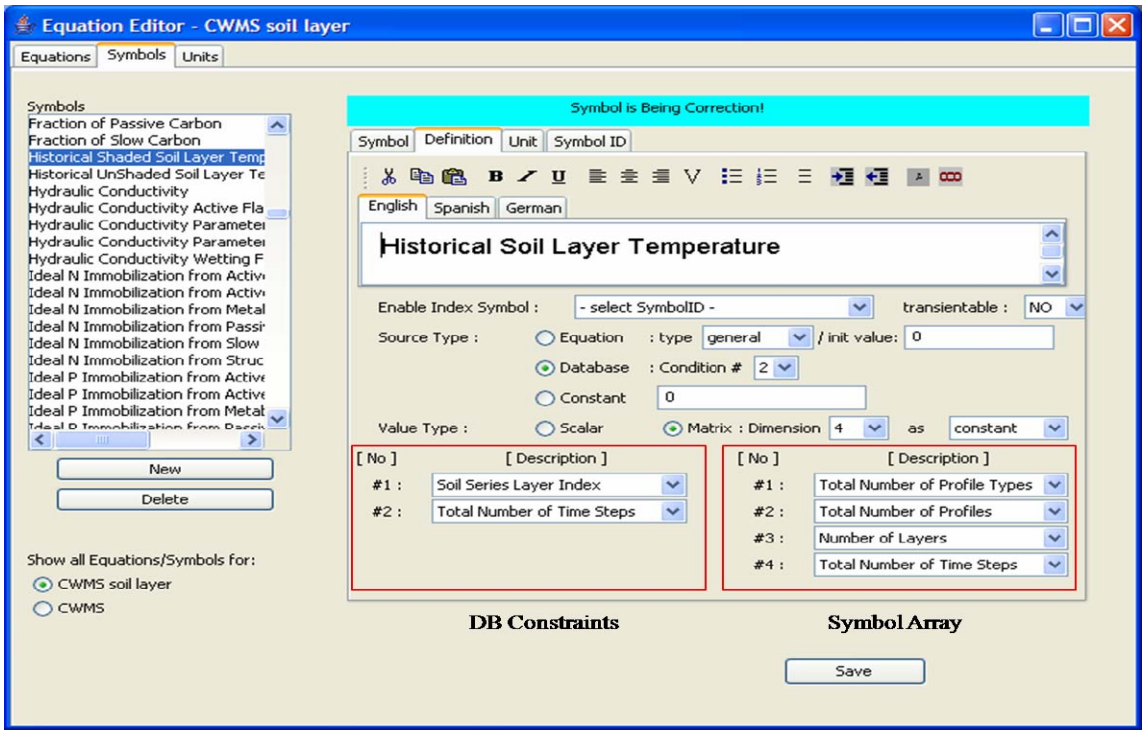


Figure 3-4. Database constraints and array dimension description of a symbol

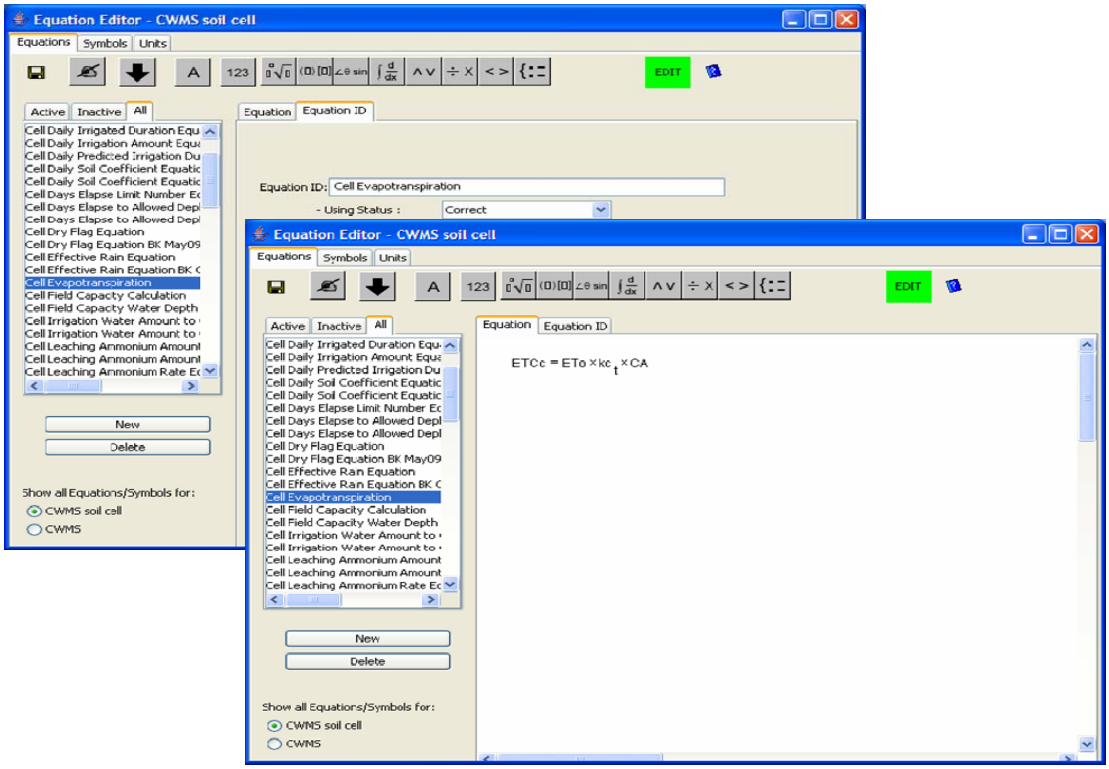


Figure 3-5. Equation ID and equation of Cell Evapotranspiration in the mathematical statement editor

The mathematical statement editor is designed to graphically create an equation from existing symbols and mathematical operator templates (Figure 3-5). An equation is an expression that has a hierarchical tree data structure composed of symbols and operators. The equal operator is the root node of the tree structure, containing a single symbol on the left branch of the tree. The value of the left side symbol is defined by the calculation of the right side terms. Thus the equation is assumed to be a function which has symbols as arguments. The editor provides an operator template which can describe specific argument sets. There are eight operator groups used to compose an equation (Table 3-1).

Table 3-1. List of operators in EquationEditor

Operator group	Operators
Exponential	Subscript, double subscript, superscript, exponent, sub and super script, function, square root, root, log
Fence	Parenthesis, bracket, brace, absolute, ceiling, floor
Trigonometry	Sine, cosine, tangent, arcsine, arccosine, arctangent
Calculus	Limit, differential, indefinite, definite, summation, product, maximum, minimum
Logic	And, or, not
Arithmetic	Add, subtract, multiply, divide, negation
Relation	Less than, greater than, less and equal, greater and equal, equal, equivalent, not equal, not equivalent, less than and less than equal to, less than equal to and less than
Case	n-case, matrix

The Unit editor is an interface to create and maintain the unit for a symbol and its compositions for representing the quantity of measurement of symbols (Figure 3-6). Unit includes not only the generic collection of global standard unit of metric system (e.g. international system of unit (SI) and the English unit system), but also domain specific units such as "cm^3 of soil" in soil engineering. It is very important to carefully track the units associated with symbols, since different models may use the same symbol but having different units. A unit is not represented by a simple string, but by a composition of symbols (like an equation). The

unit can be expressed using a composition of limited operators (multiply, divide, and power operator) and other units. Thus, basic units such as length and weight can be reused for creating a composite unit, and this makes it possible to automatically calculate conversion of units from one form to another (e.g. the English unit to the metric unit).

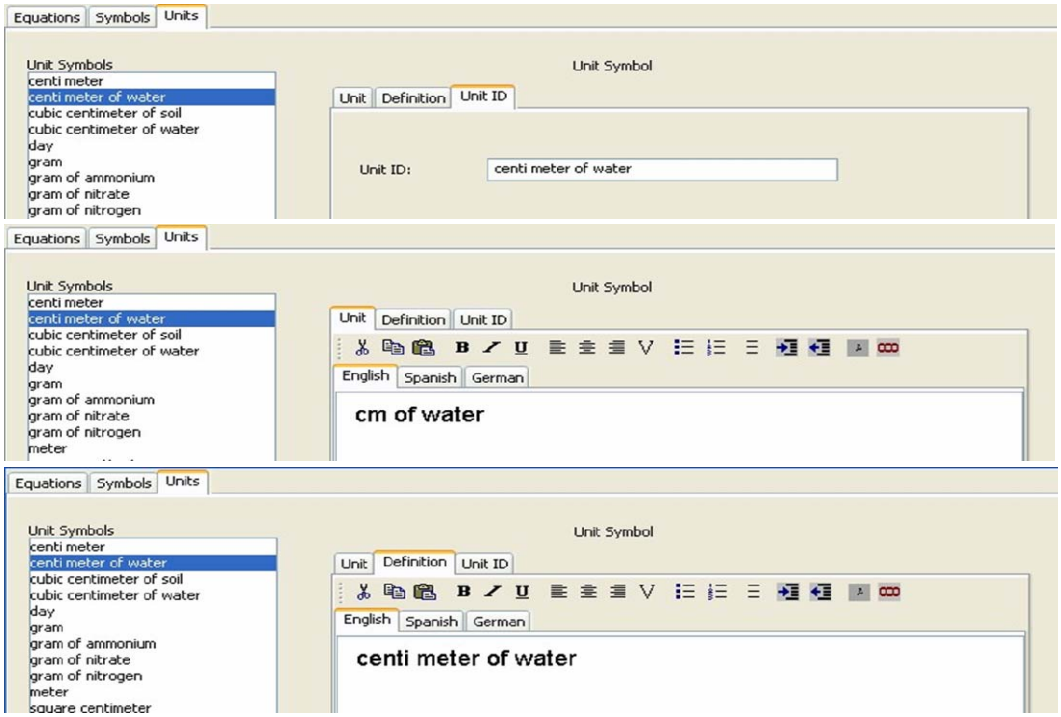


Figure 3-6. Unit ID, unit and definition of centimeter of water in unit editor

SimulationEditor

The SimulationEditor is used to describe the structure of dynamic systems using graphic elements such as source, sink, storage, and flow. It adopts concepts from the compartmental modeling technique (Peart and Curry, 1998) and Forrester notation (Forrester, 1971) which is widely used in agriculture and natural resource models. However, like the EquationEditor, these concepts are represented internally using the ontology and stored in the Lyra database. The SimulationEditor is used for specifying the overall model structure in the form of elements, and

incorporates the EquationEditor described in the previous section in order to build equations associated with each element. The SimulationEditor provides a graphic user interfaces to create and maintain a simulation system which includes a structure design interface, a simulation control interface, and a simulation result reporting interface. The SimulationEditor also contains facilities for automatically generating and running simulations and generating reports.

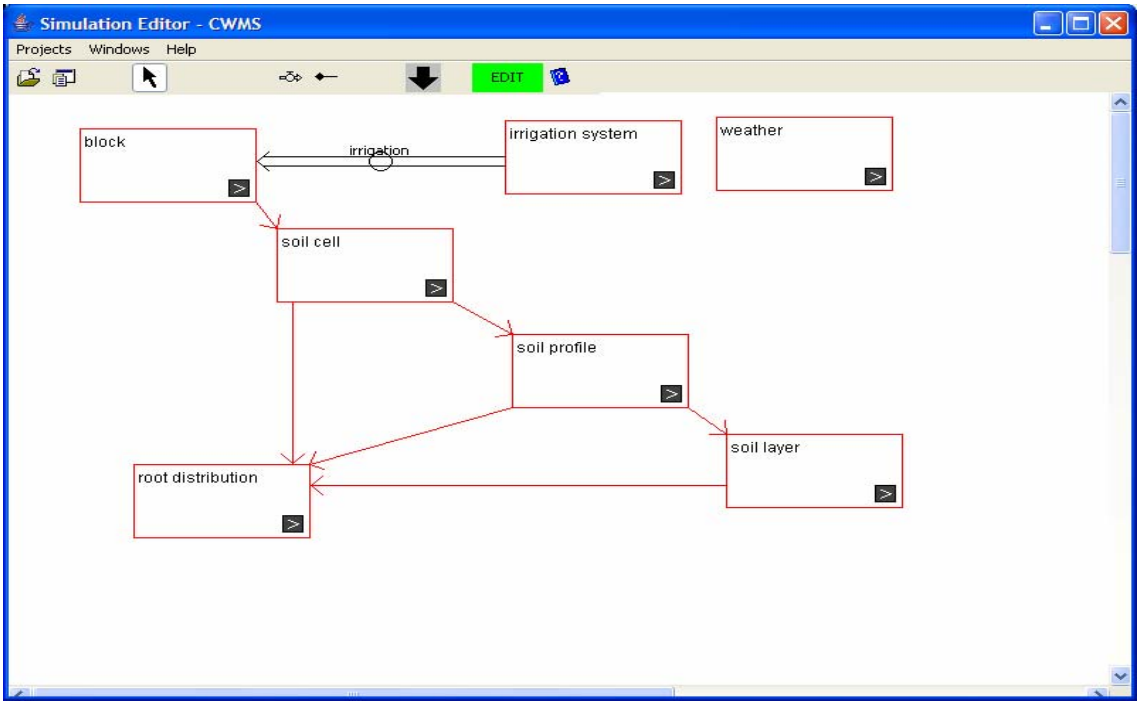


Figure 3-7. Structure editor showing a compartmental diagram of a soil-water model

The structure editor is the main interface of the SimulationEditor and provides functionalities which enables modelers to create and maintain a simulation project by designing the structure of a system, and to interact with the EquationEditor and the simulation controller. Structural design of a system is a procedure by which a modeler creates physical or environmental elements and relationships in the system by using graphic elements. For example (Figure 3-7), a 3-dimensional soil profile system may be designed as a composition of soil cell (production unit), soil profile (horizontal division), and soil layer (vertical division) concept. These three elements may be defined as an instance of storage element, and relationships

between these elements are represented by ‘Part of’ (e.g. block, soil cell and soil profile composed of soil cell, soil profile and soil layer respectively). Irrigation may be realized with the flow element representing the flow of water into the cell.

The simulation controller is a collection of simulating engines used to generate a simulation program from the mathematical model, to run the simulation, and to generate reports. For simulating a model, a simulation engine automatically converts ontology objects to program source code. It then compiles and runs the generated program to execute the simulation. Currently, Java is the target language, although in theory a simulation program may be generated using other programming language. It is not necessary for the modeler to examine, work directly with or otherwise be concerned about the generated program source code. This process is completely internal to the operation of the software, and transparent to the modeler. However, the compiled source code can be used as a component that can be accessed by other software environments after the model is developed.

The data object conversion and generation of program source code follows these steps:

- A class representing a module in the SimulationEditor forms a single class in Java. The class contains member variables and methods for all the symbols and equations in the module.
- Each symbol in the module is declared as a member variable named after the name of the symbol. If the symbol is a matrix, the member variable is declared as an array with the same dimensions as the symbol. A method is created that contains code for obtaining the value of the symbol. The name of this method is based on the name of the symbol.
    - If a symbol is a constant, the return value of the method is a constant for the symbol’s value.

- If a symbol obtains its value from a database, the method returns a value obtained by querying the database for the value of the symbol, subject to constraints specified in the symbol's properties.
- If a symbol obtains its value from an equation, the method contains code for solving the equation to obtain the value. Since the equation contains other symbols, these values of these symbols (on the right hand side of the equation), are obtained by recursively calling methods for determining their values.

Generated source code set is designed to be independent from the SimulationEditor, so that it can be used as part of a component library and inserted into other application independently. There are two levels to the system: the core level and the application level (Figure 3-8). The core level is the ontology-based simulation environment including the SimulationEditor and, the EquationEditor integrated within the Lyra OMS which also provides the database management facilities for storing the ontology objects created by the SimulationEditor and the EquationEditor. At the application level, the generated code library is used by the other applications which can be implemented independently from the core level. For example, the resulting simulation application can be integrated into a desktop application used by growers, it can be part of a larger decision support system such as DISC (Beck et al., 2004) which is a citrus planning and scheduling program or a Web-based simulation environment (users can run the simulation through a web page, or the simulation can be part of a web service that is part of a distributed simulation environment).

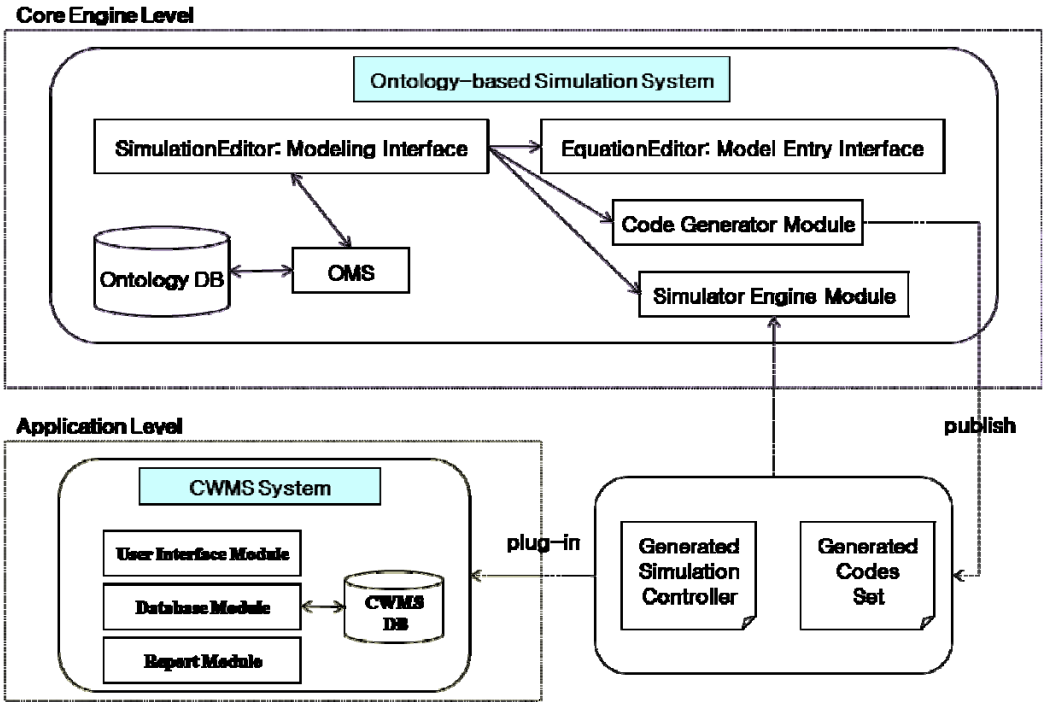


Figure 3-8. Relationships between ontology-based simulation system, generated code and application

Running a simulation involves compiling and executing the automatically generated source code. The simulation is controlled by recursively evaluating the value of a target symbol. Within the SimulationEditor, there is an interface to communicate with the model code library, which contains a method for calling the target symbol's method which results in execution of the simulation. The generated source code contains variables for storing all values of variables, which are retrieved by a report generator to display model results when the simulation has finished executing.

The report generator displays simulation results by showing the values of specific symbols in the form of a table or a graph as a function of time and proper dimension described in a symbol. A list of symbol ID which is stored in the ontology is provided to create reports, and a report is designed by selecting and adding to the target variables list and the dependent variable after simulation. A designed report form can be categorized and maintained in the ontology.

Additional Tools and Facilities

A system may be composed of many small models, and these models reference other models or equations. There is a need to verify interactions between such complex structural relationships, and to assess the behavior of models statistically. Tools are also available for exporting the model into XML in two different formats, MathML (Ausbrooks et al., 2003) and OpenMath (Buswell et al., 2004).

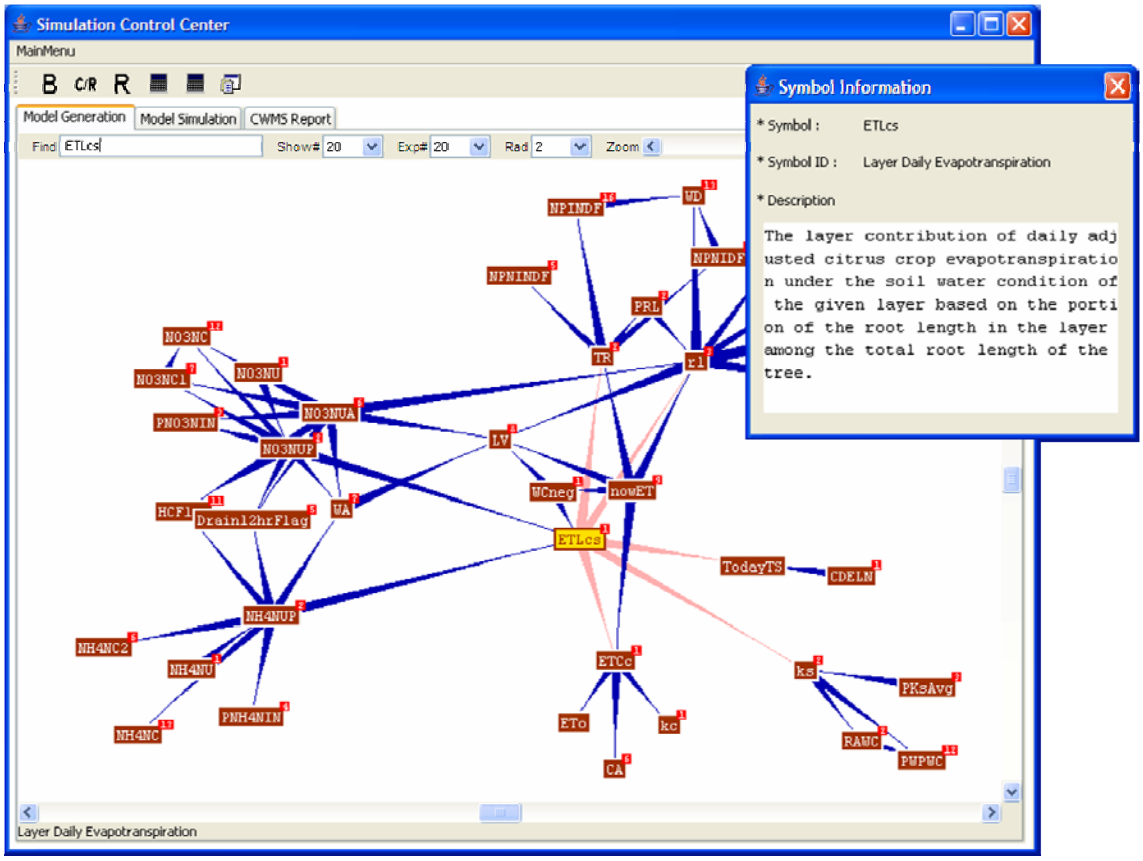


Figure 3-9. Symbol reference diagram focusing on Layer Daily Evapotranspiration

To verify the complex flow of referencing equations in a model, it is useful to visualize those flows and call sequences as a diagram. The calling sequence is generated by interpreting attributes recursively in a process that is similar to the process of generating the program code. Figure 3-9 shows an example of a calling sequence of equations which are parts of CWMS

models presented in Chapter 4. To calculate a value of a symbol such as the layer daily evapotranspiration (ETLcs), some values are required including the total root length (TR), the cell crop evapotranspiration (ETCc), the soil coefficient (ks), the today number of time step (TodayTS) and the layer root length (rl). Arrows starting from the target symbol point to other symbols which are required to calculate it. Numbers over each node indicate of nodes which are related to that node, but not shown. The calling sequence interface provides a convenient way for displaying every connected symbol as a visual network diagram, and it can be used to browse symbols and navigate the model.

A sensitivity analysis process is implemented using computer experiments. The aim of sensitivity analysis is to determine how sensitive the output of a system is with respect to the elements of the model which are subject to uncertainty or variability (Wallach et al., 2007). This is useful as a guide when the model is under development as well as to understand model behavior, to seek the main affecting factors in the system, and to figure out the significant interaction between input factors selected from the system variables. The procedure consists of two step; factor screening using Morris randomized OAT (One-factor-At-a-Time) design (Morris, 1991; Alam and McNaught, 2004) and global sensitivity analysis with screened factors from previous step. The Morris' randomized OAT design as a factor screening method is used to determine which factors are really significant when there are potentially a large number of factors involved. A computer experiment is a set of simulation runs designed to explore the model responses when the input varies within given ranges. The number of executions required to do this is dependent on a number of selected factors and levels. After choosing input factors in the system, discrete levels are automatically decided by the maximum value, minimum value and

number of levels. An experiment engine feeds factor values at a specific level, and control the iterative simulating process.

The XML generator is a tool to generate a markup language form for a model built in the ontology. XML enables the model to be shared outside of the Lyra OMS environment. Two forms of markup language, MathML and OpenMath, can be generated. MathML is an application of XML for describing mathematical notation and capturing both its structure and content. It aims at integrating mathematical formulas into Web documents. It is a recommendation of the W3C (World Wide Web Consortium) math working group. Whereas MathML has strength on presentation of formulae, OpenMath is a document markup language for mathematical formulae, which provides a mechanism for describing the semantics of mathematical symbols. To generate these XML formats from equations in the ontology, each operator template class which is declared in the EquationEditor has a method transforming operator and arguments to a string containing a XML tag expression. An operator template can have other operator templates as arguments. An equation may be considered as a tree data structure composed of operator and symbol. The XML generator traverses this tree from the root operator template (which is always the “equal” operator) to each leaf operator template, similar to the way in which the code for solving the equation is generated. An example of generating markup language is shown in Figure 3-10 which a simple equation “A=B+C” is generated in MathML and OpenMath format (generated Java code for solving this equation is shown as well).

```
[ Source Equation]
A = B + C

[ generated documents]

<!-- MathML -->
<math display='block' xmlns = ' http://www.w3.org/1998/Math/MathML'>
<mrow>
 <mi> A </mi>
 <mo>=</mo>
 <mrow>
  <mi> B </mi>
  <mo> + </mO>
  <mi> C </mi>
 </mrow>
</mrow>
</math>
```

```
<!-- OpenMath--->
<OMOBJ xmlns = "http://www.openmath.org/OpenMath" version = "2.0" cbase = "http://www.openmath.org/cd" >
<OMA>
 <OMS cd= "relationl " name= "eq" />
 <OMV name = "A" />
 <OMA>
  <OMS cd= "arithl " name= "plus" />
  <OMV name= "B" />
  <OMV name= "B" />
 </OMA>
</OMA>
</OMBJ>
```

```
<!--- Java--->

public double A()
 {
  "return B() + C()" ;
 }
```

Figure 3-10. Result of generating markup language for the equation A=B+C

In Chapter 3, methodologies were covered to represent mathematical models in the ontology using the Lyra ontology management system. To utilize the constructed model ontology for simulating models, two main tools, the EquationEditor and the SimulationEditor, are developed. The EquationEditor provides interfaces for describing symbols and equations in a model and for retrieving ontology objects, and the SimulationEditor helps to conceptualize the circumstance in which models are applied. Simulation handling process is facilitated by functions including automatic generation of program codes and reports, sensitive analysis, and calculation sequence diagram. Model representation adopting ontology-based methodologies simplifies to create a deliverable model expression such as a XML form.

CHAPTER 4
APPLICATION TO CITRUS WATER AND NUTRIENT MANAGEMENT

Ontology-based simulation methodologies covered in Chapter 3 were applied to building a model describing water and nutrient balance processes for the Citrus Water and Nutrient Management System (CWMS) (Morgan et al., 2006a). To aid growers in water management decision making, a computer-based decision support system was developed to facilitate more efficient use of water and nutrients by basing recommended application rates on site specific characteristics and local weather data. The purpose of this work was to test the feasibility of utilizing ontology-based simulation to build a moderately complex model, resulting not only in a simulation that can execute rapidly, but that also can be incorporated into a user interface for delivery to and use by growers or in other applications.

The CWMS Model

Description of Model

The CWMS model has been designed for the sandy soils of central and southern Florida which have low water and nutrient retention capacities. At citrus production sites, nutrients may be leached from the sandy soils by excessive irrigation events. The CWMS model was developed to anticipate the potential contribution to the groundwater contamination and to provide appropriate irrigation scheduling strategies. The CWMS model uses two main water inputs, rainfall and irrigation events. Rainfall amount is assumed to be affected by the canopy volume covering the soil surface. An irrigation event contains information including nutrient concentration (in the case of fertigation or injection of liquid fertilizers into the irrigation water), amount and event date, and it consists of several distinct irrigation processes. The soil water budget models in the CWMS model are based on crop water use, soil-water storage capacity, and

vertical soil water movement. Horizontal water movement is excluded due to lack of lateral movement in the sandy soil.

The model is based on a restricted area, a soil cell in a block representing a single citrus tree and the drainage field surrounding it, which is the basic unit of the geometry (Figure 4-1). A commercial block of citrus consists of many soil cells since it has many trees, but in this model to simplify the simulation process the model is based on a single soil cell, and the single tree represented by that soil cell is characteristic of all the other trees in the block. A soil cell is defined as a cubical soil area containing one citrus tree, having a depth of 200cm from the top of the soil. A soil cell is further divided into soil profiles within a cell and soil layers within a soil profile. As shown in Figure 3-7 in Chapter 3, seven concepts are defined for the model structure; block, soil cell, soil profile, soil layer, root, irrigation, and weather.

A soil cell consists of a one-tree planting row area with the tree in the center. The width and length of the cell are in-row and between-row distances to adjacent trees. It includes four-types of zones (i.e. a non-irrigated & dry-fertilized area, an irrigated & dry-fertilized area, a non-irrigated & non-dry-fertilized area, and an irrigated and non-dry-fertilized area as shown in Figure 4-2) according to the irrigation status and the dry-fertilized status, and each zone may have from 1 to 5 soil profile(s) which consist of n soil layers. The total soil layer number (n) is determined based on the particular soil type or a depth of each soil layer.

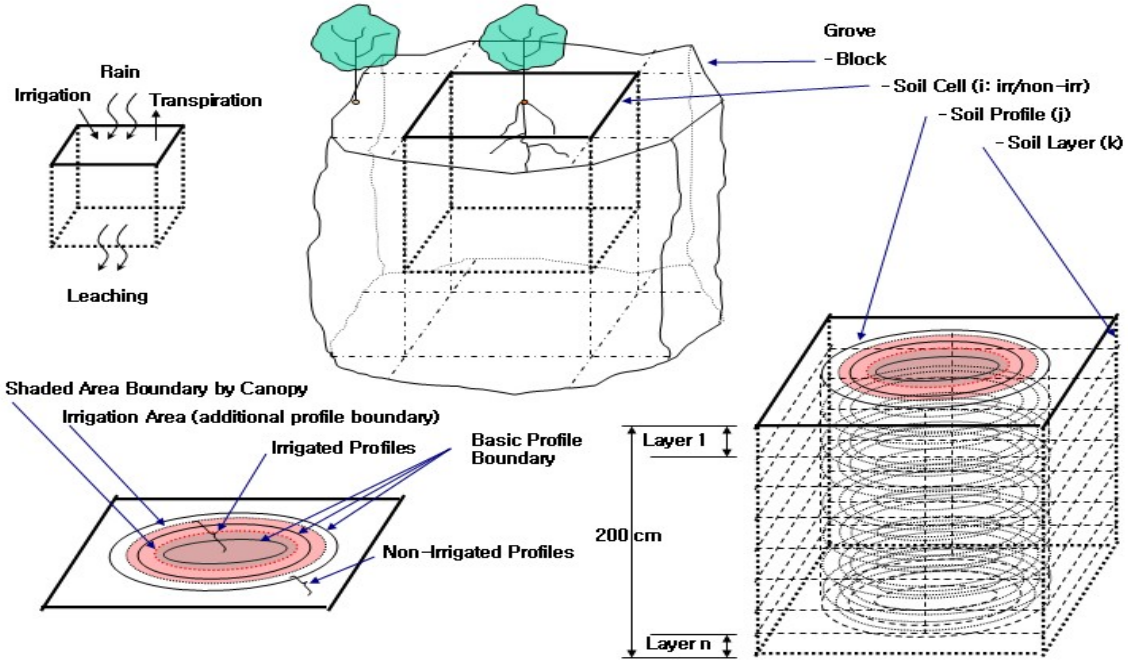


Figure 4-1. Conceptualization of soil geometry of CWMS model

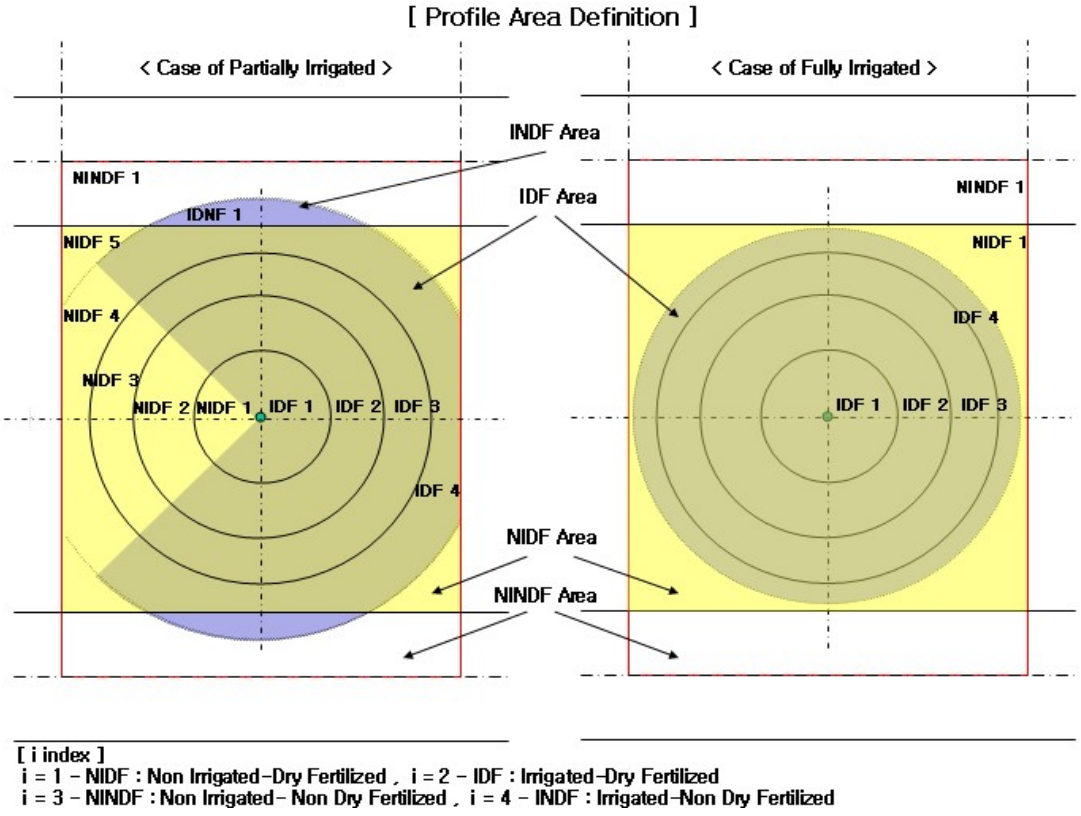


Figure 4-2. Examples of soil profile areas

Water balance for each profile is determined using rainfall and irrigation events as water inputs and evapotranspiration (ET) and leaching water as water losses from the balance. Basically, the water budget calculation is based on the tipping bucket model, enhanced by considering the effect of the delayed soil water drainage caused by the soil hydraulic conductivity during one daily time step. It is assumed that water inputs are applied at the first soil layer. Water infiltration depth is calculated as a function of the infiltration characteristics of the soil.

A pure tipping bucket model assumes that water moves the entire layer depth in one time step. Tipping bucket does not always reflect soil water content on a daily time step due to soil hydraulic characteristics. To account for the hydraulic characteristics of the soil, CWMS assumes that all irrigation, water with N application and rainfall occurs at noon and has a maximum of 12 hours to move through the soil on the first day. The model calculates the wetting front speed and the time for which the wetting front travels a layer thickness, thus to obtain the layer index of wetting front at the end of the day and let unfinished drained water continues to drain at next day.

As stated above, water loss from the water balance is water drainage below the 200 cm maximum depth and crop ET. Daily crop ET is calculated in CWMS using reference ET as user input or from weather data. A crop coefficient based on Morgan et al. (2006b) is applied to the reference ET based on seasonal variability. The crop ET deducted from each soil profile layer is proportional to the root length density of the profile layer. A layer root length density distribution is a function of tree size (Morgan et al., 2006a). An irrigation is scheduled when the CWMS determines that water content in the irrigated zone is below the allowed depletion. The irrigation

duration is determined by the water amount needed to bring water content to field capacity and is determined by the emitter flow rate, irrigation efficiency, and irrigation depth.

For nutrient management, especially application of nitrogen by irrigation (fertigation), the CWMS model provides processes for calculating nitrogen balance followed by transformation of nitrate and ammonium. Transformations are composed of complicated sub-processes and are affected by input and flow (drainage from above layer) amount of nutrient and water between layers. The model assumed that there are four nutrient flow processes by four drain events: drain by rain, pre-irrigation, during-irrigation, and post-irrigation. After four-drain steps, transformation processes is applied to ammonium and nitrate following in order of volatilization, uptake of ammonium, uptake of nitrate, and nitrification.

Model Base of the CWMS Model

The CWMS models is implemented by using a taxonomy representing physical relationship of natural resources (soil profile, crop, and environment), which consists of 4 soil related concepts (block, soil cell, soil profile, and soil layer), root density, weather, and irrigation. The system structure taxonomy is built graphically with the SimulationEditor (Figure 3-7).

For the CWMS model approximately 700 symbols and 500 equations were created. Symbols and equations developed for the CWMS model are interrelated, and their relationship can be visualized as a graph diagram (Figure 4-3), which displays connections of symbols and equations used to model the water and nitrogen balance process. Symbols and equations are represented as rectangular boxes, and the number above a box shows the count of connected boxes but not displayed. An arrow means that the target symbol is required to calculate the source equation.

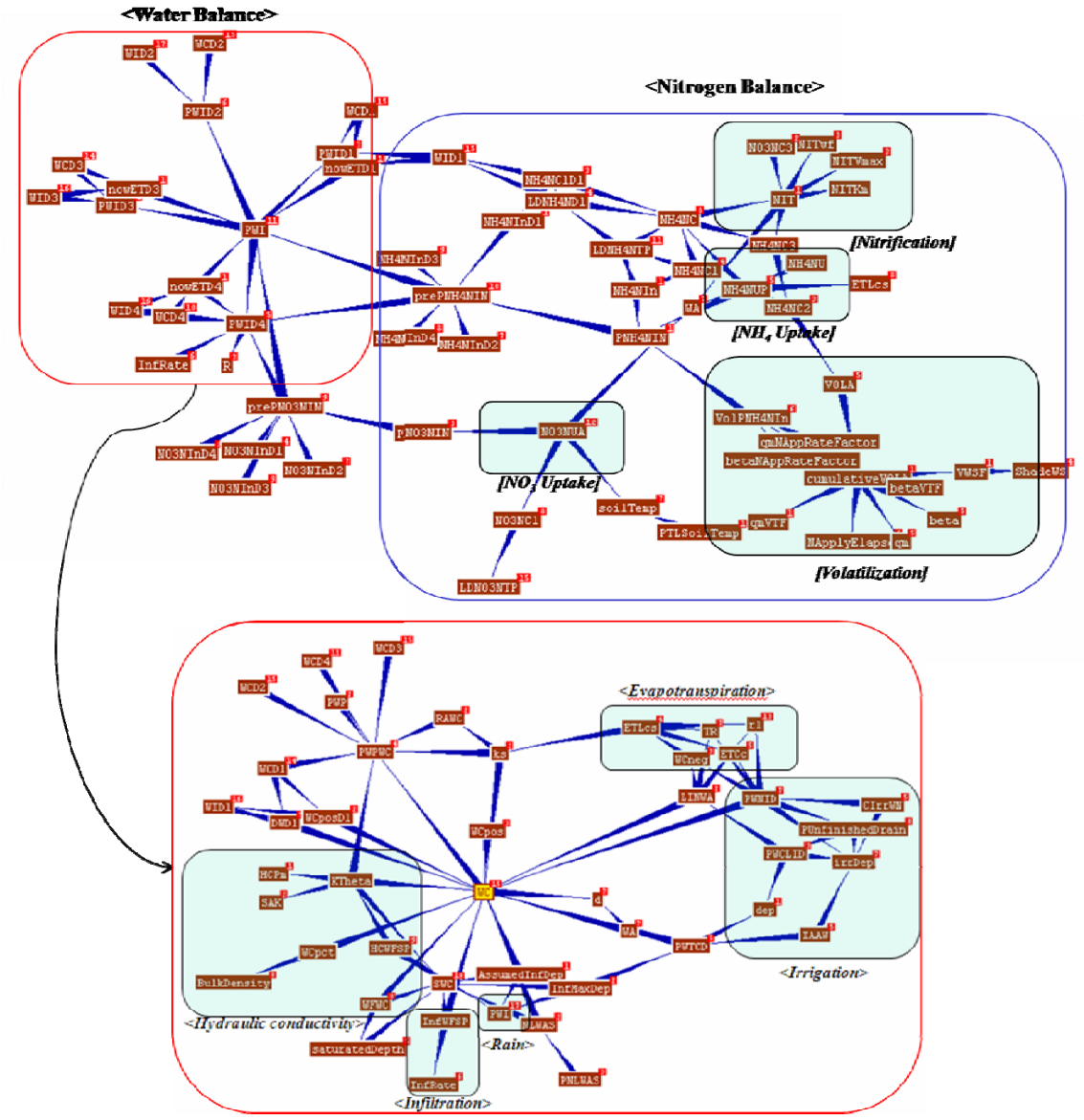


Figure 4-3. Relationship among equation symbols for water and nitrogen balance

In the diagram, nitrogen balance process group is connected with the water balance process group by referencing several equations for water balance. They can be switched with similar process groups independently. Particular processes, uptake, nitrification and volatilization, are clustered clearly from other equations in the equation group of nitrogen balance, and for water balance a similar pattern was found for processes of evapotranspiration, infiltration, and irrigation. This suggests possibilities for organizing and categorizing models and subprocesses.

The graphic in Figure 4-3 is generated automatically from the ontology objects, and an animated interface allows the model to navigate through the space of symbols.

A model base is a database of many models, model elements, equations, and symbols. It can be utilized for reusing models by applying a taxonomic organization to an ontology. In Figure 4-4, a model base is shown, which consists of equations used in the CWMS model. The taxonomy contains 6 classes including weather, water, nutrient, soil, crop and site. The water class has 5 subclasses (infiltration, evapotranspiration, precipitation, irrigation and runoff), and each subclass contains related equations and symbols. For example, the CWMS model includes two different infiltration models (Tipping Bucket Water Content Equation and Enhanced Wetting Front Water Content Equation).

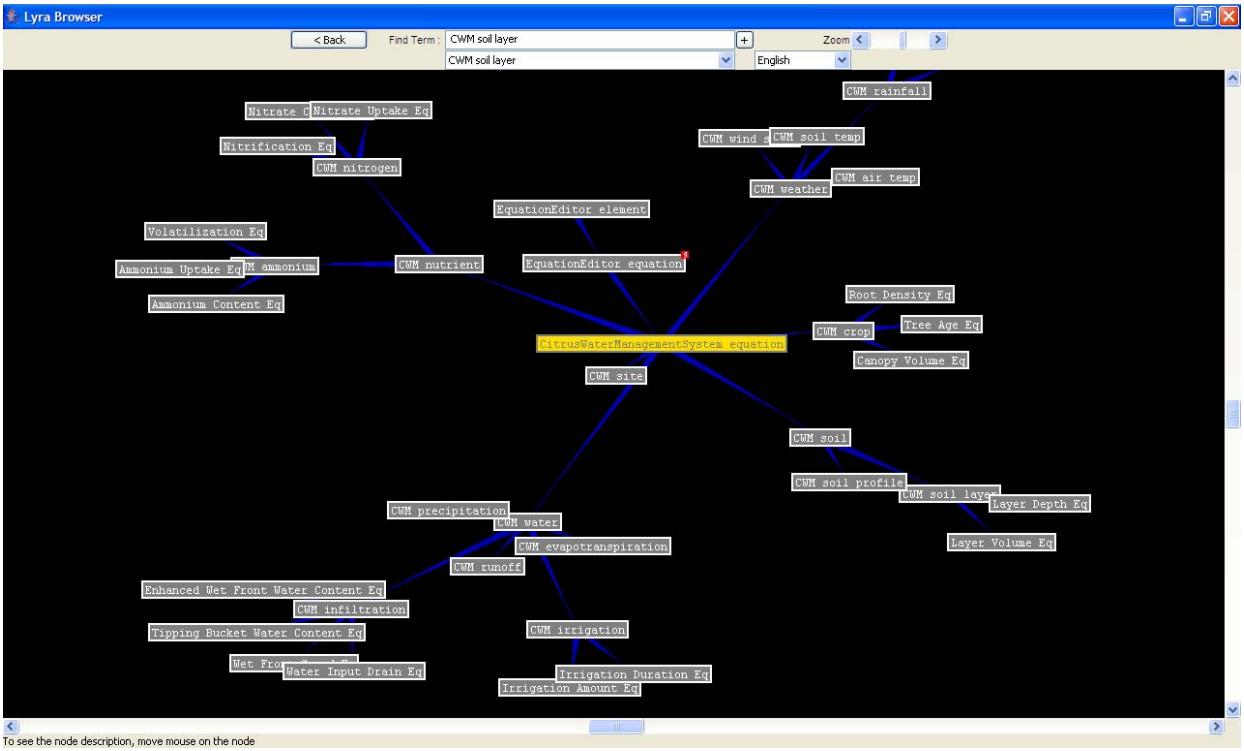


Figure 4-4. Taxonomy diagram of the CWMS model

Examples of Model Representing Process

Representing a model formed as theoretical or logical expressions (equations) in the ontology-based simulation system is a process of redefining and adjust them into a real world simulation for describing a phenomenon. Theoretical models provide the conceptual knowledge, and there are usually many reformulated models depending on assumptions and the given situation.

Morgan et al. (2006a) described how they derived the infiltration model used in CWMS from theoretical models. In summary, their infiltration model is based on Green-Ampt infiltration (Green and Ampt, 1911) and unsaturated flow based on Richard's equation (Richards, 1931) derived from Darcy's Law for irrigation and rainfall moving into soil from the surface and moving between soil layers. The Green-Ampt model in the case of no ponding at surface can be expressed as:

$$f_p = K_s + K_s M S_f / F$$

Where,

f_p : infiltration capacity of soil (the rate that water will infiltrate as limited by soil factors)

F : cumulative infiltration

K_s : the hydraulic conductivity of the transmission zone

M : the difference between initial and final volumetric water contents

S_f : the effective suction at the wetting front

Furthermore, the model adopted Mein and Larson's equation (Mein and Larson, 1973) applying the Green-Ampt model for rainfall conditions by determining cumulative infiltration at the time of surface ponding. Some assumptions addressing the situation in which the rainfall

intensity is less than the infiltration capacity of the soil are focused. The general Mein and Larson equation can be described as:

$$f_p = R = K_s + K_s MS_{av} / F_p$$

Where,

S_{av} : the average suction at wetting front

F_p : the cumulative infiltration at the time of surface ponding

R : the rainfall intensity

By considering the relation between rainfall intensity, infiltration capacity, and saturated hydraulic conductivity, the Mein and Larson equation can be written like as:

$$\text{infiltrationRate} = \begin{cases} \text{rainIntensity } (t_{ponding} \text{ will be } \infty) & \text{if rainIntensity} < Ks \\ \begin{cases} \text{rainIntensity} & \text{if } t < t_{ponding} \\ \text{infiltrationCapacity} & \text{otherwise} \end{cases} & \text{if } Ks < \text{rainIntensity} \le \text{infiltrationCapacity} \\ \text{infiltrationCapacity} & \text{if } Ks < \text{infiltrationCapacity} \le \text{rainIntensity} \end{cases}$$

Where

Ks: Saturated Hydraulic Conductivity

t: time in hours

$t_{ponding}$: Ponding time when rainIntensity>infiltrationCapacity

infiltrationCapacity: decrease as t increase

Morgan et al. assumed that no ponding occurred in the sandy soil (e.g. for Candler soil, Ks is 25 cm/hour) because rainfall is less than 5 cm/hour (except during hurricanes) and irrigation rates are typically 0.315 cm/hour or less. It was also assumed that runoff does not exist since the rainfall and irrigation intensity is usually smaller than Ks. Thus, the infiltration rate equals the rainfall rate and the amount of infiltration water equals amount of rainfall rate multiplied by time t. If rainfall rates are larger than the irrigation rate, the infiltration rate equals the rainfall intensity. Otherwise, it equals irrigation intensity. Thus, the Mein and Larson equation is simplified for such rainfall and irrigation conditions. The condition term for comparing the rain

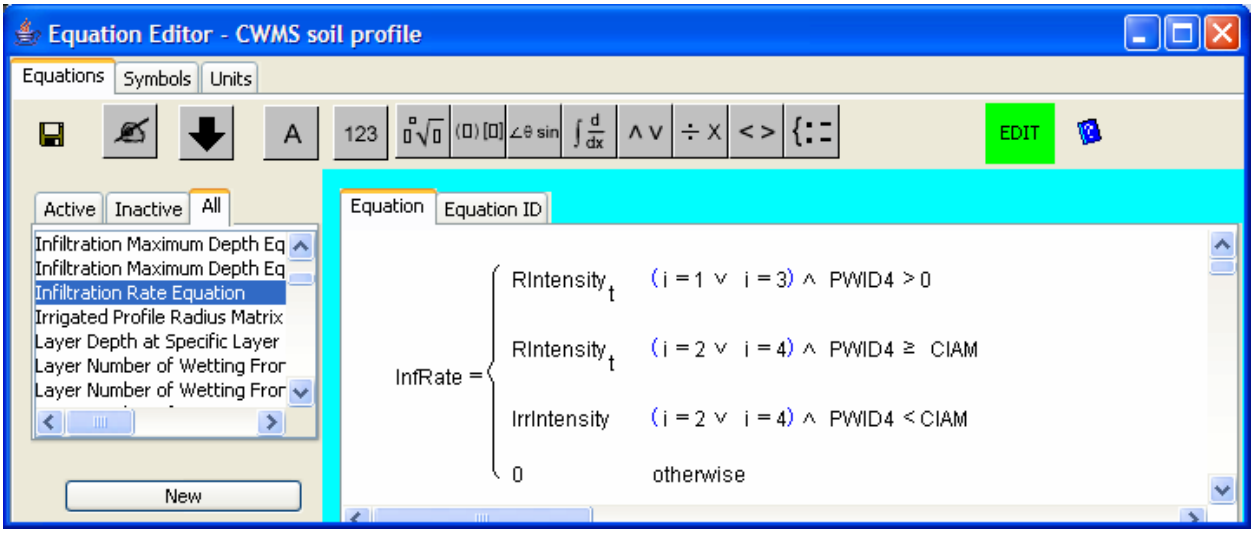
intensity with the saturated hydraulic conductivity was simplified to comparing the rainfall amount (represented by PWID4) with the irrigation amount at soil cell (represented by CIAM) for creating the average infiltration rate of soil profile. To apply the world system to the model, additional condition term s describing whether current soil profile exists in the irrigated-area or non-irrigated-area were added to the model. With the above result, an equation for the infiltration rate of soil profile was formed in Figure 4-5. CIAM is the cell irrigation amount, and i is the profile type, and numbers (1, 2, 3 and 4) represent the profile type, a non-irrigated & dry-fertilized area, an irrigated & dry-fertilized area, an irrigated and non-dry-fertilized area, and an non-irrigated and non-dry-fertilized area. SAKtop is the saturated hydraulic conductivity at surface, and PWID4 is the soil profile water input amount from rainfall effect. IAM is the equation calculating irrigation amount from irrigation duration, and IDur is the irrigation duration time.

Examples of CWMS Model Implementation

Concepts developed above were entered into the ontology system. The geometry relating soil cell and profile, soil water redistribution, and root density are given below as examples.

Soil geometric dimension

Basically, a profile is determined by the distance from the trunk of a tree to three root zone radii (75, 125, and 175cm). Other profile boundaries are the irrigation diameter and the dry-fertilized area. Depending on the irrigation type (360 degree or less than 360 degree), soil profiles can be divided into irrigated-areas and non-irrigated areas. Irrigation and dry-fertilizing events are assumed to be conducted in a soil cell area except two equipment drive paths between tree rows. Therefore, the two drive paths are always considered as a non irrigated & non dry-fertilized area (NINDF). An irrigated & non-dry fertilized area (INDF) is an irrigated area in the drive paths.



Where,

$$RIntensity = \min\left(0.8 \times SAKtop, \frac{1.75 \times R}{3}\right)$$

$$PWID4 = R \times (1 - shadeAreaRatio \times (1 - shadedRainRatio_t))$$

$$CIAM = IAM(IDur_t)$$

Figure 4-5. Morgan's infiltration rate model in the CWMS model

$$NPIDF = \begin{cases} 2 & 2 \times RZR_1 < WD \le 2 \times RZR_2 \\ 3 & 2 \times RZR_2 < WD \le 2 \times RZR_3 \\ 4 & 2 \times RZR_3 < WD \\ 1 & \text{otherwise} \end{cases}$$

$$NPNIDF = \begin{cases} \begin{cases} 4 & WD = 2 \times RZR_1 \vee WD = 2 \times RZR_2 \vee WD = 2 \times RZR_3 \\ 5 & \text{otherwise} \end{cases} & SpP < 360 \\ \begin{cases} 4 - NPIDF & WD = 2 \times RZR_1 \vee WD = 2 \times RZR_2 \vee WD = 2 \times RZR_3 \\ 5 - NPIDF & \text{otherwise} \end{cases} & \text{otherwise} \end{cases}$$

$$NPINDF = \begin{cases} 1 & WD > 2 \times DistToHedgingBoundary \\ 0 & \text{otherwise} \end{cases}$$

Figure 4-6. Equations of profile number

Equations for calculating each profile number and area are defined at the cell, and Figure 4-6 shows equations of three different profile number (profile number of a non irrigated & non dry-fertilized area is always 1 and it is defined as a constant). NPIDF, NPNIDF, and NPINDF are respectively symbols of a profile number of an irrigated & dry-fertilized area, a profile number of a non-irrigated & dry-fertilized area, and a profile number of an irrigated and non-dry-fertilized area. RZR is a symbol of the root zone radius matrix, and WD is a symbol of the wetting diameter, and SpP is a symbol of the spray pattern.

A soil layer is one vertical element of a soil profile, and the number of soil layers in a soil profile is determined by layer thickness and total depth of the soil profile, whose maximum depth is 200cm. The thickness of soil layers can be grouped, and it is represented as a matrix as in Figure 4-7. Each row is a layer group, the first column is a thickness of layers in a group, and the second column is the number of layers in a group, and third column is a cumulative layer number to that group.

Symbols belonging in concepts, block, soil cell, soil profile, and soil layer, are required dimensions. The time dimension is a common dimension required by most symbols as one dimension of the matrix. Symbols in block and soil cell need only the time dimension, whereas those in soil profile need three dimensions, one for time, one for soil profile type, and one for soil profile number. Symbols in the soil layer need four dimensions, and they include three dimensions from soil profile and one for soil layer number. For example, a symbol, historical soil layer temperature, defined in soil layer has four dimensions, and it is described through the EquationEditor (Figure 4-8).

$$LThickRangeArr = \begin{vmatrix} 5 & 10 & 10 \\ 10 & 6 & 16 \\ 15 & 6 & 22 \end{vmatrix}$$

Figure 4-7. Layer thickness matrix

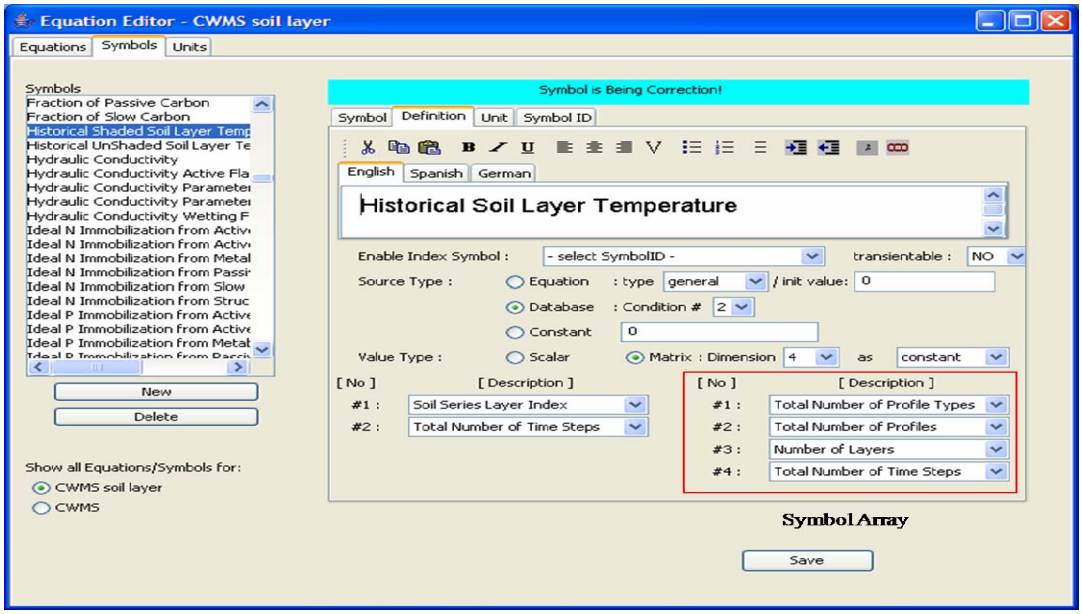


Figure 4-8. Example of dimension description of a symbol in soil layer

Time step

The main time step for the model is daily. Rain event, irrigation event, and fertilizer applications are assumed to occur at 12:00 pm, but adjustments to the time period of 0-12:00 pm and 12:00 pm - 24:00 pm are controlled by using some time flag symbols. The minimum period of simulation which can be executable is 14 days. The first 13 days (for 14 days calculation) or first 5 years (for 20 years calculation) are used to initialize and stabilize values of symbols whose initial condition are not known at the simulation starting time. For example, the initial values of soil water content is usually unknown, but assumed to be a default value and computed over the 13 days (or 5 years) to initialize the values.

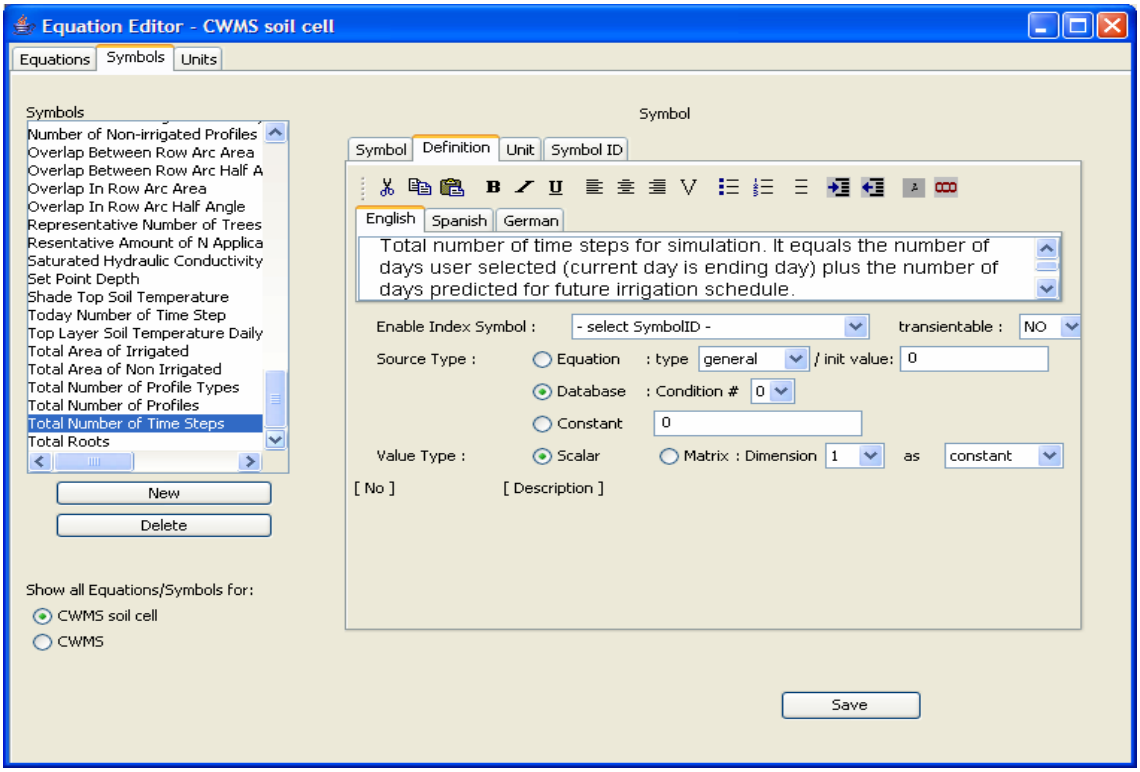


Figure 4-9. Total number of time steps symbol, t

There are two concepts related with time. One is Total Number of Time Steps for assigning system time dimension size, a value that is stored in and obtained from the database (Figure 4-9). The other concept related with time is Index variable of Time Step, t, which is used as the general variable for the current time.

Root density

As shown in Figure 4-10, root density is represented as a matrix from the model for each soil depth and root sections based on root density distribution as a function of tree size (Morgan et al., 2006a). A column is a root section and a row is a soil layers group to a specific depth. Following Morgan's model, the root horizontal area is divided into four sections (0-75 cm, 75-125 cm, 125-175cm and 175cm-boundary), and 10 soil layer groups are used. The first 6 rows have thicknesses 15 cm and last 4 rows have 30 cm thicknesses, which are calculated by proportional equations based on the root density value of 6th soil depth group. RD is a symbol of

the root density, and cv is a symbol of the canopy volume, and RSL is a matrix symbol of the root density regression parameters for layers below 6th soil depth group.

The root density equation is designed for specific soil layer depths and root ranges. The CWMS model utilizes it for an equation of LRD which is the layer root density (Figure 4-11). LD and LT are symbols of the layer depth and thickness of a layer at specific depths.

$$
RD = \begin{vmatrix}
\begin{cases} 1.2 + 0.023 \times cv & 0 < cv \le 15 \\ 1.1 + 0.043 \times cv - 0.00088 \times cv^2 & 15 < cv \le 35 \\ 1.45 + 0.0022 \times cv & 35 < cv \le 50 \\ 1.3 + 0.006 \times cv & cv > 50 \end{cases}
\begin{cases} 0.2 + 0.027 \times cv & 0 < cv \le 20 \\ 0.26 + 0.024 \times cv & 20 < cv \le 50 \\ 1.1 + 0.007 \times cv & cv > 50 \end{cases}
\begin{cases} 0.005 \times cv - 0.01 & 2 < cv \le 15 \\ 0.02 - 0.0075 \times cv + 0.0007 \times cv^2 & 15 < cv \le 35 \\ 0.26 + 0.01 \times cv & 35 < cv \le 50 \\ 0.5 + 0.005 \times cv & cv > 50 \end{cases}
\begin{cases} 0.054 \times cv - 0.8 & 14.8 < cv \le 32 \\ 1 - 0.002 \times cv & 32 < cv \le 50 \\ 0.55 + 0.007 \times cv & cv \ge 50 \end{cases} \\
\begin{cases} 0.3 + 0.02 \times cv & 0 < cv \le 15 \\ 0.3 + 0.03 \times cv - 0.0007 \times cv^2 & 15 < cv \le 35 \\ 0.6 - 0.0026 \times cv & 35 < cv \le 50 \\ 0.22 + 0.005 \times cv & cv > 50 \end{cases}
\begin{cases} 0.1 + 0.02 \times cv & 0 < cv \le 15 \\ 0.07 + 0.035 \times cv - 0.0009 \times cv^2 & 15 < cv \le 35 \\ 0.19 & 35 < cv \le 50 \\ 0.02 \times cv - 0.81 & cv > 50 \end{cases}
\begin{cases} 0.0053 \times cv - 0.008 & 1.5 < cv \le 15 \\ 0.008 \times cv - 0.04 & cv > 15 \end{cases}
\begin{cases} 0.005 \times cv - 0.125 & cv > 25 \\ 0 & \text{otherwise} \end{cases} \\
\begin{cases} 0.12 + 0.012 \times cv & 0 < cv \le 15 \\ 0.1 + 0.019 \times cv - 0.0004 \times cv^2 & 15 < cv \le 35 \\ 0.35 - 0.002 \times cv & 35 < cv \le 50 \\ 0.005 \times cv & cv > 50 \end{cases}
\begin{cases} 0.01 + 0.012 \times cv & 0 < cv \le 15 \\ 0.019 \times cv - 0.004 - 0.0004 \times cv^2 & 15 < cv \le 35 \\ 0.16 + 0.0005 \times cv & 35 < cv \le 50 \\ 0.02 \times cv - 0.8 & cv > 50 \end{cases}
\begin{cases} 0.002 \times cv - 0.002 & 1 < cv \le 15 \\ 0.0043 \times cv - 0.037 & cv > 15 \end{cases}
\begin{cases} 0.002 \times cv - 0.05 & cv > 25 \\ 0 & \text{otherwise} \end{cases} \\
\begin{cases} 0.07 + 0.013 \times cv & 0 < cv \le 15 \\ 0.06 + 0.016 \times cv - 0.0002 \times cv^2 & 15 < cv \le 35 \\ 0.13 + 0.007 \times cv & cv > 35 \end{cases}
\begin{cases} 0.01 + 0.006 \times cv & 0 < cv \le 15 \\ 0.01 \times cv - 0.05 & 15 < cv \le 50 \\ 0.2 + 0.005 \times cv & cv > 50 \end{cases}
\begin{cases} 0.0013 \times cv & 1 < cv \le 15 \\ 0.012 \times cv - 0.16 & 15 < cv \le 35 \\ 0.09 + 0.005 \times cv & cv > 35 \end{cases}
\begin{cases} 0.0018 \times cv - 0.045 & cv > 25 \\ 0 & \text{otherwise} \end{cases} \\
\begin{cases} 0.07 + 0.008 \times cv & 0 < cv \le 20 \\ 0.03 + 0.01 \times cv & 20 < cv \le 50 \\ 0.23 + 0.006 \times cv & cv > 50 \end{cases}
\begin{cases} 0.02 + 0.004 \times cv & 0 < cv \le 15 \\ 0.015 \times cv - 0.15 & 15 < cv \le 50 \\ 0.45 + 0.003 \times cv & cv > 50 \end{cases}
\begin{cases} 0.001 \times cv - 0.0008 & 0.8 < cv \le 15 \\ 0.013 \times cv - 0.18 & 15 < cv \le 35 \\ 0.01 \times cv - 0.075 & 35 < cv \le 50 \\ 0.22 + 0.004 \times cv & cv > 50 \end{cases}
\begin{cases} 0.001 \times cv - 0.025 & cv > 25 \\ 0 & \text{otherwise} \end{cases} \\
\begin{cases} 0.01 \times cv - 0.007 & 0.7 \le cv < 20 \\ 0.013 \times cv - 0.06 & 20 \le cv < 50 \\ 0.29 + 0.006 \times cv & cv \ge 50 \end{cases}
\begin{cases} 0.0015 \times cv - 0.002 & 1.4 < cv \le 15 \\ 0.01 \times cv - 0.13 & 15 < cv \le 50 \\ 0.12 + 0.005 \times cv & cv > 50 \end{cases}
\begin{cases} 0.0008 \times cv - 0.0009 & 1.2 < cv \le 15 \\ 0.009 \times cv - 0.12 & 15 < cv \le 35 \\ 0.006 \times cv - 0.005 & cv > 35 \end{cases}
\begin{cases} 0.0008 \times cv - 0.02 & cv > 25 \\ 0 & \text{otherwise} \end{cases} \\
RSL_1 \times RD_{61} \quad RSL_1 \times RD_{62} \quad RSL_1 \times RD_{63} \quad RSL_1 \times RD_{64} \\
RSL_2 \times RD_{61} \quad RSL_2 \times RD_{62} \quad RSL_2 \times RD_{63} \quad RSL_2 \times RD_{64} \\
RSL_3 \times RD_{61} \quad RSL_3 \times RD_{62} \quad RSL_3 \times RD_{63} \quad RSL_3 \times RD_{64} \\
RSL_4 \times RD_{61} \quad RSL_4 \times RD_{62} \quad RSL_4 \times RD_{63} \quad RSL_4 \times RD_{64}
\end{vmatrix}
$$

Figure 4-10. Root density matrix

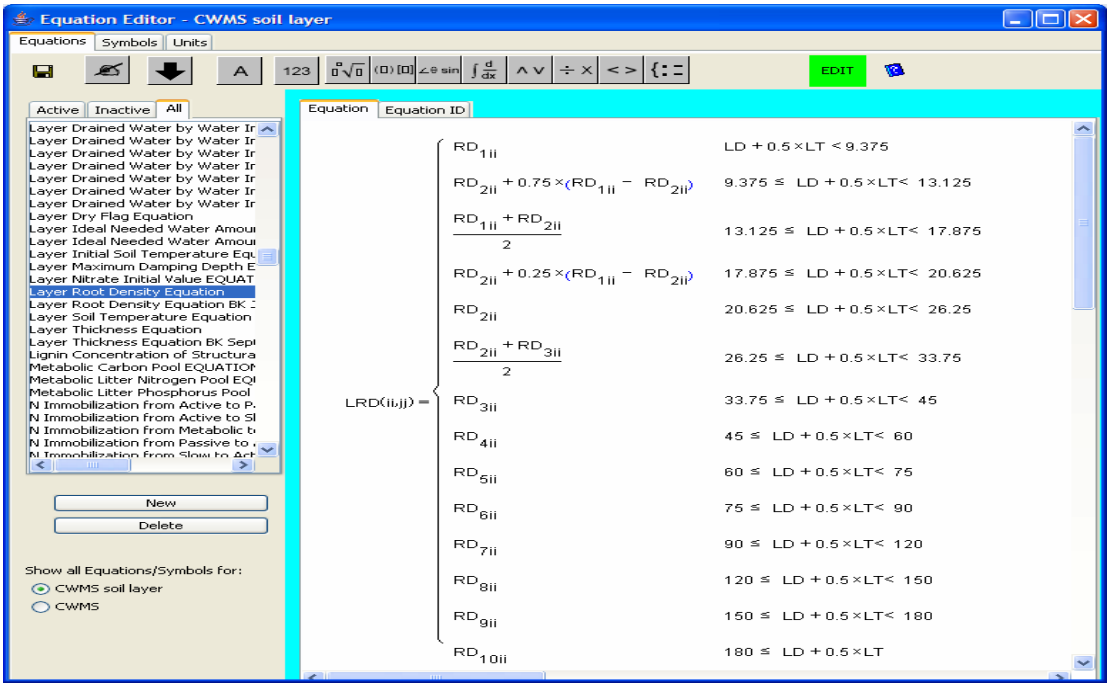


Figure 4-11. Layer root density equation

Water dynamics

The water balance model consists of rainfall, irrigation, evapotranspiration, and infiltration. As stated previously, surface runoff and subsurface lateral flow are not considered due to the high saturated hydraulic conductivity of sandy soils. Basically, the water budget calculation is based on the tipping bucket model, enhanced by considering the effect of the delayed soil water drainage which is caused by the soil hydraulic conductivity during one daily time step.

Rainfall and irrigation are water inputs into the system, and it is assumed that they are applied at the first layer. The symbol Profile Water Input (PWI) in the soil profile module represents input water amount from water resources into the soil profile. According to the CWMS model, it considers the complicated nutrient management processes by calculating different sources of water and nutrient separately. In the equation for PWI, sources of water inputs are distinguished as 4 different types depending on the considering event: irrigation (water), N application, post N application, and rainfall. Since the system time step is daily and

there is no sub-time step, symbols are created for every stage and distinguished by subscript number. These are four-drain process named. Figure 4-12a shows related PWI equations (PWI1, PWI2, PWI3, and PWI4), where it is assumed that irrigation and N application are applied to just irrigated-area (i=2).

The symbol WI (Figure 4-12b) is the layer water input, and the amount is determined by the difference of amount of input water into a layer from environment (PWI) or from the upper layer (DW) and the amount of layer evapotranspiration (nowET). For the four-drain process, calculation of layer water input is conducted for every stage separately. The symbol WIflag is for indicating the status of the remained water drain by the hydraulic conductivity.

A layer water content is represented by the symbol WC whose amount is calculated by the difference of increasing amount (WCpos) by drained water and decreasing amount (WCneg) by evapotranspiration during the previous time step. At the start of simulation all layer water content has same amount calculated with constant depletion level. For the four-drain process, a layer water content at time t would be a WCD4 of previous time step which is the layer water content applying irrigation, N application, post N application, and rainfall (Figure 4-12c).

The CWMS model enhanced the pure tipping bucket model by computing the wetting front moving speed during the simulation, whereas the pure tipping bucket model assumed that water moves the entire layer depth in one time step. The model assumed that all irrigation, water with N application, water with post N application and rainfall occurs at noon and has a maximum of 12 hours to move through the soil on the first day after irrigation, water with N application, water with post N application or rainfall. And, the model calculates the wetting front speed (Figure 4-13) and the time for which the wetting front travels a layer thickness, thus to obtain the layer index of wetting front at the end of the day and let unfinished drained water continues to drain at

next day. WFSP is the layer wetting front speed, and it can be calculated by the symbol of the infiltration WFSP (Figure 4-13b) or the symbol of the hydraulic conductivity WFSP (Figure 4-13c). Figure 4-13d is the equation for hydraulic conductivity.

$$PWI = PWID1 + PWID2 + PWID3 + PWID4$$

$$PWID1 = \begin{cases} CIAM & i = 2 \\ 0 & \text{otherwise} \end{cases} \qquad PWID2 = \begin{cases} IAM(preApplication + withApplication) & i = 2 \\ 0 & \text{otherwise} \end{cases}$$

$$PWID3 = \begin{cases} IAM(postApplication) & i = 2 \\ 0 & \text{otherwise} \end{cases} \qquad PWID4 = R \times (1 - shadeAreaRatio \times (1 - shadedRainRatio_t))$$

A

$$WI_t = \begin{cases} WID1 + WID2 + WID3 + WID4 & FourDrainPerDayFlag = 1 \\ \begin{cases} PWI - nowET \times LT & PWI \geq nowET \times LT \\ PWI & \text{otherwise} \end{cases} & WIflag = DF\_12hrTdyAir \vee (k = 1 \wedge HCFlag = 0) \\ \begin{cases} DW_{k-1} - nowET \times LT & DW_{k-1} \geq nowET \times LT \wedge PWI > 0 \\ DW_{k-1} & \text{otherwise} \end{cases} & k > 1 \wedge (WIflag = DF\_12hrTdyAbvLyr \vee HCFlag = 0) \\ \begin{cases} DW_{k-1t-1} - nowET \times LT & DW_{k-1t-1} \geq nowET \times LT \\ DW_{k-1t-1} & \text{otherwise} \end{cases} & k > 1 \wedge t > 1 \wedge WIflag = DF\_24hrYstrdyAbvLyr \\ \begin{cases} DW_{k-1} - nowET \times LT & DW_{k-1} \geq nowET \times LT \\ DW_{k-1} & \text{otherwise} \end{cases} & k > 1 \wedge WIflag = DF\_24hrTdyAbvLyr \\ \begin{cases} DW_{k-1t-1} + DW_{k-1} - nowET \times LT & DW_{k-1t-1} + DW_{k-1} > nowET \times LT \\ DW_{k-1t-1} + DW_{k-1} & \text{otherwise} \end{cases} & k > 1 \wedge t > 1 \wedge WIflag = DF\_Ystrdy12hrTdyAbvLyr \\ \begin{cases} DW_{k-1t-1} + DW_{k-1} - nowET \times LT & DW_{k-1t-1} + DW_{k-1} > nowET \times LT \\ DW_{k-1t-1} + DW_{k-1} & \text{otherwise} \end{cases} & k > 1 \wedge t > 1 \wedge WIflag = DF\_Ystrdy24hrTdyAbvLyr \\ 0 & \text{otherwise} \end{cases} \quad \text{otherwise}$$

B

$$WC_t = \begin{cases} WCD4_{t-1} & t > 1 \wedge FourDrainPerDayFlag_{t-1} = 1 \\ WC(d) & t = 1 \\ WCpos_{t-1} & t > 1 \wedge PWI_{t-1} > nowET_{t-1} \times LT \wedge (WIflag_{t-1} = DF\_12hrTdyAir \vee (k = 1 \wedge HCFlag = 0)) \\ WCpos_{t-1} & t > 1 \wedge k > 1 \wedge DW_{k-1t-1} > nowET_{t-1} \times LT \wedge (WIflag_{t-1} = DF\_12hrTdyAbvLyr \vee HCFlag = 0) \\ WCpos_{t-1} & t > 2 \wedge k > 1 \wedge DW_{k-1t-2} > nowET_{t-1} \times LT \wedge WIflag_{t-1} = DF\_24hrYstrdyAbvLyr \\ WCpos_{t-1} & t > 1 \wedge k > 1 \wedge DW_{k-1t-1} > nowET_{t-1} \times LT \wedge WIflag_{t-1} = DF\_24hrTdyAbvLyr \\ WCpos_{t-1} & t > 2 \wedge k > 1 \wedge DW_{k-1t-2} + DW_{k-1t-1} > nowET_{t-1} \times LT \wedge WIflag_{t-1} = DF\_Ystrdy12hrTdyAbvLyr \\ WCpos_{t-1} & t > 2 \wedge k > 1 \wedge DW_{k-1t-2} + DW_{k-1t-1} > nowET_{t-1} \times LT \wedge WIflag_{t-1} = DF\_Ystrdy24hrTdyAbvLyr \\ \max(WCpos_{t-1} - WCneg_{t-1}, PWPWC) & \text{otherwise} \end{cases}$$

C

Figure 4-12. Water balance equations: A) profile water input amount equations, B) layer water input amount equation, and C) layer water content equation

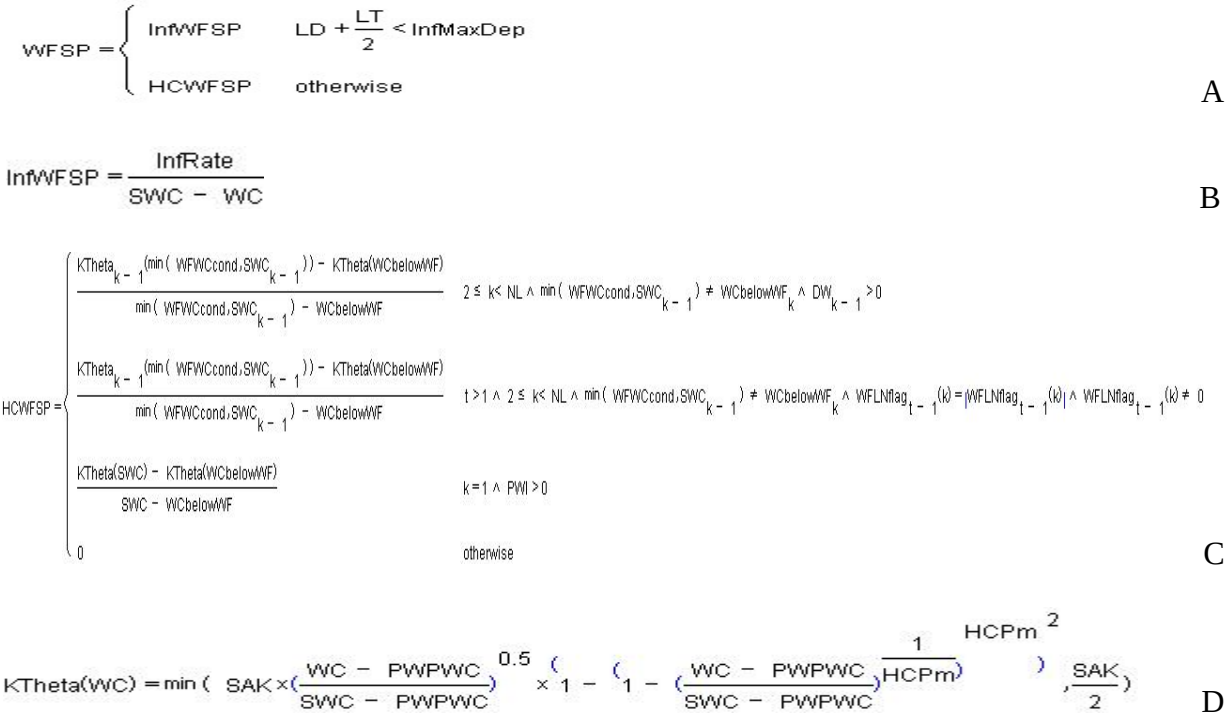


Figure 4-13. Enhanced hydraulic conductivity related equations in CWMS model: A) Wetting front speed equation, B) infiltration wetting front speed equation, C) hydraulic conductivity wetting front speed equation, and D) hydraulic conductivity equation

Nitrogen balance

For nutrient management, especially application of nitrogen by irrigation (fertigation), the CWMS model provides processes for calculating nitrogen balance followed by transformation of nitrate and ammonium. Transformations are composed of complicated sub-processes and are affected by input and flow (drain from above layer) amount of nutrient and water between layers. The model assumed that there are four nutrient flow processes by four drain events: drain by rain, pre-irrigation, during-irrigation, and post-irrigation. After four-drain steps, transformation processes is applied to ammonium and nitrate following in order of volatilization, uptake of ammonium, uptake of nitrate, and nitrification.

The amount of nitrogen input into a soil profile is an equation formed with the dissolved ammonium (NH_4) and nitrate (NO_3) nitrogen amount of dry fertilizer by rain or irrigation and

fertilizer amount during the fertigation. Nitrogen drain amounts (ammonium and nitrate) of a layer from the above layer are represented by symbols, Layer Drained Nitrate and Layer Drained Ammonium, and they are calculated by equations of soluableRate. For uptake amounts of nitrogen, passive uptake of ammonium and active/passive uptake of nitrate are formed as an equation. Also, the model assumed that the uptake process of ammonium occurred after volatilization and nitrification follows a nitrate uptake process, and they are utilized by using separate symbols for each stage.

The amount of nitrification is represented by symbol NIT, and its equation includes the rate of maximum nitrification as a function of ammonium content (NH_4NC_3), maximum nitrification amount at a time (NITVmax), half-saturation constant of nitrification (NITkm), and soil moisture factor (NITwf). Nitrification is allowed till 80% of current ammonium content (Figure 4-14).

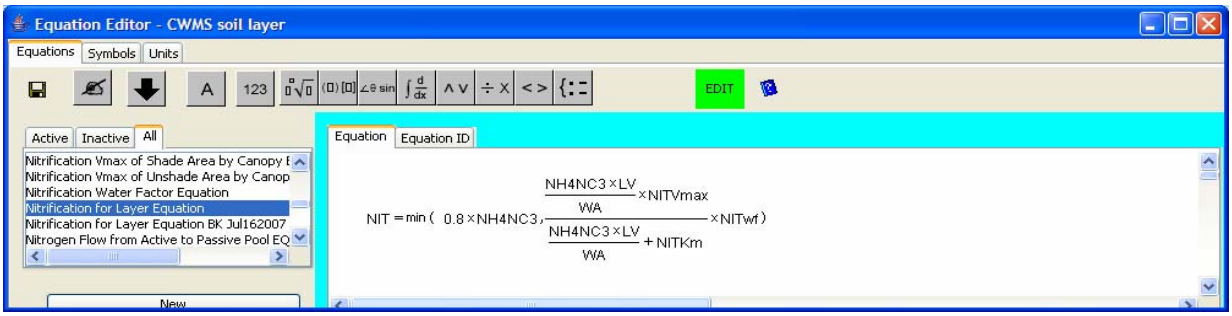


Figure 4-14. Layer nitrification equation

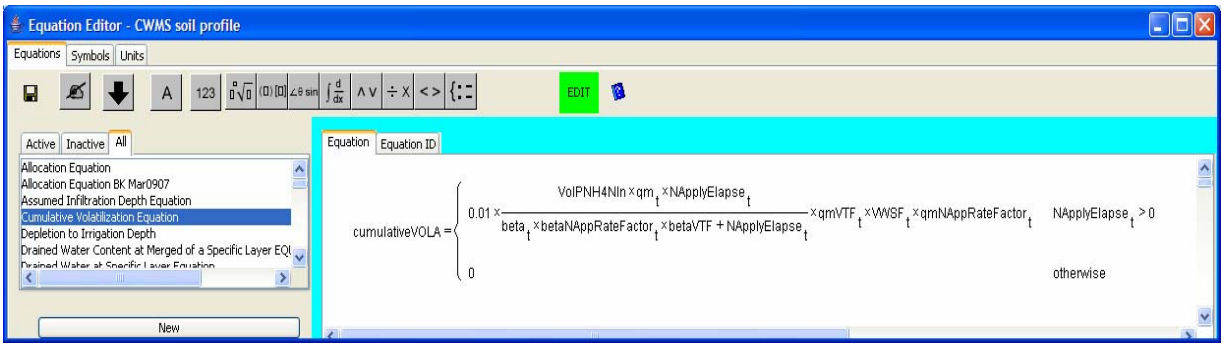


Figure 4-15. Accumulated profile volatilization equation

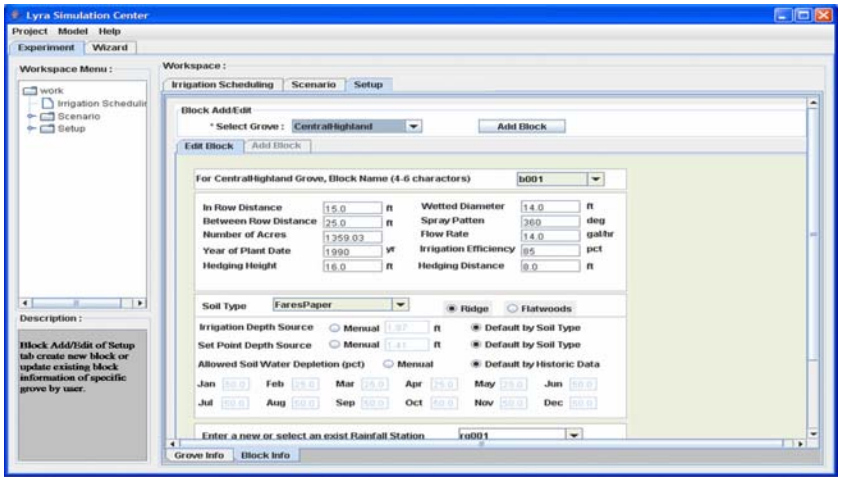
Volatilization (cumulativeVOLA) is created at the soil profile module, since volatilization occurs till 5cm soil depth from the surface. It represents a cumulative volatilization loses over a day, which is determined by the relationships between ammonium content ($VolPNH_4NIn$), days counting from the volatilization starting time (NApplyElapse), percentage of maximum cumulative volatilization (qm), and site-specific temperature/wind parameters (Figure 4-15).

Application Implementation

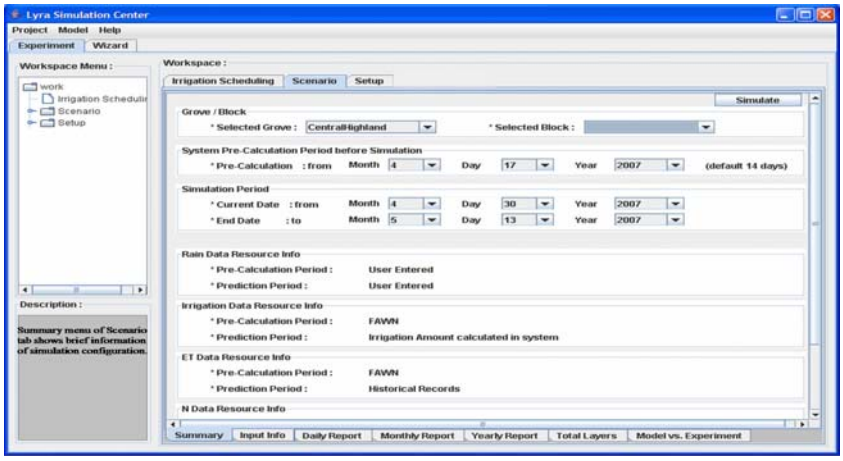
The CWMS model is used to implement a CWMS application program for use by grower that utilizes crop, soil and weather data. A CWMS application consists of the automatically generated simulation code and a graphic user interface. The generated simulation code is plugged into the graphic user interface without further coding required.

A graphic user interface allows growers to interact with the system through three phases: the setup, the irrigation scheduling, and reporting. The setup phase is for configuring the cell and block information for a particular grove (Figure 4-16a) and for describing simulation site, start/end data, and resource location (Figure 4-16b). The simulation period is separated into an initializing period and a simulation period. For a long term simulation, an initializing period can be longer than 14 days which is the default initializing period for farm irrigation scheduling.

The irrigation scheduling phase, shown in Figure 4-17 provides irrigation scheduling information to growers. By default, it is based on a 14-day simulation followed by a 3-day prediction period (the simulation period can be extended) to provide immediate term recommendations on irrigation rates. In order to plan a strategy on irrigation scheduling, simulation system tested for full seasons (over 250 days per year and over 30 years).



A



B

Figure 4-16. Setup Phase: A) grove/block and B) simulation period

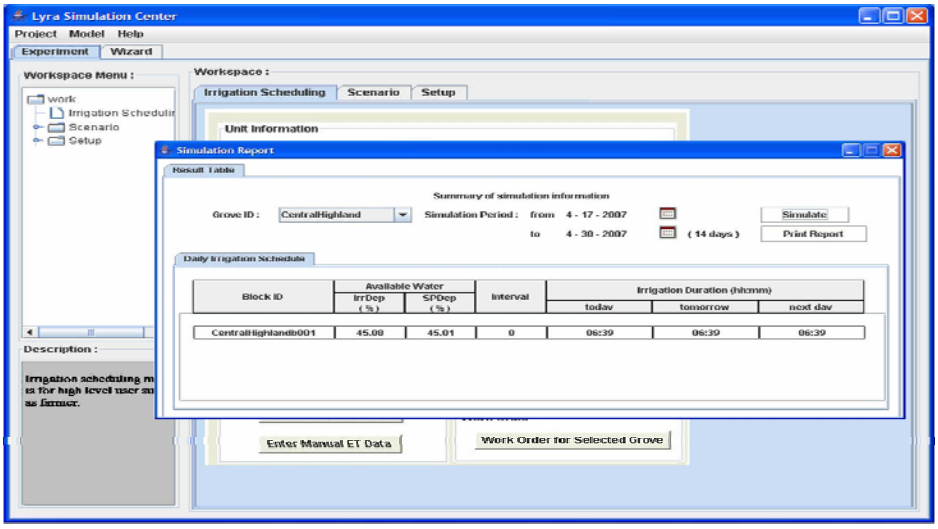
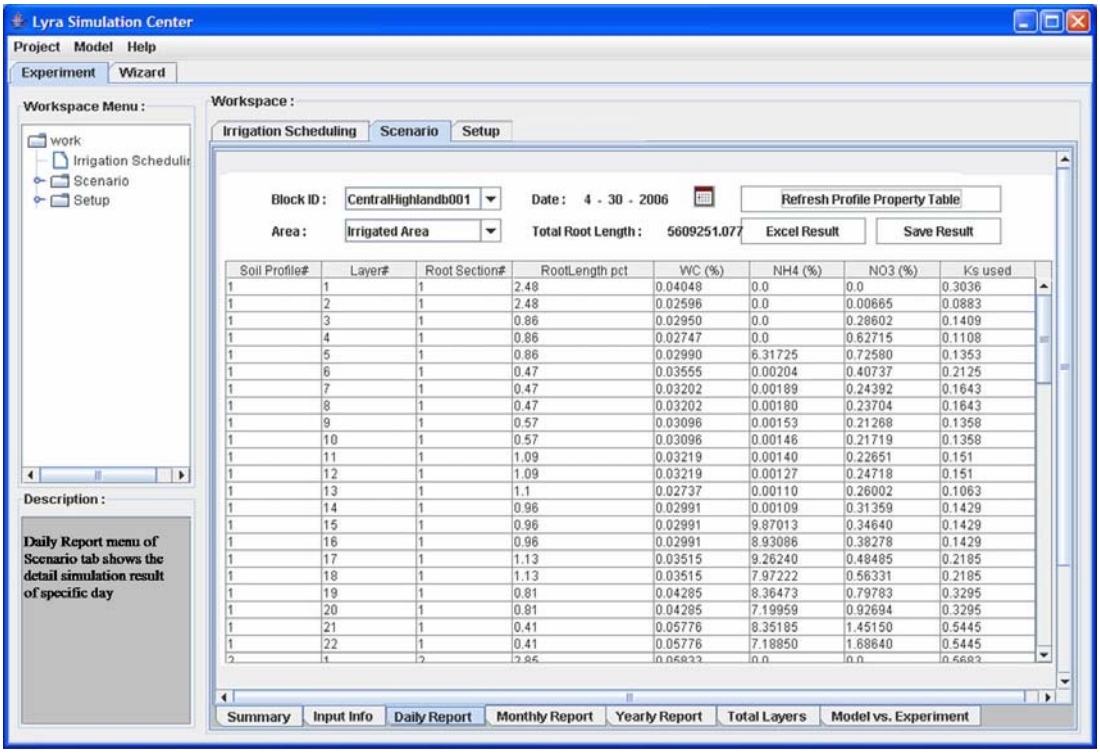
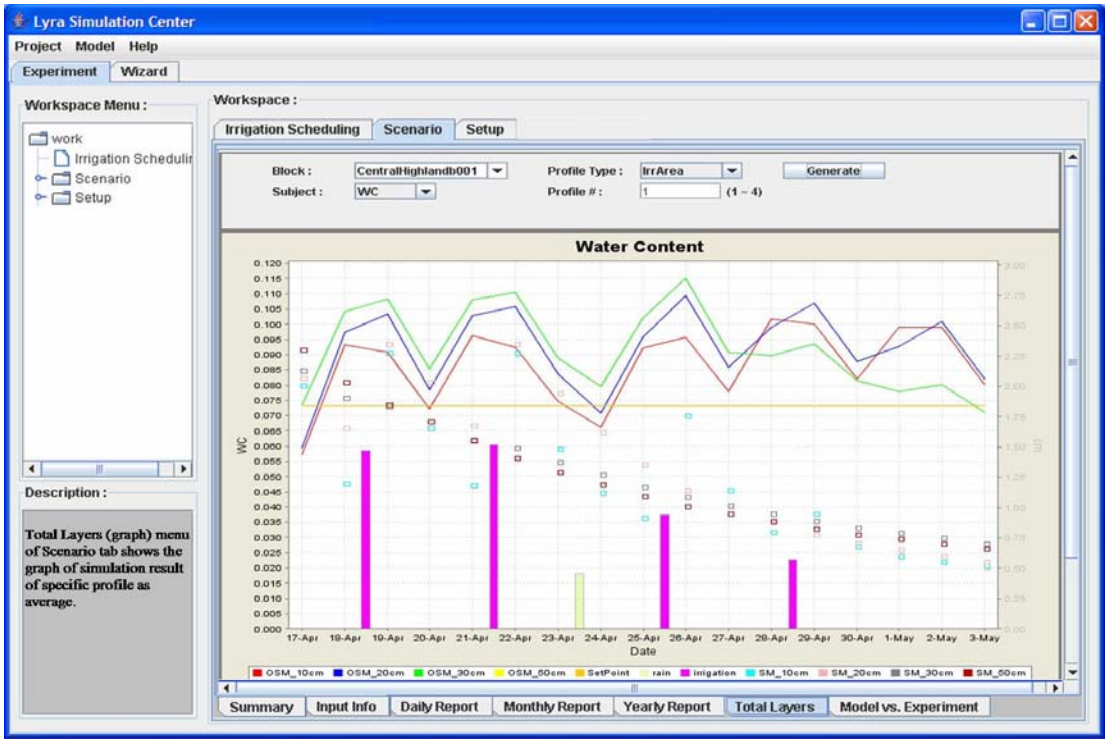


Figure 4-17. Irrigation scheduling result



A



B

Figure 4-18. Simulation results: A) table and B) graph

Detailed simulation results are provided in the form of daily, monthly, and yearly reports (Figure 4-18). The daily report contains each layer's root length, water content, nitrate and ammonium content, and soil coefficient. Data can be browsed by selecting a specific date and profile type. The monthly report shows data for a particular month including irrigation interval days and duration, evapotranspiration, crop coefficient, soil coefficient, water and nutrient leaching amount at 2 m depth and irrigation depth, rain, and irrigation. The yearly report provides the monthly total value of irrigation, rain, water and nutrient leaching amount at 2 m depth and irrigation depth, and fertilizing amount. Water, nitrate, and ammonium content contained in the daily report can be displayed as a chart.

Model Extension

The CWMS Java code was generated automatically by the SimulationEditor and the EquationEditor, and can be used as a software component that can be used independently of the model building environment. The compiled Java code can be easily connected to other user interfaces or simulation system. For example, the Watershed Assessment Model (WAM) which is used as a part of a larger FDACS BMP simulation, adopted the CWMS model as a sub-component of land use in citrus production. The CWMS model provides information about leached water and nutrient amounts to the host simulation system.

A key issue was how easily the CWMS model could be modified for integration with WAM. A water and nitrogen balance model needed by the WAM was required to use several new soil types, and modifications to the model were made to support these new parameters. Using the EquationEditor, new symbols for soil types and parameters were created and existing equations were modified by replacing old symbol and by adding new formula, and some new equations calculating required values by the WAM were added into the model. This was all

accomplished with less than 10 hours of work including creation of required file input/output protocol by WAM (that took about 80% of total work hours).

Model Performance

Simulation of the CWMS model containing approximately 700 symbols and 500 equations uses different numbers of equations depending on the combination of processes (e.g. use process of tipping bucket or effect of hydraulic conductivity). To test the performance of the CWMS model for the maximum number of processes, the combination including hydraulic conductivity, four-drain process and moving wetting front is chosen, which consists of 330 equations. Applying dimension size to these equations, total number of calculation at double precision level is 330,000 for 14 days period. It takes approximately 5 seconds by a computer with Intel Pentium 1.7GHz CPU speed and 1G RAM. Calculation time for 1, 10 and 30 years are 24 seconds, 5 minutes and 15 minutes, respectively. For an extension for WAM which contains process of tipping bucket and moving wet front, it takes 5 minutes for 30 years simulation. In order to validate the accuracy of the model, Morgan (Morgan et al., 2006a) compared the observed water contents at soil depth 10, 20, 30 and 50cm from foil surface with 2 years simulation result for two different sites. According to the validation result, R^2 values were varied in the range between 0.46 and 0.75, and for soil depth 10 and 20 cm it gave 0.7 R^2 average value which is higher than another two points. The validity of the model depends on the accuracy of the equations and parameters, and is impacted by the quality of the model implementation platform.

Model Sensitivity Analysis

Sensitivity analysis is useful method to guide model development as well as to understand model behavior when the model is under construction. This method is applied to the CWMS model for identifying most significant factors to Cell Water Amount (CWA) and determining their interaction, which has been implemented at the SimulationEditor as an additional feature.

The procedure consists of two steps: a factor screening with Morris randomized OAT design and a global sensitivity analysis with screened factors.

At the factor screening step, a variable (e.g. CWA, a sum of water amount in the soil cell) is selected to analyze the response of the system to the CWMS models' water balance processes. Variables related with the tree characteristics, water inputs (rain and irrigation) and water movement are selected as an input factor (Table 4-1).

Table 4-1. Input factors related with water input and hydraulic conductivity

no	Symbol ID	Symbol	min	max	unit
1	Canopy Volume	cv	3.2	12.6	m^2
2	Emitter Flow Rate	EFR	20	70	L/hr
3	Hydraulic Conductivity Parameter n	HCPn	2.6	4.6	-
4	Initial Depletion	Dini	0.09	0.19	-
5	Irrigation efficiency	IE	79	89	%
6	Readily Available Coefficient	KRA	0.03	0.13	-
7	Wetted Diameter	WD	100	500	cm

The selected variable used for tree characteristic was canopy volume (CV, volume of a citrus tree as function of tree age). Selected water input variables were emitter flow rate (EFR, the volume of water discharged from the emitter within a period of time), initial depletion (Dini, the initial condition of depletion), and irrigation efficiency (IE, the percentage of water pumped into the irrigation system that actually gets distributed by the emitter) and wetted diameter (WD, the diameter of the irrigation emitter). The selected variables for water movement were soil hydraulic conductivity (HCPn), was assumed to same for all soil layers, and readily available coefficient (KRA, coefficient used to calculate the readily available water content for uptake for uptake).

The minimum and maximum values of factors six different variables in Table 4-1 were applied. Six orientation matrices are generated according to the Morris factor-screening design, and the respective elementary effects for 7 different factors per orientation matrix are estimated

from the simulation response for CWA. Following Morris OAT design 8 simulation configurations are generated for each of six orientation matrices. In each orientation matrix, the first row represents the base case (configuration) and the remaining 7 are used to determine the elementary effects for all 7 factors involved.

After comparing the elementary effects of 7 factors for 6 different trajectories and the corresponding mean and variance of the distribution, factor 7, the WD, appears significantly separated from the other factors and it means that the wetted diameter dominate the simulation result. The WD increases value of CWA since it determine direct water input amount from irrigation event, but its effect compared with other factors was explained before this analysis. Whereas, factor 5 and 6, IE and KRA, has lower mean-variance relation value than other factors, so that model results are less sensitive those two factors were screened before sensitivity analysis.

At the sensitivity analysis step, 3^5 complete factorial design makes 243 scenarios with the 5 factors selected by the Morris OAT screening-factor method and 3 different factor levels. The analysis of variance on the simulation result of CWA was performed, which included interactions between two different factors. The results presented in Table 4-2 shows the sum of squares and the sensitivity index which is calculated by dividing the sum of squares with the total variability.

From the result of sensitivity analysis, the CWA was apparently governed by the WD, and Dini with a significant impact on the system than other factors. The HCPn was more sensitive than the CV and the EFR. The EFR appeared as the least sensitive factor among the main factors. The WD related the water input to the amount of irrigation. Thus, water balance could be affected significantly by the irrigation amount when there was less rainfall. For the interaction between two factors, the interaction of the WD and the CV was more significant than others, and

interactions with the HCPn had relatively larger value than other interactions because it contributed to increase water amount in deep soil layer. The CV affected rainfall into the system by blocking direct rain, and limited amount of rain could reach to soil.

Table 4-2. Sensitivity analysis result including main effects and two-factor interactions

Effects	SS ($x10^6$)	Sensitivity Index	Effects	SS ($x10^6$)	Sensitivity Index
cv	7,915	0.00102	cv*WD	7,847	0.00101
EFR	805	0.00010	EFR*HCPn	493	0.00006
HCPn	2,084	0.00027	EFR*dini	82	0.00001
dini	$120x10^3$	0.01545	EFR*WD	171	0.00002
WD	$7.64x10^6$	0.98102	HCPn*dini	63	0.00001
cv*EFR	145	0.00002	HCPn*WD	914	0.00012
cv*HCPn	993	0.00013	dini*WD	99	0.00001
cv*dini	19	0.00000	residuals	5,919	

Sensitivity analysis result provides information about impact factors and related factors impacts. It may be useful to reconfigure model parameter and to create other models using these symbols.

In Chapter 4, the CWMS model developed by Morgan et al. (Morgan et al., 2006a; Morgan et al., 2006b) is implemented using ontology-based simulation methodologies and tools covered in Chapter 3. Soil geometry structure is designed with 4 concepts, soil block, soil cell, soil profile, and soil layer and their dimensions are defined with index concepts describing array size. With the existing mathematical models symbols and equations are defined and entered into the ontology, and they formed a model base containing symbols and equations and structuring relation between them. Model performance is tested under two different simulation conditions, and using a sensitive analysis tool, critical input factors and the associated factor relations are revealed for water amount in the soil system. Through these processes the CWMS model is created and executed efficiently by the graphic interface program.

CHAPTER 5
SUMMARY AND FUTURE WORK

The following methodologies were developed utilizing ontology-based simulation techniques to build mathematical models.

1) The EquationEditor includes a symbol dictionary for entering symbols appearing in the equations along with their definitions and units. Symbols are defined by specific concepts. Equation are rendered visually using classic mathematical notation, but internally a hierarchical data structure (tree) is used for storing operators and symbols. The equal operator is the root node of the equation tree. Operators (like + and -) used in the equation become a node in the tree with child nodes being additional operators or symbols. The Equation Object Model (EOM) used in the Equation Editor is a collection of basic objects which represent information describing a mathematical expression and defining data type of attributes, and which communicate with ontology-based database system to retrieve data.
2) The SimulationEditor incorporates the EquationEditor and is designed to represent the structure of dynamic systems using graphic elements. The SimulationEditor also contains facilities for automatically generating and running simulations and providing reports. The SimulationEditor provides a graphic user interface to create and maintain a simulation system; a structure design interface for the simulation system, a simulation control interface, a simulation result reporting interface, and some additional interfaces including a math markup language generator and a statistical model analyzer.

These methodologies were applied to develop a model of the Citrus Water Management System. Approximately 700 symbols and 500 equations are conceptualized and stored in ontology database using the SimulationEditor and EquationEditor. A Java program for running the simulation was generated automatically from the modeling environment and incorporated into both a stand-alone application for grower and WAM. The modeling environment provides adequate tools to create and modify models without any programming knowledge. From the results, it can be concluded that ontology-based simulation offers a significant improvement in the methodology for building, publishing, and managing model.

For the next step, it will be useful to study model reusability within the existing model base of the CWMS model. Issues on model reusability are related with the scale of models in the problem domain, which requires the consistency of the temporal and spatial scale to guaranty compatibility in models (Leon et al., 2002). For a similar scale domain problem with the CWMS model, such as models using different soil profiles, limitation placed on reusing these sub-models are that they have rigid and sophisticate connections with other processes such as a hydraulic conductivity which has strict requirement for spatial scale. On the other hand, from an extension study of the CWMS model, WAM, in which two different models cooperate independently keeping the internal scale of the model may cause significant inefficiency of simulation time. There are needs for an efficient way to organize and classify models and processes within a model base and for a flexible way to constructing a set of simulation model for different project and modeler by switching with a different process. Diverse level taxonomic categories may help the model base to be handled more intuitively.

The data reusability could follow the model reusability. Especially, relational databases are important sources of data for simulation model, but it is expensive to identify existing data, to

determine the exact format of data and to use data in a model. There has been research to convert directly relational databases directly to ontology using a mapping language (Barrasa et al., 2004) and to transform/service various heterogeneous database sources including database as ontologies (TopBraid, 2003). It is difficult to provide a formal way to use databases as ontologies since security and restriction level of data varies and case depends on the domain. Therefore, it will be useful to study sharing databases as a form of ontology for a simulation model in the agriculture domain to build an efficient simulation model network. This study can include methods to publish/search databases, negotiate/communicate automatically to get wanted data, and provide a protocol for networking within the domain. Finally, a visual environment will be required to enhance the reusability of models and data and ontology since they have a complicated relationship and structure. There are some studies on solving complexity problem in displaying ontology visually (Bosca et al., 2005; TouchGraph, 2005), but it needs to develop methods focusing on the relations in model and data.

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