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About Models

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1. Introduction - Models

In agricultural sciences mathematical models were not popular until the 1960s. There are now numerous models in existence that simulate growth processes. They differ in their objectives, levels of complexity and relation to other agricultural components. Model applications ranging from data interpretation to technology transfer, to decision support e.g. AusVit (developed by the Cooperative Research Centre for Viticulture) have not only advanced our understanding of growth processes but have also provided a theoretical basis for management.

Although vine growth models are still premature in terms of making regulatory management decisions and they are mostly at the research stage, they have been used to analyze real-world problems (France and Thornley 1984; Godwin and Jones 1991). These include fertilizer management (Ma et al. 2001), yield estimation (Schultz 1995; Williams 1996; Iacono and Sommer 1996), berry characteristics (Ebadi et al. 1996) and disease incidence models at various scales (Broome et al. 1995). On the other hand, Tedeschi (2006) suggests that methods used to model a plant may sometimes mislead and need checking.

Models are made up of sub-models. The process of breaking down a complex model of vine growth using sub-systems and their relationships is part of a **Systems Approach.** This is a method that helps us comprehend aspects of many scientific disciplines where due to the complexity of the vine growth processes and their dynamic responses to environmental conditions, it is beyond our mind's ability to quantitatively synthesize all the knowledge available.

Types of Models

Most models are either **empirical** (also called functional) or **mechanistic**. The best-known empirical models are soil nitrogen (N) test correlations. In these, large numbers of field trials are combined to predict the optimum N inputs, usually based on measurement of soil nitrate, for achieving maximum crop yield or maximum economic yield and in some cases taking into account possible environmental outcomes. The N input recommendations are specific to crop and soil type and may be modified according to expected moisture conditions. Empirical models are usually well accepted by practitioners because they are based on extensive field data and experience. It is noteworthy that soil test correlation results are often adjusted according to the experience of the expert recommendation committee and further modified by practitioners in the field. While N recommendations based on soil nitrate tests are effective for annual crops, they are less useful for perennial crops that have the capacity to store limited N in tissues from season to season. Predicting these N requirements requires an understanding of soil processes, especially mineralization and immobilization of N, which are best described by mechanistic models.

While empirical models are effective, they are not robust. They cannot be easily transferred from one location to another, nor can they easily accommodate new considerations or new information that was not included in the original model development.

Mechanistic models are more robust than empirical models because they are based on scientific formulae and describe the actual physical and biological processes in the soil-crop system. They have been less common as they are more difficult to design.

Mechanistic models (Figure 1 and 2) are increasingly based on Object Oriented Programming (OOP) (Meyer 1988; Lemmon and Chuk 1997; Sequira et al. 1997).

Model Components

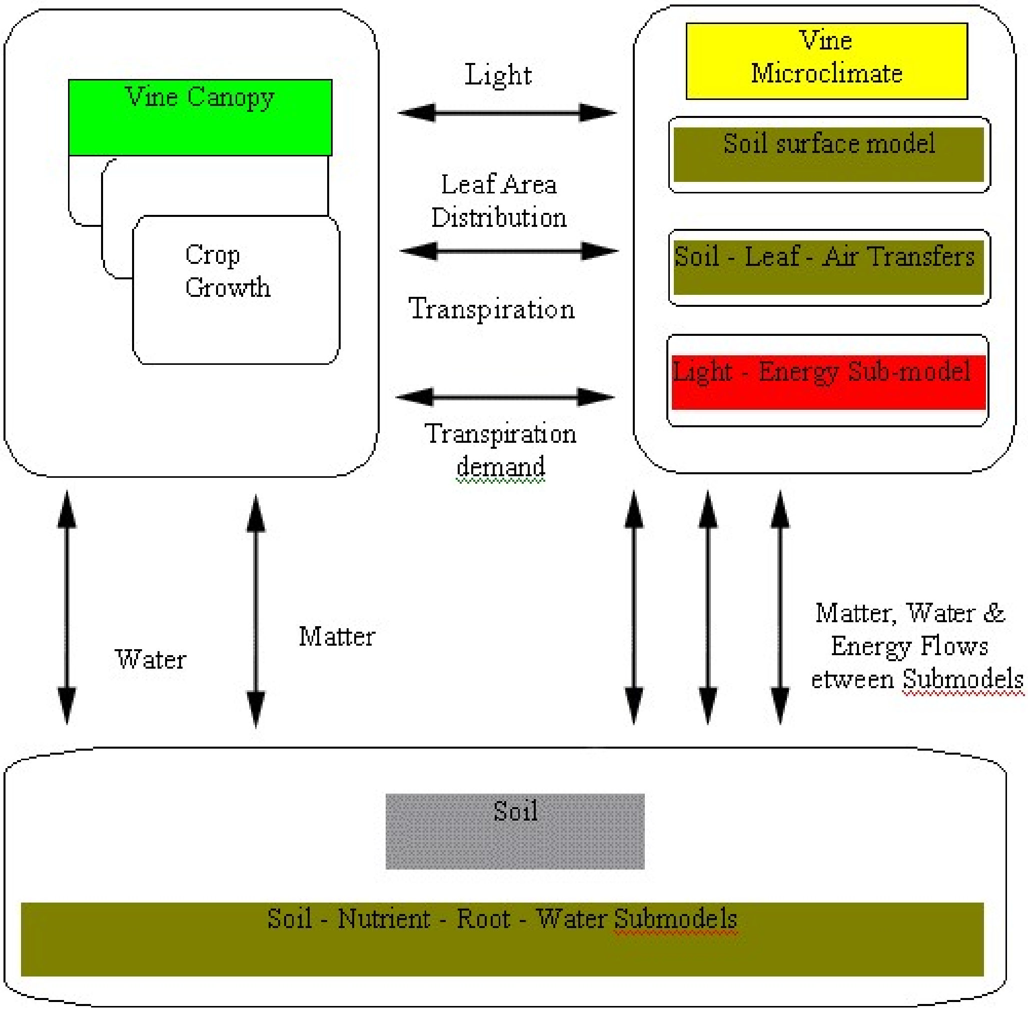
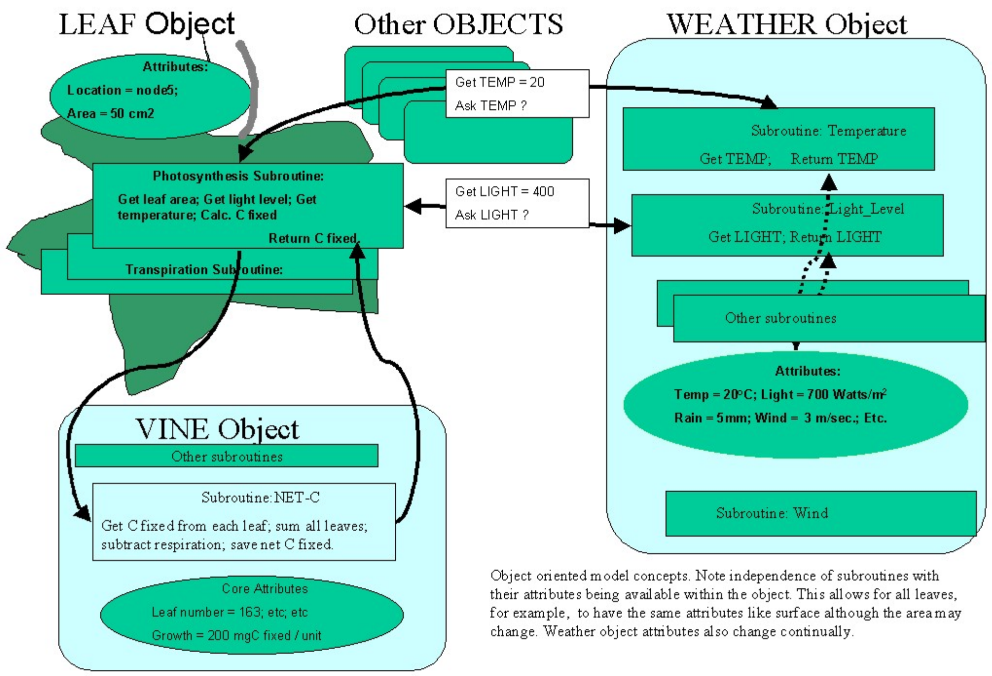


Figure 1: Object Oriented models - A schematic model overview shows flow of information, energy and matter with arrows. The boxes represent modules of a program. One module is used to contain all the plant part model internal relations (a box is used to show this). The model designers can then specify what inputs and outputs a particular programming module has which allows easier overall control of the programming of complex relationships such as occur in the vine. This method is sometimes called Object Oriented Programming because we think of the objects in a simulation, like a leaf or berry, rather than complex, interrelated equations which may be hard to follow.

These models consist of sub-models that *make common sense* in terms of the relationship of the parts. OOP also allows common sense inheritance to occur. Therefore, if you have a sub-model of a leaf then any new leaf inherits leaf like properties. This becomes useful if you are modelling a vine and need to add new leaves at the end of a shoot. You can just say *add new leaf* as the computer program runs instead of specifying all leaf characteristics again for each new leaf.



Object oriented model concepts. Note independence of subroutines with their attributes being available within the object. This allows for all leaves, for example, to have the same attributes like surface although the area may change. Weather object attributes also change continually.

Figure 2: Object oriented model concept. Note inter-dependence of sub-routines with their attributes being available within the object. The leaf object *asks* the weather object for the temperature. The weather object gets the temperature from its attributes (which change continually) and returns the information to the leaf object. The leaf needs the temperature to help calculate photosynthesis for the vine (also an object). Whilst apparently cumbersome, this method allows quick duplication of leaves or vines as modules with their own characteristics i.e. all leaves are flat and can photosynthesize. The new leaf is said to *inherit* the attributes of the existing leaves. This both speeds up programming and reduces mistakes.

Is the Model Valid?

Most model developers provide experimental data in support of their model. Growth models have a history of being difficult to parameterise, especially after the introduction of multiple resource pools such as soil nutrients or sub-model objects. Pool sizes and associated rate parameters are difficult to measure. A model that consistently performs well may be accepted, but its validity may be demonstrated only for use in particular situations (Molina and Smith 1998). Whitmore (1995) and others have pointed out that the disagreement between simulated and measured soil N model values, for example, may be due to problems in getting accurate samples in the field. Diekkruger et al. (1995) concluded as a result that it is sometimes more important to improve field measurement than to develop new models.

One difficulty with models is determining the rate coefficients used for various process simulations, which may be various mathematical functions (first-order, zero-order, or Michaelis-Menten kinetics for some enzyme rates). Occasionally, a mathematical algorithm is used for some simpler models (France and Thornley 1984).

Another problem is validating the effect of sub-system interactions on results in the field. The rate coefficients may be constants, but often are modified for soil type, temperature, and variety effects (Beckie et al. 1995). Most models are still using a zero to one index for each environmental factor, but some integrate response curves for the combined environmental effects. VineLOGIC integrates the effects of each of these environmental factors by determining which is the most limiting on any one day and using that to modify plant growth processes.

When data for validation are lacking, using the opinions of experts to gain confidence in a model, called a subjective face validity approach, was suggested for multi-criteria analysis projects by Qureshi et al. (1999). This approach helps to engage large numbers of knowledgeable specialists in the process of model validation and was used in the early stages of VineLOGIC development. Engaging a larger population of model users is useful because the majority of data and knowledge for model inputs resides with possible model users.

Fundamental misunderstanding of the modelling process can sometimes cause errors. Lee et al. (1996) reviewed several reports in which groundwater modelling was used to choose the best actions to remediate groundwater contamination. Mistakes in model use, found in every report, included misunderstanding the models, improper application of boundary conditions, poor estimation of input data, lack of validation or calibration and misinterpretation of results. Of these *inappropriate input parameters* is rated as the worst problem. This study shows an urgent need for increased education in the use of models especially when the model use may influence industry policy.

The topic of model validation and testing continues to be examined. Although vine growth models cannot ever be absolutely validated because not all cases can ever be tested, there exists a considerable body of test data for most of the major models (Greenspan et al. 1996).

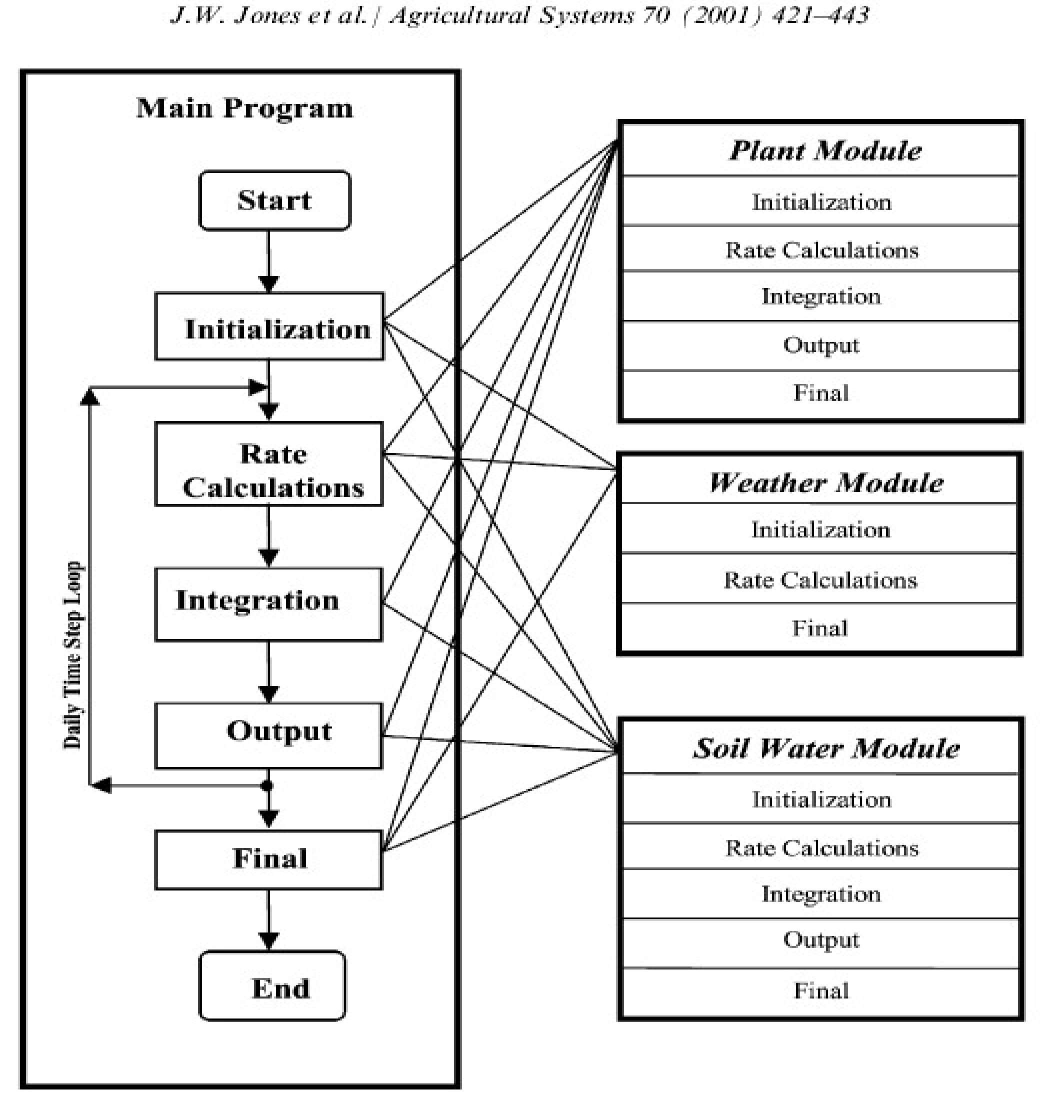


Figure 3: Example vine sub-model components on the right used in a mechanistic simulation of the plant's growth. Many of the *boxes* would contain other sub-models and so on. The OOP models use the same sub-models it is just the programming of the interactions which is different.

From Jones JW; Keating BA & Porter CH, (2001): Approaches to modular model development. Agricultural Systems, 70: 421-443.

Advantages of a Graphical Interface

The principal advantage of a graphical interface for models is that symbols take the place of programming code or numbers. To the user, the graphical model is transparent rather than a black box, for example, the dynamic TOMGRO model of Jones et al. (1991) showing tomato growth and fruiting on screen. Dynamic, mechanistic vine models are inherently very complex because of the many processes involved, but the graphical format enables non-programmers to more easily understand the structure and assumptions of the model. As discussed above, users must understand models to use them correctly. The user can reflect on the model construction and assess if the modeller has included all essential system elements (Diekkruger et al. 1995). In part, understanding of the model is gained from being able to access output data from many parts of the model at once.

In addition to the model, a simulation requires an interface displaying the simulation in a proper way and some facility to change the parameters while the model is running (Gary et al. 1995). Simulations designed to support learning must have user interfaces that reflect the model so that the learners can create a mental model of the vine growth and performance.

Another important outcome of the graphical interface is that it places some of the responsibility of model validation in the hands of the user. Given that models can never be validated for every location and circumstance, a solution is that users carry out the validation for their own needs and environment. The graphical interface enables users to observe any flow or transformation of the simulation. Users can then compare model performance with their own data as well as personal experience. In this way, the vast knowledge of non-modellers can gradually be incorporated into future versions.

Future Directions

Given the current status of vine models, the question needs to be asked - where are we headed? From the research side, a more mechanistic, process focused approach to modelling is emerging with help from object-oriented languages and tools such as C++, Java and Python languages (Booch 1991). There is also more emphasis being placed on waste water for irrigation purposes and salinity issues, and future progress will depend on correctly addressing interactions between processes and developing methods to more effectively parameterize all levels of models. Evaluation of environmental impact using the Life Cycle Assessment modelling (Canals et al. 2006) is an emerging technique which will impact on viticulture model use.

Previously, use of models has largely been restricted to research and graduate level education (Gunn et al. 1999). These writers found that models with easy-to-use interfaces, databases, and supporting material were an effective educational tool for early undergraduate education, for example models may serve as a general introduction to students about the fundamental components of the vine growth cycle. For advanced students, the model provides direct access to the equations, and information about sources of the equations, with the possibility of carrying out research by exploring alternative algorithms (Bittman et al. 2001).

Students taking advanced courses in horticulture and viticulture can explore the mechanics of the model, the sub-model relationships and learn about some of the assumptions. They can game-play with the model and test sensitivity. These students will gain understanding about the behaviour of systems in general and the vine system in particular. At the graduate level, there is potential to adapt a model to suit specific needs, such as looking at new varieties, pruning methods, considering fluctuating watertables, etc.

Knowledge of the vine system through simulation models is no longer the domain of modellers alone but essential for everyone involved in managing resources on farms and in the environment. This knowledge is required to generate better agricultural practices and environmental policies. When many field workers and specialists are trained in vineyard simulations, the quality and validity of models will improve, and more managers will be inclined to make use of the resource. Also, there may be fewer cases of model misuse.

Summary

Thanks to advances in computer hardware in recent years and the sophistication of the modelling platforms including object-oriented programs, graphical versions of dynamic vine models can be run efficiently, even while generating substantial graphical and tabular output. Therefore, the graphical interface is now more than a teaching tool; it is also a convenient platform for routinely running the model.

With the rise of the Internet and instant access users are demanding models that are easy to use and that have accessible databases. This will soon mean models that can be accessed and run on the Internet with data found on the Internet. There are several advantages to developing and running vine models on a graphical platform.

(1) There is no source code
(2) The entire model is visible - not a black box
(3) Model construction is rapid and requires little technical programming skill.

The graphical interface makes models accessible to more people involved with management issues. This approach involves the user in the validation process and encourages users to obtain the required input parameters, and perhaps even to develop better techniques for measuring the parameters.

While involvement with graphical models does not require knowledge of programming it does require an understanding of systems, modelling, and simulation. Due to the complexity of the processes, the model may be difficult to grasp without instruction. For example, it potentially may be a useful tool for teaching the water balance system specifically and *system thinking* in general. Students may learn first by operating the model, then by manipulating it, and finally by modifying and enhancing it. Having these future resource managers skilled in graphical modelling will help to prevent the misuse of models, which is a growing concern as policy-makers rely increasingly on models for political decisions. For example, climate change models.

The ability of vine models to make projections of future outcomes of management scenarios with respect to key environmental areas such as nitrate leaching, carbon sequestration, and emissions of greenhouse gases has generated intense interest in using them as regulatory tools. Criteria need to be developed for model certification if they are to be used in regulation (Shaffer and Hansen 2001).

With the introduction of crop yield monitors and global positioning systems (GPS), interest has been generated in the potential use of models for site-specific or precision management. The use of vine growth models like VineLOGIC with real-time remote sensing data will enhance our ability to predict vineyard dynamics and plant biomass productivity.

Development and implementation of these models will have a major impact on projections of management effects on the environment. Models have provided tools for use in estimation of nitrogen fertilizer requirements, water use patterns, berry growth and canopy distribution affecting light interception. Farmers can be readily shown the impacts of their management on the environment and given answers to *what-if* questions regarding crop response to management practices. However, because farmers may not be able to use models directly, a model-based information-decision support database is often needed for extension and technology transfer.

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2. Soil Water Balance Model Example

In many systems the model is divided into sub-models. An example is the SOIL-WATER sub-model. In terms of the whole model this *black box* feeds information regarding the availability of water to the PLANT GROWTH and PHENOLOGY sub-models. It takes as input some plant values, from the PLANT GROWTH sub-model and from the PHENOLOGY sub-model. Below we want to illustrate how a SOIL-WATER sub-model might work. Note that this is purely an example and is not necessarily descriptive of VineLOGIC versions.

The role of the soil water sub-model (or object) is to predict the proportion of the water stored in the root-zone which is available to the crop, and incorporate this into the crop Growth Factor used in the simulation.

Water availability in the root-zone is largely determined by the water balance in which rainfall, run-off, and evapotranspiration (E) - incorporating plant transpiration and soil evaporation are the main factors. Rainfall minus run-off is called effective rainfall. Solar radiation and temperature influence both the amount of evapotranspiration (E) and the rate of dry matter production through photosynthesis.

A comparison of different models, under a wide range of rain-fed and irrigated conditions, has shown that a 'single reservoir' model is capable of estimating the soil water use by most crops. These models are based on the maximum rooting depth, where water holding parameters are averaged over the entire rooting depth without making allowances for different water holding capacity by layer or soil type.

The crop water requirements are calculated from a reference crop evapotranspiration estimated by the modified Penman-Monteith equation (Doorenbos and Pruitt 1977). The reference crop evapotranspiration is modified by a crop factor (K_{vine}) that depends on the stage of growth information provided from the PHENOLOGY sub-model to obtain the maximum potential evapotranspiration. So perhaps when there are few young leaves the crop factor will be lower than at full leaf phenological stages. The Penman-Monteith equation used resulted from the work of Penman (1948) at the Waite campus of Adelaide University in South Australia and modified by Monteith in the 1960s and is now used very widely.

Soil specific parameters in the sub-model are the volumetric water content at field capacity (FC) and at permanent wilting point (PWP). They are averaged over the depth of the root zone although they may be weighted by the relative thickness of every horizon in the root zone (as is done in VineLOGIC). Here we consider the simpler method.

Volumetric water content at soil matric potential of 10 and 1500 kPa is used to estimate field capacity (FC) and permanent wilting point (PWP) respectively for vines, however these values of FC and PWP differ for each crop and variety.

Water balance in the model may then be estimated daily using the following criteria:

1. The evapotranspiration procedure calculates the maximum potential evapotranspiration for the vine, E_{max} (mm/day), from the product of the modified Penman reference evapotranspiration E_{ref} and the crop factor, K_{vine} mentioned above. The crop factor may be calculated according to the procedure of Doorenbos and Pruitt (1977) or determined from experimental work. The average K_{vine} is about 0.45.

2. Maximum evapotranspiration, E_{max} (mm/day) is compared with the effective rainfall or irrigation additions. If the effective rainfall/irrigation is sufficient to meet the demand there is no soil water deficit. If E_{max} is higher than effective rainfall/irrigation, there is a water use (deficit) that could be met by extracting some of the soil water stored in the root zone.

3. If the available soil water is above a critical level, the deficit could be met by soil water. The critical fraction of the maximum water storage in the root zone, given the symbol 'p', is tabulated in Doorenbos and Pruitt (1977) as a function of E_{max} (ie reliant on atmospheric demand) and type of crop. Experiments can provide data of the form shown in Figure 1. This shows that at some point between wilting point (PWP) and field capacity (FC) water does not limit the crop growth. Between that soil water value and wilting point it becomes more and more difficult for the plant to extract the water. This relationship may be shown by a second order polynomial regression between the tabulated values of p and E_{max} values for vines allowing a continuous relationship to be used in the model. An example fit gives a relationship of the type:

$$p = 1.036 - 0.133E_{max} + 0.006E_{max}^2 \qquad \text{(eqn.1)}$$
$$= \text{(no units)-(mm/depth)+(mm/depth)}$$
$$= 0.69 \text{ for a } E_{max} \text{ of 3.0 mm per day in this example.}$$

Critical water storage (M) is calculated as:

$$M = p \times W_{tot} \qquad \text{(eqn.2)}$$

where W_{tot} is the maximum water storage in the root zone (mm).

So the soil water **not** readily available for crop use:

$$= (1 - p) \times W_{tot} \qquad \text{(eqn.3)}$$

When the actual water storage is higher than the critical storage level, the roots are able to easily extract water to meet crop requirements and the actual rate of evapotranspiration E_a is equal to the crop water requirement ie E_{max}. However, when the water storage in the rootzone is lower than this critical level, the actual water use E_a is lower than the requirement and the relative reduction in water use is the ratio of the actual storage and the storage at the critical level (see Fig 1).

In order that this instantaneous relationship is calculated for the time interval of the model (usually one day) then we need to integrate small time intervals of evapotranspiration E_{max} during the day to get a daily E_a figure of actual crop water use as mm per day.

E_a = soil water at start of day x exp [E_{max} / (1-p) W_{tot}]

{Note that E_a is the change in daily soil water plus irrigation additions or rainfall}

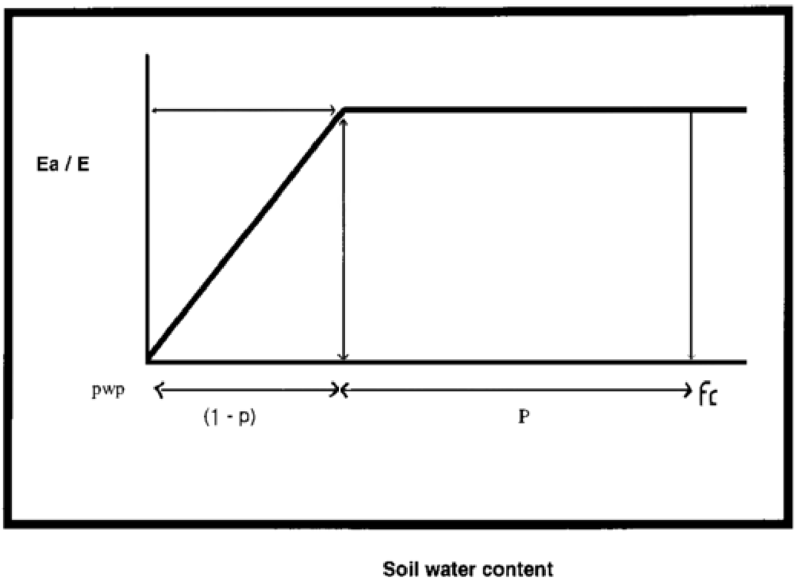

Figure 4: The relative crop water use as a function of the water storage in the root-zone (Doorenbos and Pruitt 1977). FC = field capacity; PWP = permanent wilting point, p = fraction of total soil water above PWP which is easily extractable by the crop; (1 -p) = fraction of soil water difficult to extract; E_c = crop water requirement (mm/day); E_a = actual crop water use (mm/day).

When the soil water content in the root-zone falls below a critical value, the rate of water uptake by the plants and the rate of growth are reduced. Moisture stress is assumed to occur below the critical moisture content in the soil and to be related directly to the E_a.

In a model a growth factor associated with the water availability may be included such that:

Growth Factor = E_a / E_{max}

And this growth factor will be 1.0 until a critical level of soil drying is reached. Then the growth factor is reduced to zero as the soil dries to permanent wilting point. This growth factor is called by the VINE object in the model to help determine the amount of carbon (C) that can be "fixed" for each day, here depending on the soil water levels.

Other things like light levels and available nutrients for growth will also affect the Growth Factor. Other sub-models would calculate these.

Partly adapted from A. Shepherd A., McGinn, SM and Wyseure, GCL (2002), Ecological Modelling 147 (2002) 41-52

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