QUEENSLAND WATER MODELLING NETWORK

Water planning, integration and management

# MEDLI Science Review: Synthesis report

## Final report

Report prepared by

Prof Ted Gardner

For the Queensland Water Modelling Network

Queensland Government

The Queensland Water Modelling Network (QWMN) is an initiative of the Queensland Government that aims to improve the state's capacity to model its surface water and groundwater resources and their quality. The QWMN is led by the Department of Environment and Science with key links across industry, research and government.

Prepared by: Prof Ted Gardner (Victoria University)



Citation

Ted Gardner (2021). MEDLI science review: Synthesis report. Report to the Queensland Water Modelling Network, Department of Environment and Science.

Acknowledgements

QWMN commissioned a review of MEDLI (Model for Effluent Disposal using Land Irrigation) to assess the science underpinning its Hydrology, Nutrient & Pond Chemistry modules, to identify gaps, and suggest possible improvements. This Synthesis report is one of five reports written for the MEDLI Science Review by a team led by Prof Ted Gardner (Victoria University). Other reports from the MEDLI Science Review are "Hydrology – Model and process" by Dr Tony Ladson; "Pond chemistry module" by Dr Mike Johns and Dr Bronwen Butler; "Methodologies used by biophysical models for simulating soil nutrient pools and processes in pasture systems - Carbon, nitrogen and phosphorus" by Dr Phil Moody; and "Modelling of Water and Solute Transport in MEDLI" by Prof Freeman Cook.

# Table of Contents

## Abstract

A review of MEDLI model was commissioned by QWMN to assess the science underpinning its Soil Hydrology, Nutrient & Pond Chemistry modules, and to identify gaps and suggests possible improvements, given that MEDLI was released in the mid-1990s. The hydrology review concluded that the Cascading bucket-CN-Ritchie evaporation structure was still relevant and fit for purpose, although some changes were suggested to the soil evaporation, soil water distribution, and solute leaching algorithms.

The algorithms used in the N module are similar in concept, if not detail, with the more sophisticated N models used in APSIM and DAIRYMOD. However, MEDLI does not contain a soil carbon model, but its relevance to *cut and cart* pasture is questionable due to minimal stubble residue. A major concern is for realistic denitrification prediction, and a critical value is the maximum denitrification rate. A detailed literature review on this topic is warranted. MEDLI must also consider the substantial volatilization loss (>= 50% TAN) from high pressure spray irrigation.

MEDLI uses the Freundlich equation to calculate sustainable soil phosphorus life. Given its cost and measurement difficulty, its discontinuation is recommended for all but very sandy soils in close hydraulic connection to surface receiving waters. It should be replaced (after appropriate testing) with the more easily measured Colwell-P:PBI ratio method described by Moody (2021).

The P export pathways of most environmental concern are via sediment attached and dissolved forms in the surface runoff. Sediment loss is unlikely in permanent cut and cart pasture. The loss via dissolved P can be estimated from soil solution P predictions and a soil solution P-runoff P relationship. It is unlikely the magnitude of dissolved P loss (< 1 kg P/ha/yr) is worth significantly extra modelling effort in MEDLI, but the effort is warranted for other QWMN models.

The Pond Chemistry module, which models pond nutrient loss, has been identified as the process most in need of improvement in MEDLI. Alternative empirical, but physically sensible algorithms have been recommended for predicting the reduction in soluble N and TP. However, nutrient loss via the settling of the nutrient rich algal biomass remains a vexing question. Future focus should be on treating low strength sewage effluent rather than high strength agri-industrial wastewater.

Perhaps the biggest conceptual challenge in modifying MEDLI algorithms is experimental evidence that the changes will predict more realistic/accurate outcomes. This applies particularly to the soil hydrology processes and denitrification.

# 1. Summary

QWMN commissioned a review of the MEDLI model to assess the science underpinning its Hydrology, Nutrient & Pond Chemistry modules, to identify gaps, and suggest possible improvements given that MEDLI was released in the mid-1990s. The reviews were undertaken by Dr Tony Ladson, Dr Phil Moody and Drs Mike Johns and Bronwen Butler respectively. This report draws heavily on their work.

**Soil Hydrology Module**: After reviewing 18 one-dimensional hydrology models in detail (see **Appendix A**), it was concluded that the Cascading Bucket-Runoff Curve Number-Ritchie evaporation structure was still relevant and fit for purpose, although some changes were suggested to the soil evaporation, soil water distribution, and solute leaching algorithms. A major issue identified was the absence of experimental data sets to confirm or otherwise MEDLI predictions, especially deep drainage. A more physically based infiltration algorithm (Green & Ampt equation) is worth investigating for runoff prediction from irrigation areas. However likely gains in precision from adopting the physically rigorous SWIM module (based on the Richards equation) is probably not worth the effort for most MEDLI applications. Informed choice of more physically rigorous, deep drainage and solute leaching algorithms will require input from an appropriate (soil physics) specialist after a comprehensive literature review (see Cook 2021).

**Nitrogen Module:** The Michaelis-Menten type algorithms and scaling factors used in the N module are similar in concept, if not detail, with the more sophisticated N models used in APSIM and DAIRYMOD. However, MEDLI does not contain a dynamic soil carbon input model, which is essential to model the N (and P) transformations from organic surface residues. Having soil C dynamics driving the N processes is mechanistically correct, is intuitively logical, and could be incorporated into MEDLI reasonably easily, but its relevance to cut and cart pasture is questionable (due to minimal stubble residue). A more important concern is appropriate denitrification prediction, and this is difficult to improve given the general absence of independently measured experimental data, although choosing a well justified maximum rate (kg N/ha/day) is essential for all subsequent calculations. A literature review to better define this value is warranted. Other assumptions in the denitrification algorithms tend to reduce the predicted loss, in that labile C is often assumed to be limited to the top 10 cm or so of soil, which will drain to the DUL within a day or so. Hence the opportunity for denitrification is limited by both the assumed depth of labile C and the duration of waterlogged conditions. The predicted denitrification response to less conservative assumptions is worthy of investigation. Unlike other N models, MEDLI must consider substantial volatilization loss (>= 50% TAN) from high pressure spray irrigation, but the value is probably best informed by experimental measurement rather than theory.

**The phosphorus model** in MEDLI uses the Freundlich adsorption isotherm equation to calculate the irrigation time (years) corresponding to significant breakthrough in soil solution P concentration at the "compliance" soil depth (=> rooting depth). Given the cost and difficulty of obtaining the adsorption data, and the low risk of its off-site movement in groundwater, its discontinuation is recommended for all but very sandy soils in close hydraulic connection to surface receiving waters. It is recommended it be replaced (after appropriate testing) with the more easily measured Colwell-P:PBI ratio to predict soil solution P using the algorithms developed by Moody (2021). The P export pathways of most environmental concern are via sediment attachment and dissolved forms in the surface runoff. Sediment loss is unlikely in permanent cut and cart pasture, but the HowLeaky model provides guidance if this assumption were to prove incorrect. The loss via dissolved P can be estimated from soil solution P predictions (based on the Colwell-P: PBI ratio) and a soil solution P-runoff P relationship, although the latter function is rather uncertain. It is unlikely that the magnitude of dissolved P loss (< 1 kg P/ha/yr) is worth significantly extra modelling effort in MEDLI, but the effort is warranted for other QWMN models.

**The Pond Chemistry module** has been identified as the process most in need of improvement in MEDLI because of errors of overestimation in nutrient "loss" via sediment settling, and conceptual errors in the main N loss processes from ponds. Alternative empirical algorithms have been recommended for predicting reduction in **soluble** N and TP, and both have had some degree of validation. However, the settling of algal biomass which sequesters substantial amounts of soluble N

and P remains a vexing question. It is recommended that future changes to MEDLI focus on treating relatively low strength sewage effluent in a multi pond system, given high strength agri-industrial wastewater is now usually treated using engineered systems that produce an effluent of consistent composition.

Perhaps the biggest conceptual challenge in modifying MEDLI algorithms is experimental evidence that the changes will predict more realistic/accurate outcomes. Algorithms with increased complexity and physical realism will not necessarily achieve this outcome because of difficulties in estimating input parameter values.

Some recommendations are made as to how similar future similar model reviews should be managed by the commissioning client and executed by the selected contractor(s).

# 2. Introduction

A review of MEDLI model was commissioned by QWMN to assess the science underpinning its Soil Hydrology, Nutrient & Pond Chemistry modules, and to identify gaps, and suggests possible improvements given that MEDLI was released in the mid-1990s. The reviews were undertaken by Dr Tony Ladson, Dr Phil Moody and Drs Mike Johns and Bronwen Butler respectively and followed a three-phase process:

1. Describe Methodology and provide a first pass of key science elements and knowledge gaps. List of other QWNN models that could potentially benefit from the review
2. Final reports from sub-contractors
3. Synthesis report drawing together key findings of the three reviews and a list of recommended changes to MEDLI

This report is the Synthesis task and draws heavily on the text from the three reviews, whilst the following graphics (Figures 1, 2 and 3) provide a schematic of the biophysical issues considered in the three reviews. The essence of the methodology was to undertake a broad-brush Scopus search on appropriate words which included models (e.g., ANSWERS) as well as processes (e.g., deep drainage) followed by a selection of apparently relevant references. Over 7000 abstracts were "scanned" for relevance, followed by selection of about 800 manuscripts which were then shared, via the Elsevier sharing tool Mendeley. In addition, individual reviewers used their own search resources, which involved access to a university library. The DES library staff at EcoSciences Precinct provided invaluable support in assisting with literature searches, obtaining pdfs of manuscripts, and setting up the shared Mendeley folder. In addition, various modelling experts were polled for their advice on key hydrology-plant growth models, as well as journals that were more likely to publish articles of relevance to the review.

Because of the broad spectrum of issues covered by the review tasks (hydrology-nutrients-pond chemistry) there was a tension between allocating time to an encyclopaedic but broad-brush review of published models, and a detailed examination of the science used in the various algorithms. For example, infiltration under rainfall has been described using physically rigorous, numerical solutions to fundamental flow equations (e.g., Richards equation), a simplified numerical approach (e.g., Green & Ampt), and the empirical but widely used Curve Number approach. Similarly, for a process such as solute movement (critical for nitrate leaching predictions), the alternatives include numerical solution to the convective dispersion equation, Transfer Function models which measure the distribution of solute travel times from the soil surface to a reference depth, and semi empirical equations (e.g., Burns equation) which assume simple convective flow with the deep drainage water, adjusted by a soil water mobility coefficient. Superimposed on these options is the fundamental philosophy of the MEDLI model which uses a pragmatic top-down approach to algorithms structure, and cognizance of the relative degree of difficulty confronting a MEDLI user in obtaining the necessary input parameter values. Generally, the more biophysically rigorous the algorithm, the more complex the input parameters required (such as soil hydraulic functions for numerical flow models). As Stirzaker et al. (2010) commented on this conundrum - *the more accurately the processes are described, the greater the error that can be introduced through incorrect parameterization. Hence, it is often better to have a simpler model that we understand, and understand the limitations of, than a complex one we do not understand.*

To help resolve the frequent tensions between breadth vs depth, the reviewers regularly sought feedback from the DES project manager (Alison Vieritz). Hence for the Hydrology review, it was considered more important to undertake a comprehensive review of the more common one-dimensional hydrology models (which were chosen in part from their number of hits in the Scopus search) than delve into the soil physics underpinning them. This "omission" was partially resolved by adding a separate review reported in the appendices of this synthesis report, which was enhanced by a subsequent more detail soil physics review by Prof Freeman Cook (2021). However, for the Nutrient review, it was considered more important to understand the structure of the algorithms that described nitrogen volatilization/mineralization/immobilisation/nitrification/denitrification than undertake an encyclopaedic description of the many N models developed over the past three or four decades. For

this approach to work well, the models chosen for detailed examination needed to represent the "best in class" and included APSIM, DAIRYMOD and DNDC. The structures were directly compared with those in MEDLI where equivalent algorithms occurred (e.g., MEDLI has no dynamic carbon model for external inputs of C). For the phosphorus module, Dr Moody developed some original algorithms to replace the complex Freundlich based approach. For the pond chemistry review, it was clear that adoption of complex dynamic biokinetic models would move MEDLI well outside its *raison d'être*. Hence, the review focused on the algorithms underpinning MEDLI, nutrient transformation and loss processes, and suggestions for more physically sensible, but empirical algorithms for N and P removal.

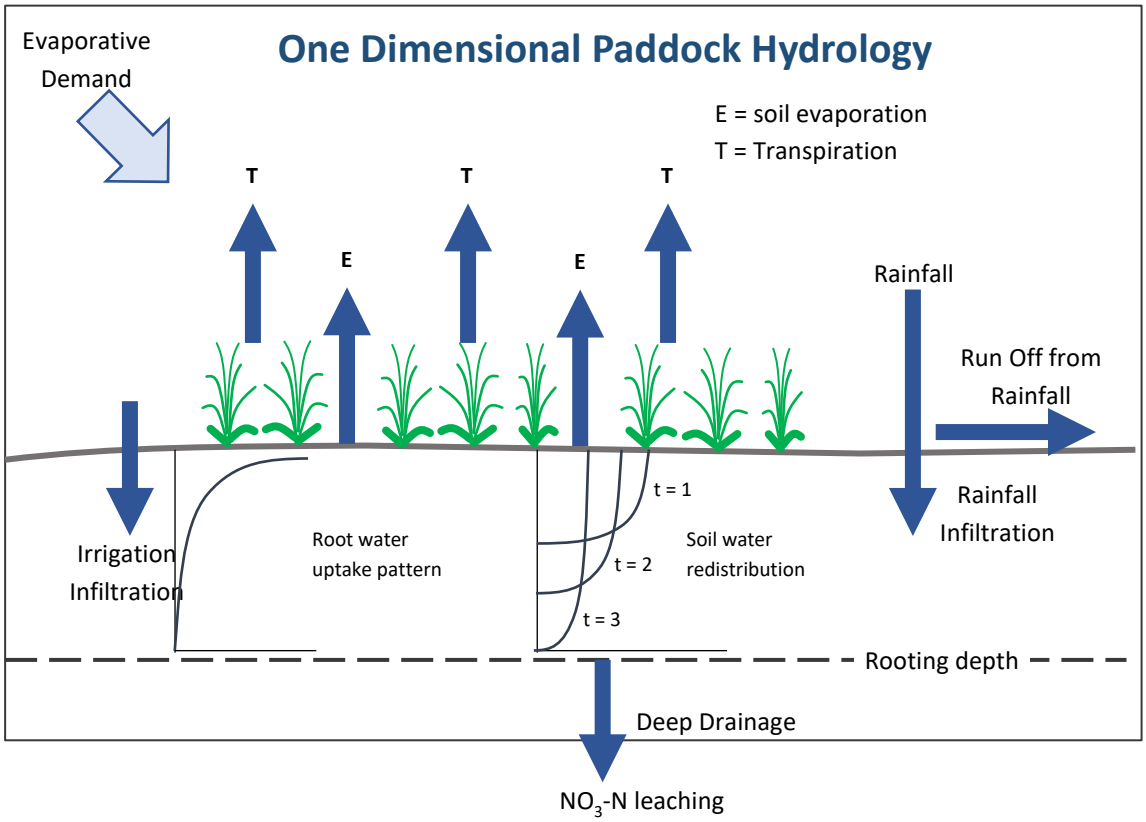



*Figure 1. Schematic of an effluent irrigated pasture showing the complete infiltration of irrigation and the often partial infiltration of daily rainfall. Redistribution of water down the profile (t1, t2, t3) occurs in a non- linear manner as the soil gradually de-saturates. Once the wetting front moves below the root zone, it is classified as deep drainage. Solutes in the soil solution (e.g., NO3-N) move with the deep drainage in a convective and dispersive manner. Water loss is partitioned into soil evaporation and plant transpiration, both of which are affected by atmospheric demand and crop cover. Root water extraction is primarily driven by the root distribution (root density decreases from top to bottom) and modified by the soil water status of each soil layer.*

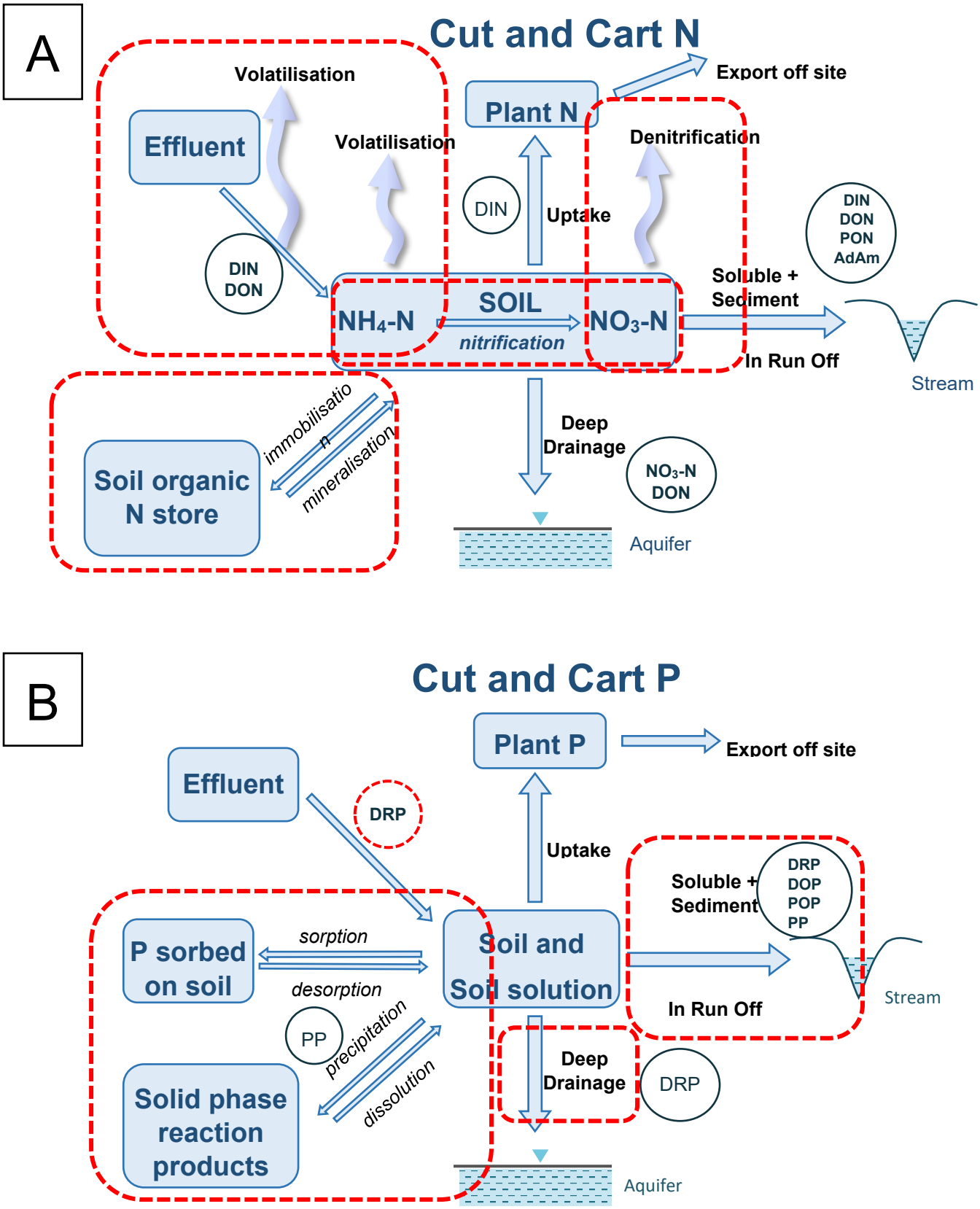



*Figure 2 (A). Nitrogen pools and processes considered in the daily N budget of MEDLI. Abbreviations (e.g., DIN) are assigned to the processes discussed in this review. (B). Phosphorus pools and processes considered in the daily P budget of MEDLI. Abbreviations (e.g., DRP) are assigned to the processes considered in this review.*

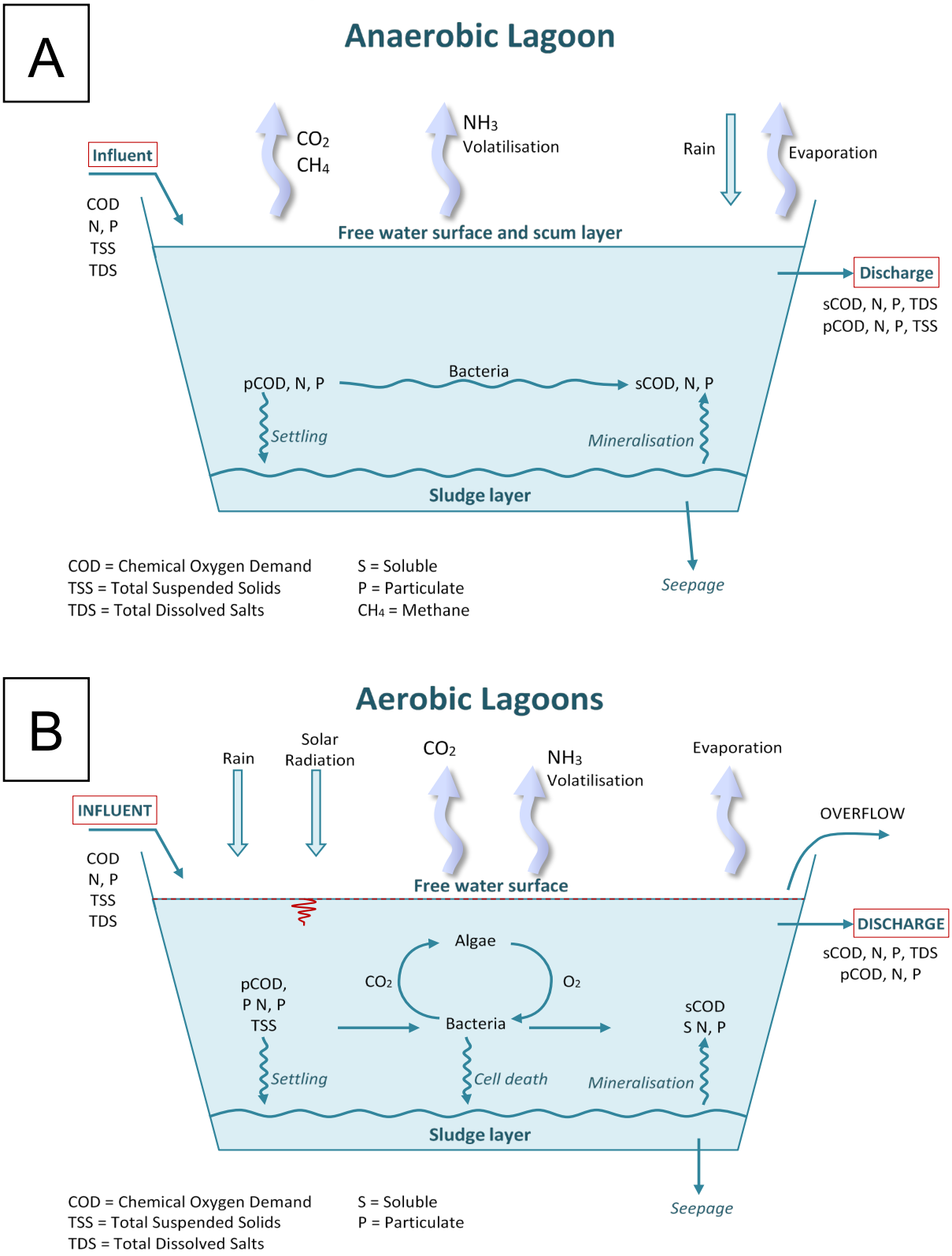



*Figure 3. (A). Schematic of an anaerobic lagoon showing the partitioning of the incoming suspended solids into the settled sludge, as well its partial conversion into soluble forms of C, N and P. The anaerobic process converts COD into methane as well as a suite of other gases (e.g., $NH_3$, $CO_2$, $H_2S$). (B). Schematic of an aerobic lagoon showing the partitioning of the incoming suspended solids into the settled sludge, as well its enhanced conversion into soluble forms of C, N and P via aerobic processes driven by oxygen from water column mixing and algal growth. The aerobic process converts COD into $CO_2$ as well as other gases (e.g., $NH_3$). Penetration of solar radiation into the water column is essential for vigorous algal growth.*

# 3. Hydrology

The hydrology report by Dr Tony Ladson (2021) highlighted the key scientific elements of MEDLI and the knowledge gaps in the Hydrology module. The hydrology aspects include:

- Infiltration runoff
- Soil water redistribution (+ leaching of N and P)
- Soil evaporation
- Transpiration
- Pond evaporation
- Ground water transport of contaminants

The report summary states:

- Most of the hydrologic aspects of MEDLI are fit for purpose and consistent with current well-regarded modelling approaches
- Alternatives to Class A pan evaporation should be considered such as Penman-Monteith and FAO 56 - but there are unresolved issues with estimating the new crop coefficients.
- Pond evaporation is often not a straightforward relationship with Class A pan. There is an opportunity to improve the modelling of pond evaporation and provide better guidance to users.
- MEDLI is a One-D model – but should take the opportunity to consider run-on and lateral sub surface flow to cope with more complex landscapes and climates (e.g., cold, wet winters).

## 3.1. MEDLI in context

Over 100 related models were reviewed such as SWAT, CREAMS, SWMM, WEPP, HowLeaky etc. These deal with similar physical processes but vary in their spatial/temporal scales, input data needs, algorithms used to represent physical processes, and the type of problem addressed (crop yield, water quality, etc).

MEDLI aims to quantify the water, nutrient and salt balances of pasture and crops irrigated with treated effluent. It operates at a daily temporal scale and is suitable for spatial scales up to about 1 ha and on gentle slopes. The limitations on size and slope are because lateral flow and run-on are not modelled as they are for example, in APSIM. MEDLI simulates processes at a single point in the landscape so lacks the capability of models that operate on a grid where cells can interact and allow sediment and pollutants to be routed across the landscape.

Compared to other similar models (a subset of the 100 mentioned in the text), MEDLI:

- Uses Class A pan to estimate potential evaporation that drives evaporation & transpiration
- Estimates soil evaporation as a 2-stage process (demand and supply control respectively)
- Uses Curve Number to estimate runoff & hence infiltration
- No consideration of water loss by spray irrigation (drift and evaporation) or canopy interception
- Erosion is not modelled
- Export of dissolved nutrients in (rainfall) runoff not considered

## 3.2. Potential Evaporation

Class A Pan data has had a long history of criticism because its value is very sensitive to the surrounding environment (green vs. dry) and its response to the climate variables driving it (solar radiation, wind speed, temperature, and relative humidity) can be very different to the response of a *short green crop freely supplied with water.* Consequently, there are many proponents arguing that potential or reference crop transpiration should be calculated using more physically rigorous metrics such as the Penman-Monteith equation or its variant in FAO 56. The SILO data base provides a

range of potential evaporation estimates (Class A pan, Morton, FAO 56, Penman -Monteith), and any one of these could be adapted for use in MEDLI. However, this implies that the relationship between Class A and say Penman-Monteith needs to be explored to assess the quantum of the likely change by climate zone, as well as the generic change in crop coefficients for a range of crops. This issue is beyond the scope of this review and is being followed up by the SILO climate group (Dr Juliusz Zajackkowsk, DES, pers. comm.). Notwithstanding these issues, a recent review by McMahon et al. (2013) noted that Class A Pan data was one of four equally preferred methods for estimating potential evaporation for rainfall runoff modelling.

However, from a scientifically rigorous point of view, using FAO 56 methods (see Allen et al. 1998) in MEDLI should be actively considered, especially given that Class A pan data is being rapidly phased out by the BOM. Part of this change over should include some validation experiments that the new evaporation metric actually provides a potential ET estimate that is in agreement with independently measured ET (for well-watered, short green grass). This will not be the last time that a recommendation for validation will be made in this report, especially for “hard to measure” water balance components. However, one could reasonably argue that the transpiration of irrigated crops/pasture is a well-researched area, and that the literature may be sufficient to give confidence in alternative algorithms. This literature review needs to be a separate study to this review.

## 3.3. Soil Evaporation

The soil evaporation approach used in MEDLI is a two-stage process based on an algorithm proposed by Ritchie (1972).

- Stage I soil evaporation is at the potential soil evaporation rate modified by crop cover and/or crop residue. The maximum amount of soil water that can be removed during Stage I is the input parameter **U** (mm)
- Stage II soil evaporation is controlled by the rate that water can move through the upper soil layers. The rate is specified by an input constant, **CONA** (mm/day1/2)

The two stage approach dates from Philip (1957) and Gardner and Hillel (1962) and was developed into a practical approach by Ritchie (1972). The Ritchie model has been widely adopted by most daily time step hydrology models, with the main point of concern being choosing the appropriate values of U and CONA for different soil textures. Values are listed in MEDLI based on results from Knisel (1980) and Ritchie and Crum (1989) which related U and CONA to the Clay% of the soil.

The Ritchie model has been well validated for bare soil conditions by Foley and Fainges (2014) who also reported that the CONA value was responsive to seasonal evaporative demand, with the value almost halving in winter compared with summer.

In MEDLI, bare soil evaporation is reduced by the fraction of green plant cover and dead residue cover. That is, the fractional covers are additive to obtain the net effect, with a 100% cover corresponding to a potential soil evaporation of zero. This assumption ignores the findings that soil evaporation is very responsive to both the amount of stubble cover (t/ha) and the fraction of cover (%) (Adams et al. 1976; Bond and Willis 1970). HowLeaky and APSIM have separated the green cover and residual loads into two separate functions, with potential soil evaporation being a **linear** reducing function of increasing **green** cover, going to zero at 86%, and a **non-linear** function of increasing surface residue load. The latter function is shown in Figure 4.

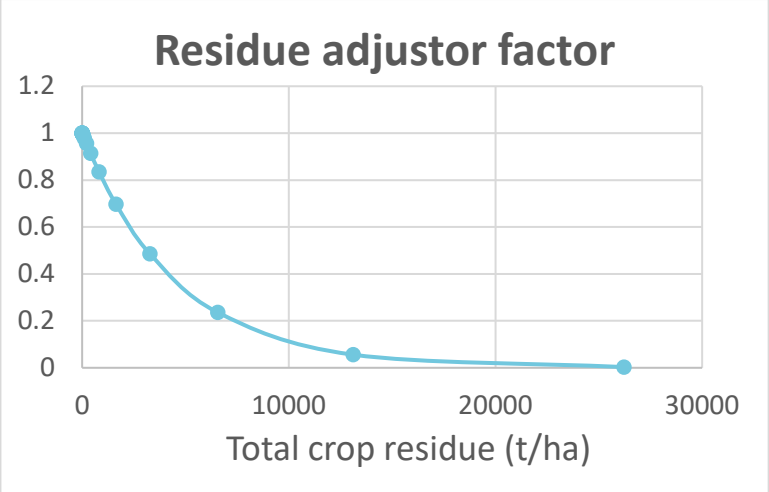



*Figure 4. The effect of mass of crop residue on the soil evaporation adjustor factor. For zero residue, the factor equals one allowing soil evaporation to occur at the potential rate (from HowLeaky manual).*

It is recommended that MEDLI consider changing its cover-effect adjustors for potential soil evaporation to correspond with those in HowLeaky, as the frequent wetting of an irrigated soil is likely to maximize the water loss response to differences in these functions. In MEDLI, for example, zero evaporation occurs at 100% green cover compared with 87% in HowLeaky. Similarly, 100% dead cover reduces evaporation to zero irrespective of its thickness (mm) or mass (kg/ha) in MEDLI. A recent MEDLI run in Beaudesert showed that relatively small changes in the assumed dead cover fraction changed predicted irrigation demand by around 150mm/yr due to changes in predicted soil evaporation.

It is further recommended that the effects of MEDLI cover adjustments and HowLeaky cover adjustments on irrigation demand be explored by multiple runs to assess their effects on the quantum of irrigation demand. Of course, comparing simulations does not provide validation as to the superior algorithm, but the experimental difficulty of undertaking rigorous evaporation experiments (e.g., Foley and Whish 2015) makes the practicality of independent validation unlikely.

APSIM has an alternative soil water balance module (infiltration, evaporation, deep drainage) called SWIM that is based on numerical solution to the Richards equation. Foley & Fainges (2014) reported that SWIM did not provide a more accurate prediction of measured soil evaporation from lysimeters than the Ritchie model. Overall, it is recommended that the Ritchie soil evaporation model be retained but with possible adjustments to the green & dead cover functions to better line up with the HowLeaky/APSIM cover functions.

A more detailed discussion of the cover functions (and second stage drying behaviour) is reported the **Appendix B**.

## 3.4. Transpiration

In MEDLI, plant transpiration is a function of:

- The amount of water in the soil profile
- Fractional plant canopy cover
- Potential evapotranspiration adjusted by a maximum crop coefficient, and a pan coefficient.

The actual transpiration rate depends on the amount of water available in the soil profile.

- MEDLI first partitions the potential transpiration rate amongst the layers in the soil profile based on the **relative plant available soil water**. The upper two soil layers are weighted more highly to reflect that these layers are usually favoured for water extraction since they usually contain more roots

- The relative plant available water content is the difference between the current soil water content (SW) and the lower soil limit, divided by the maximum plant available water (DUL – LSL).
- The relative plant available water content is then combined with the weighting function (mentioned above) to determine the water to be supplied from each layer
- The actual transpiration from each layer is then limited to the amount of plant available water in that layer. Hence for any soil layer k
- $TRANS_k$ = MIN{$potential_k$, $SW_k - LSL_k$}

However, the algorithm implies that transpiration will continue at the potential rate until the soil water content is reduced to the lower soil limit, at which point transpiration will reduce to zero. An alternative approach is to reduce the transpiration rate as the soil water content approaches the lower soil limit. This approach is used in the EPIC model where transpiration rate is reduced once the plant available water is below 25% of the maximum available (Jones and Kiniry, 1986; Sharpley and Williams, 1990).

**It is recommended that a modified algorithm be explored for use in MEDLI to capture the generally accepted understanding that transpiration falls below the potential rate once the relative PAWC falls below a certain value** (say 0.25, see Ratliff et al. 1983).

## 3.5. Infiltration and Runoff

The Curve Number algorithm is one of the most commonly used rainfall/runoff algorithms used in daily step hydrology/water balance models. The model comes out of the ARS group of the USDA and has been well accepted and tested to predict runoff from dryland soils in the USA. Basically, it calculates runoff from the equation:

$$R = \frac{(P-0.2S)^2}{(P+0.8S)}$$

Where R is the runoff, P is the rainfall and S is a retention parameter, which is the maximum amount of water (mm) that can be retained before runoff commences.

The shape of this response can be seen in Figure 5 for a rainfall event of 50mm

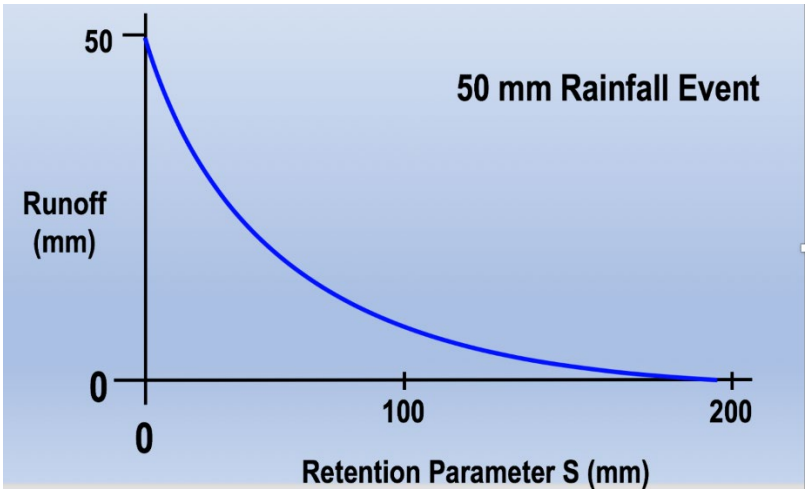



*Figure 5. The relationship between the retention parameter S and runoff for a 50mm rainfall event.*

For a given soil, S varies with the antecedent soil water content and the maximum value of the retention parameter, Smax, via the equation:

$$S = S_{max}\left[1 - \sum_{i=1}^{n} WFi * \frac{SW_i + AD_i}{SW_{max} + AD_i}\right]$$

Where **$WF_i$** is the weighting factor for layer i ( upper soil layers have a higher weighting than lower soil layers ), **$SW_i$** is the pre storm soil water content of layer i, **SWmax** is the saturatedwater content of layer i, and**$AD_i$** is its air dry moisture content.

**Smax** is calculated from the equation

$$S_{max} = 254\left[\frac{100}{CN1} - 1\right]$$

Where **CN1** is the Curve Number for a specific soil at its driest antecedent moisture content.

CN1 is calculated from CN2

$$CN1 = -17 + 1.35CN2 - 0.014CN2^2\ 0.00012CN2^3$$

Where CN2 is the curve number for average antecedent moisture conditions after adjustment for crop residue cover and soil tilth (surface roughness).

Cover of 80% will reduce CN2 value by 20 units, which is the maximum reduction.

Figure 6 shows the relationship between Smax and CN1.

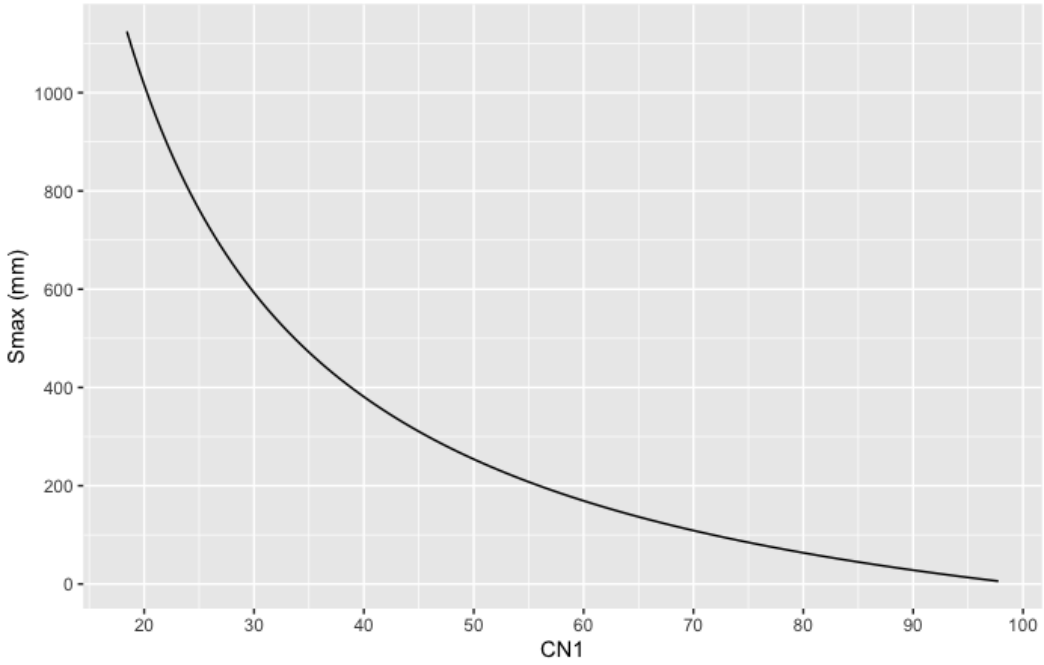



***Figure 6**. Relationship between Smax and CN1 (driest antecedent conditions)*

The curve number method has been criticized because of its lack of physical realism and because it lumps many processes into a single parameter. For example, the approach does not consider how runoff is produced: for example, by Hortonian runoff (rainfall rate > infiltration rate) or saturation excess mechanisms. There is also no consideration of infiltration processes, nor the effect of rainfall intensities. In reality, it is the amount of infiltration that determines runoff. This is the opposite of the approach taken in the curve number model which first calculates runoff, with infiltration being the rain that is left over.

Ponce and Hawkins (1996) consider alternatives to the curve number method including infiltration equations such as Green & Ampt (Mein and Larson, 1973). They point out that real soils are far from homogeneous and will have cracks and roots which make theoretical approaches difficult to apply. A lumped single parameter model such as the curve number method represents about the right level of sophistication given inherent uncertainties and our state of knowledge. They also point out that there has been a large investment in relating soils to curve numbers and that any alternative would need to offer the same convenience.

The curve number method is commonly used in modelling and is incorporated into APSIM, GRASP, GLEAMS, CREAMS, HowLeaky and PERFECT.

**In summary, the curve number approach is widely used and has been found to produce results that are fit for purpose. It seems appropriate for use in MEDLI.**

The CN approach has been validated in dryland catchments in the USA and Australia (e.g., Littleboy et al. 1992,1996, Silburn and Freebairn 1992, Ghahramani et al. 2019) but less so for irrigated land uses. By happenstance, rainfall runoff was measured from effluent irrigated paddocks at Beaudesert, with a value of about 250 to 300mm/yr in 2018. In comparison, MEDLI simulations for the same period predicted values of up to 100mm/yr. This difference is important as the mass balance structure of MEDLI partitions the reduced runoff into infiltration and hence deep drainage, with its implications for nitrate leaching etc.

There seems to be a compelling case to take a more proactive monitoring approach of (effluent) irrigation areas to confirm, or otherwise, the accuracy of the runoff predictions from CN method. This experimental effort should be complemented by a more rigorous consideration of the much more physically based, but computationally complex Green & Ampt equation for unsteady rainfall conditions (see Figure 7). More detail on the use of Green & Ampt for *steady* rainfall conditions is given in **Appendix C**.

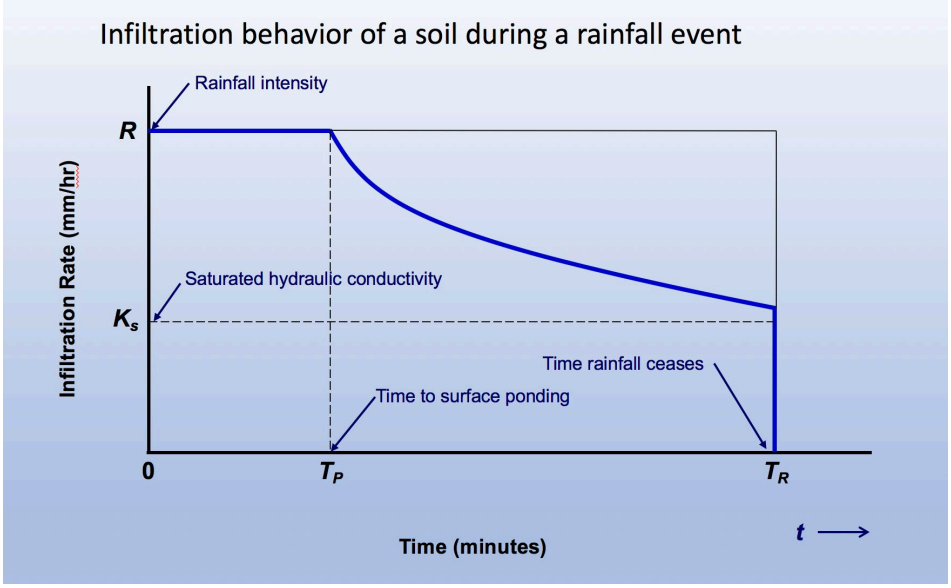



*Figure 7 .A schematic of infiltration into a soil under steady rainfall rate **R** mm/day. Up to the time to surface ponding **Tp** all the rainfall enters the soil as the rainfall rate is less than the soil infiltration rate. When this condition no longer applies, surface ponding occurs and the infiltration continues to decrease in a nonlinear manner with time as the total hydraulic gradient reduces with the increased wetting depth. The long-term infiltration rate is the saturated hydraulic conductivity, **Ks**.*

## 3.6. Deep Drainage

If the soil water content of any soil layer exceeds its DUL value, the excess water is routed downwards to the next layer as drainage. If the drainage passes below the rooting depth, it is no longer available for transpiration and hence is considered as **deep drainage**. MEDLI predicts this redistribution of water in excess of the DUL using algorithms adapted from CREAMS (Knisel, 1980) and EPIC (Sharpley and Williams, 1990). Basically, the drainage rate is the product of a single valued soil specific scaling factor **ti,** and the size of the current Drainable Porosity store ($\theta$ – DUL), which has a maximum value of $\theta$s – DUL for a given soil layer. The **ti** in turn is calculated from an exponential function with **TTi** which in turn is the ratio of the total drainable porosity (DP) and the saturated hydraulic conductivity Ks, as per the following equations taken from the MEDLI technical manual.

$$Dr_i = \text{MINIMUM}\left[ t_i \times (sw_i - fc_i),\ Ksat_i \times \text{TimeFact} - \text{overflow} \right] \quad \text{.....Equation 5.14}$$

$$t_i = 1 - e^{\frac{-1}{TT_i}} \quad \text{.....Equation 5.15}$$

$$TT_i = \frac{(sw_{max_i} - fc_i)}{ksat_i} \quad \text{.....Equation 5.16}$$

where:

| | | |
|---|---|---|
| TTi | = | travel time for layer i |
| $t_i$ | = | drainage factor for layer i |
| $sw_i$ | = | soil water content of layer i |
| $sw_{maxi}$ | = | maximum soil water content of layer i |
| $fc_i$ | = | upper storage limit of soil layer i |
| $Ksat_i$ | = | maximum saturated hydraulic conductivity for soil layer i (*mm/d*) |

As **ti** is a fixed value, the drainage rate on successive days is a constant fraction of the remaining drainable porosity (DP) leading to a steep decrease in drainage rate with elapsed time, which reflects real world behaviour of a draining profile. Figures 8 and 9 show this response for three different values of **ti** assuming a DP of 10mm and it is evident that **ti** must be < 0.5 for a substantial change in the draining behaviour. The question arises as to whether the **ti** values reflect real world behaviour, given that **ti** values reduce as the **TTi** values increase (see Figure 10). In fact, small values of **TTi** correspond to larger value of **ti**, and soils with large values of **Ks** will have smaller values of **TTi.** Hence, high permeability sandy soils will tend to high **ti** values and hence rapid drainage behaviour, as occurs in the field (see Figure 11). Given that DP varies between soils by a factor of 2 or possibly 4, whilst **Ks** varies by orders of magnitude, it follows that the highly permeability soils are likely to have small **TTi** values, high **ti** values, and hence rapid predicted drainage. Consequently, the drainage algorithm in MEDLI reflects in a general sense the real-world behaviour of different soil textures **and hence is fit for purpose.**

Nonetheless, the use of travel time **TTi** to characterise different unsaturated drainage behaviour, whilst computationally useful, does not capture the true drainage behaviour of soils which is driven by their K- $\theta$ function, an example of which is shown in Figure 12. A more physically rigorous description of unsaturated drainage from a soil layer would be using the K- $\theta$ function to estimate K for every day, or part day, and then calculating the drainage flux (mm/day) using Darcy's Law with an assumed unit hydraulic gradient (i.e., due to gravity alone). If a numerical solution of Richards equation is used (as per the SWIM module in APSIM) the assumption of unit gradient can be discarded since the change in matric potential (calculated from the $\psi$–$\theta$ function) is also considered and used to calculate the *total hydraulic gradient* across the soil layers (Huth et al. 2012).

The challenge in using this Darcian/Richards approach is that the K- $\theta$ (and $\psi$–$\theta$) functions must be known for the soils/soil layers of interest and this will be particularly challenging for MEDLI users. One approach is to use the Campbell soil hydraulic functions (Campbell 1974) to characterize K- $\theta$ relationship, viz:

$$K/Ks = (\theta / \theta s) \exp 2+3\ \gamma / \gamma$$

where $\gamma$ in the exponent is the negative slope to the slope of the moisture characteristic ($\psi$ – $\theta$) when expressed in a semi log format.

Because Ks can be strongly influenced by a few macropores, it is often best to use a slightly unsaturated K to scale the K/Kw function; say the K (and $\theta$) at -10 or -20 cm of soil suction. Tension infiltrometers are well suited for these sorts of measurements (White et al. 1992). An alternative approach is to measure the $\psi$ – $\theta$ relationship on undisturbed soil cores (at say -100, -300, -1000 and 15000 cm of suction) and use a paired unsaturated K- $\psi$ – $\theta$ measurement to match the theoretical functions (Cook and Cresswell 2007). However, this requirement is so onerous, it moves MEDLI beyond the scope of a pragmatic effluent irrigation design model used by consultants.

However, Huth et al. (2012) describes a simpler methodology to calculate these functions from the traditionally measured soil water inputs (SAT, DUL, 15 bar, Air Dry, Ks) and some assumptions about the unsaturated K value at the DUL. This information is used with the Campbell (1974) functions to generate a K- $\theta$ function with matching K at saturation (the measured Ks) and K at the drained upper limit ($K_{DUL}$) which is assumed to have a nominal value of 0.1mm/day. See Figure 13. The actual calculations are more complex than the curves might suggest because the driving equations incorporate a soil matrix conductivity function (active at $\theta$ =< DUL) and soil macropore flow function (active at $\theta$ > DUL).

Another simpler approach is to use pedo-transfer functions which are empirical equations for estimating the various exponents of the functions based on soil texture etc. They were developed predominately for USA soils (Zhang and Schaap 2017, Vereecken et al. 2010, Patil and Singh 2016 but see Cichota et al. 2013). The question is whether this increase in computational complexity and data inputs lead to more accurate predictions of deep drainage. A literature review to address this question seems warranted[1], (see for example Verburg et al. 1995) along with a review of explanations of the methods to estimate K- $\theta$ and $\psi$–$\theta$ from relatively simple soil water measurements (which may include the K at the moisture content corresponding to a soil suction of a few tens of cm).

The Huth calculation protocols for soil hydraulic functions are used in the APSIM technical manual and the question that presents itself is whether the SWIM module provides a better estimate of Deep Drainage than the cascading bucket module. Huth et al. (2012) provide a comparison for multi-year field data for a self-mulching vertosol and a poorly drained chromosol (measured by others) and argue that the APSIM-SWIM model captured the major differences in *time tend of soil water content* for cropping and pasture treatments. Other comparison studies which also measured deep drainage (using lysimeters?) showed fair to good agreement for flood irrigated sugar cane in the Burdekin (Stewart et al. 2006) and dryland wheat on a deep sandy soil in WA (Asseng et al. 1998) noting the latter study used the SoilWat module in APSIM, not the SWIM module. Other studies that used SWIM to predict deep drainage include Lucerne on a vertosol in the Riverina (Verberg et al. 2007,1995), Eucalyptus trees on a freely draining chromosol at Wagga (Snow et al, 1999) and various high production dairy pasture experiments on permeable soils in high rainfall areas of New Zealand (Chichota et al. 2012, Vogeler et al. 2016, Buckthought 2013). Overall agreement between measured and predicted cumulative deep drainage was good to excellent, giving confidence to the various modellers that APSIM- SWIM could be used as a surrogate of *hard to measure* deep drainage, to test the viability of simpler farm management models such as OVERSEER (Vibart et al. 2015).

Of the 18 models reviewed in detail by Tony Ladson (Ladson 2021), only one model used the Richards equation approach to simulating soil water redistribution with APSIM-SWIM. This was applied relatively successfully to estimate deep drainage and nitrate leaching under sugarcane in the Burdekin Delta (Stewart et al. 2006).

[1] It's possible that published deep drainage studies used to calculate soil hydraulic functions (the instantaneous profile method e.g. Watson 1966 and van Bavel et al 1968) could provide some experimental data sets for this comparison.

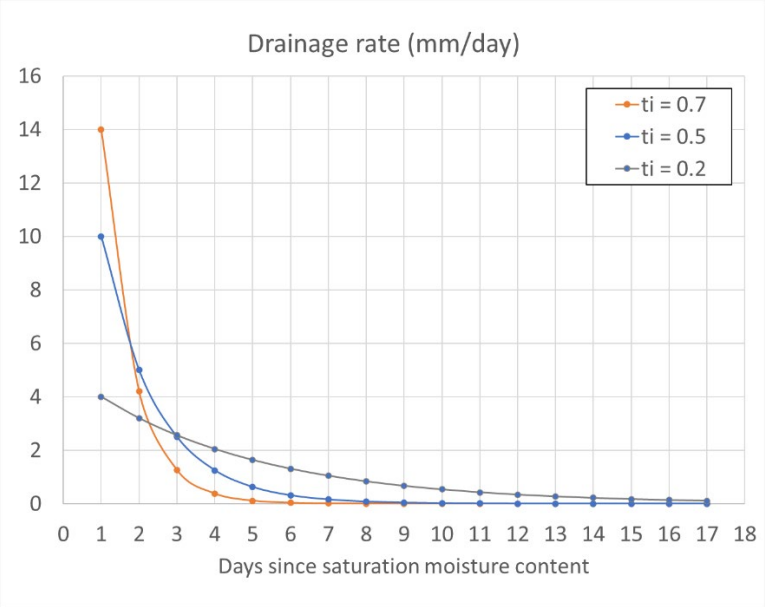



*Figure 8. The effect of the value of the Drainage Factor (ti) on the drainage rate from a soil layer with a total Drainable Porosity of 10mm as a function of time from saturation.*

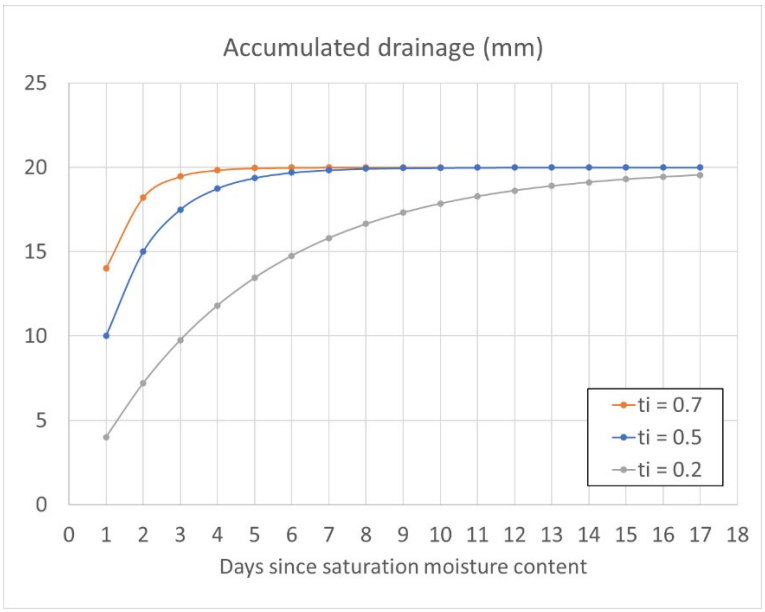



*Figure 9. The effect of the value of the Drainage Factor (ti) on the cumulative drainage from a soil layer with a total Drainable Porosity of 10mm as a function of time from saturation.*

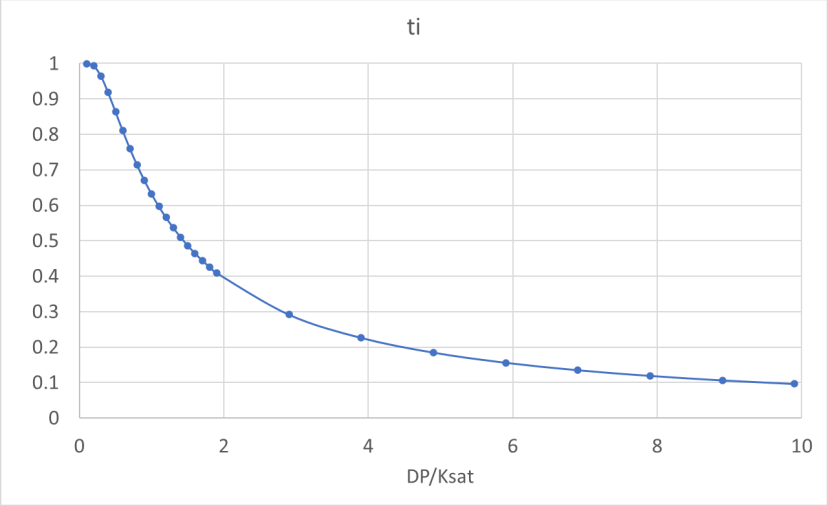



*Figure 10. The relationship between the Drainage Factor ti and the Travel Time TTi value defined as the ratio of total Drainable Porosity (DP) to saturated hydraulic conductivity (Ksat).*

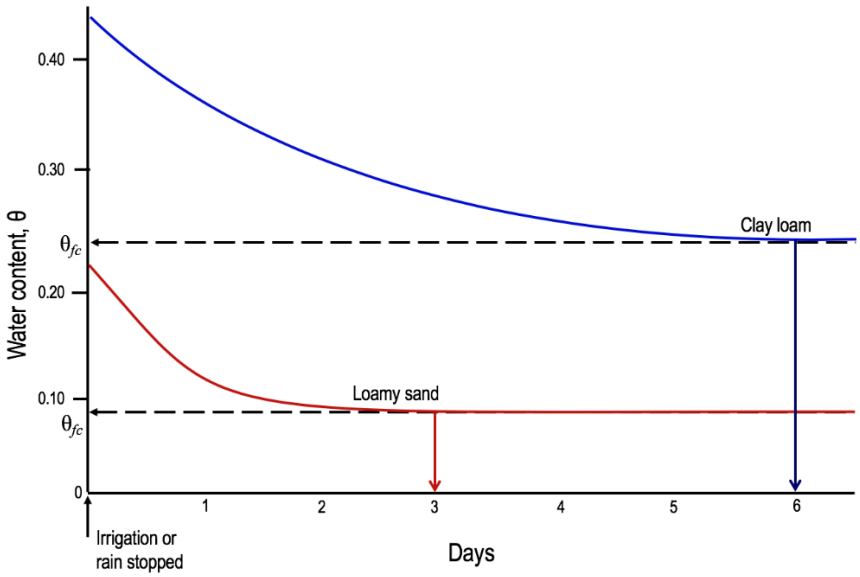



*Figure 11. The change is soil water content with draining time for two soils of contrasting texture. The sandier soil has a steeper reduction in K with reducing θ and hence reaches Field Capacity (θfc) sooner (3 days vs 6 days for the clay loam).*

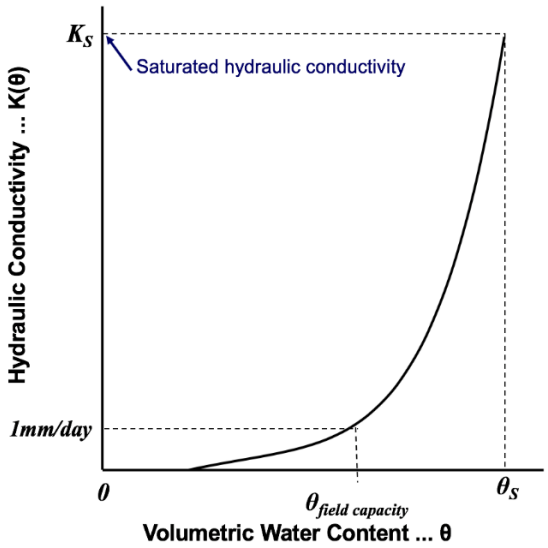



*Figure 12. The Relationship between unsaturated hydraulic conductivity K and volumetric soil water content $\theta$ for a generic light textured soil. Assuming downward drainage materially ceases at 1mm/day, the corresponding moisture content is the USL or Field Capacity.*

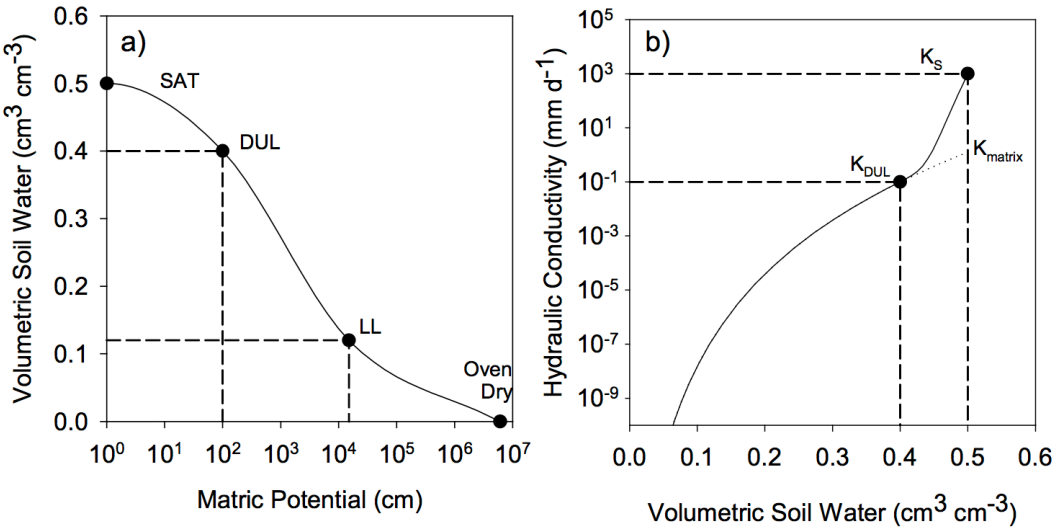



*Figure 13. Demonstration on how basic soil hydraulic properties are mapped into continuous hydraulic property functions for matric potential (a) and hydraulic conductivity (b) (From Huth et al 2012)*

## 3.7. Solute Leaching

Solute leaching is a critical part of MEDLI both because of soil salinity control (effluent is often saline) as well as $NO_3$ leaching. The algorithm in MEDLI assumes the fully mixed solute in one soil layer moves with the deep drainage flux into the next layer where it fully mixes again before moving into a lower layer until it runs out of drainable water or passes below the soil depth of interest (usually the rooting depth). The literature (e.g., Biggar and Nielsen 1976) shows that solute movement is a convective diffusive process that has historically been described by the Convective Dispersion Equation (CDE). However, there are considerable doubts that this equation can predict solute leaching in the field because of the very large variation (log normal distribution) in the calculated pore water velocity and the Diffusion coefficient. Consequently, Jury and colleagues (Jury 1982, Jury et al. 1982,1986,1990) developed and/or applied a Transfer Function Model (TFM) to capture the

stochastic convective nature of solutes moving through *virtual* stream tubes at different velocities, thereby generating the vertical spread in concentration of a surface applied solute leaching through a soil. For the TFM to be used in MEDLI (to predict $NO_3$ leaching), the probability density function (pdf) of the solute transit time (for given soil) needs to be calculated *a priori* using its mean and variance values. It is uncertain if the TFM can be used for practical modelling in irrigated soils without prior solute leaching measurements.

A simpler version of the TFM appears to be the much earlier empirical Burns leaching equation (Burns 1975,1976,1982, Scotter et al. 1993, Magesan et al. 1999) which requires only the amount of deep drainage and the effective or mobile soil water content transporting the solute, to estimate the fraction of solute retained in Z cm of soil after leaching. It appears that this effective moisture content is <DUL value reflecting that only some of the soil water is "mobile" (Addiscott 1977, Addiscott and Wagenet 1985, Clothier et al. 1992,1995).

The Burns leaching equation may be written (as modified by Towner 1983 and discussed by Scotter et al. 1993) as:

$$F = exp\left(-Z\theta/_{DD}\right)$$

Where F is the fraction of the mass of resident solute (say $NO_3$) in the soil profile that is leached below any depth Z cm after a given amount of Deep Drainage (DD mm) passes below this depth. **θ** is the mobile water content which, to a first approximation, is assumed to equal the DUL moisture content (i.e., Field Capacity).

The equation appears to describe a variety of field leaching data reasonably well except in swelling and cracking soils (Burns 1975, 1976). It is recommended that an expert opinion be sought to assess the practicality of using the TFM or the Burns equation or some other similar type of analytical function for use in MEDLI (see Cook 2021).

More detail on solute leaching models is given in **Appendix D.**

## 3.8. Erosion and Nutrient Export

If there is an interest in modelling the export of sediment-attached nutrients and pollutants, then it will be important to model erosion and transport of sediment. This capability is available in several models (AGNPS, ANSWERS, APSIM, CREAMS, EPIC, HowLeaky, HSPF, PERFECT, RSULE, and WEPP).

Sediment enrichment refers to the preference for nutrients and pollutants to be attached to fine particles, combined with the preferential transport of these fine particles. Thus, the sediment transported from a hillslope can have much higher nutrient content than the average concentration of soil.

It is unlikely that sediment loss from permanent cut and cart pasture, as often used in effluent irrigation, will have substantial erosion (and hence nutrient export) as the permanent cover % is far greater than the threshold when substantial erosion can occur (< 50%, Silburn et al. 2011). However, if the cropping system predisposes the paddock to erosion (say annual row crops) then the erosion/sediment enrichment algorithms from HowLeaky could be added into MEDLI.

In HowLeaky, soil erosion is estimated on a daily basis using functions reported by Freebairn and Wockner (1986) that relate soil erosion to runoff volume, surface and crop cover, rainfall erosivity, soil erodibility, management practice and topography. This sub model predicts soil erosion for each runoff event which is modified by a sediment enrichment algorithm to estimate the export of P and N.

## 3.9. Groundwater

MEDLI simulates the concentration of solutes in groundwater to determine if groundwater quality is protected at some defined distance from the edge of the irrigation area. The algorithm is based on an

analytical approach to groundwater modelling described in Dillon (1989), the PLUME model. The algorithm has been tested against analytical solutions and detailed numerical models.

The modelling approach involves

- Leachate mixes with groundwater that flows beneath the site
- Dispersion occurs in the direction of flow
- Dispersion occurs in the vertical direction
- Lateral dispersion is neglected
- Concentrations are calculated on a vertical profile
- Groundwater mounding is not modelled

This approach is likely to be conservative, predicting pollutant concentrations that are higher than actual because lateral dispersion is ignored. MEDLI is usually applied to small areas so there will be many situations where the scale of the aquifer is larger than the irrigated area. This means that lateral dispersion could be substantial. MEDLI ignores this lateral dispersion so will predict values that are too high.

Application of the model is dependent on detailed knowledge of the aquifer system (e.g., flow rate, and solute dispersion coefficients) which is unlikely to be available for “normal risk” effluent irrigation areas. If on the other hand, there is a high risk of groundwater contamination of an adjacent aquifer, then more detailed investigation of aquifer parameters is warranted, and a more sophisticated groundwater model should be considered (e.g., MODFLOW or MT3D).

Overall, the inclusion of an analytical groundwater contamination module in MEDLI is a conceptual overreach and serious consideration should be given to its deletion and replacement by appropriate numerical groundwater models, which is the usual domain of expert groundwater hydrologists.

Ladson’s review of 18 mainstream hydrology models (Ladson 2021) identified that inclusion of a groundwater module was very unusual, with GLEAMS being a possible exception.

# 4. Nutrients

## 4.1. Nitrogen

The partitioning of applied nitrogen is one of the most important processes considered in MEDLI since the $NO_3$ contamination of groundwater is one of the key environmental assessment criteria used by the regulatory agency. The N cycle is very complex and involves:

- The addition of N in the effluent
- Volatilization loss of ammonia ($NH_3$) to the atmosphere during and after effluent irrigation.
- Mineralization (in the soil) of **organic** forms of N which includes organic N in the effluent and dead plant material and its transformation into soil ammonium
- Immobilization - the conversion of **inorganic** N into organic compounds which are then not available to plants.
- Nitrification - the conversion of soil ammonium ($NH_4^+$) into nitrate ($N0_3^-$) that is more mobile.
- Denitrification - the conversion of nitrate to nitrogen gas (and its forms) which is then lost from soils to the atmosphere

The various processes depend on temperature, soil water status, pH and other properties of the soil. For example, the processes of mineralization and immobilization depend critically on the carbon/nitrogen ratio. If the C:N ratio is high (greater than about 30:1), N is more likely to be immobilized (Godwin and Jones, 1991). It is for this reason that the more complex crop-nitrogen models incorporate a carbon module since it is the C:N ratio that determines the ultimate partitioning of N into the various organic and inorganic stores.

Considering the importance of the N (and C) cycle to agriculture, it is not surprising that a wide range of N models have been developed over the last few decades. Moody (2021), in his review of N models, suggested that the models can be classified as either mechanistic (e.g., WNMM, DNDC and DAYCENT), or empirical (e.g., APSIM and DAIRYMOD). The way that the processes are handled in the mechanistic models can be conceptually different from the empirical model treatments; for example, in APSIM, the processes of nitrification and denitrification are described as an empirical reaction, expressed via Michaelis–Menten type equations, whereas DNDC uses a microbial growth model (see Moody 2021-Table 1).

Despite the commonality across the models in factors considered to modify process kinetics such as soil water content, temperature and pH, the scaling modifiers used in the models for processes such as nitrification and denitrification can be different between models (as illustrated in Moody 2021 - Fig. 1.1). Therefore, it is not surprising that models often simulate different outputs for specific N processes from the same input data. Moreover, Moody notes that model outputs are most applicable over longer timeframes (weeks) and are generally poor at predicting daily fluxes for processes such as denitrification (e.g., APSIM and DAIRYMOD: Harrison et al. 2018; APSIM and DNDC: Vogeler et al. 2013).

Given the general lack of consistency in modelled N processes when models are compared, Moody argues there is no compelling case to suggest that the MEDLI N process components should move from their current empirical basis to a more mechanistic basis.

Moody recommends that consideration could also be given to revising MEDLI to include a carbon component that would be the driver for the ammonification process (organic matter decomposition). Having soil C dynamics driving the N processes is mechanistically correct, is intuitively logical, and could be incorporated into MEDLI reasonably easily following the APSIM or DAIRYMOD exemplars. However, a C model involves a substantial increase in complexity and inputs for an uncertain quantum of accuracy gains for a typical effluent irrigated *cut and cart* pasture where crop residue mass is likely to be small compared to that for harvested grain crops.

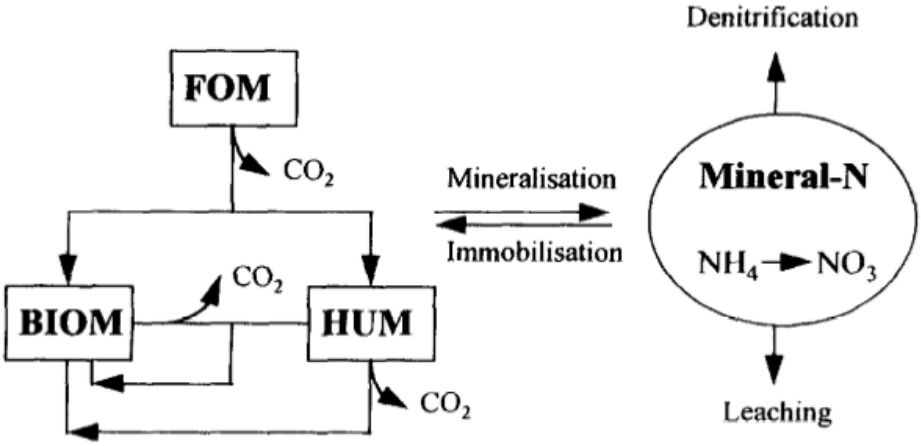



*Figure 14. Carbon and mineral N pools in APSIM's N module. Reproduced from Fig. 3 of Probert et al. (1998).*

Figure 14 shows the conceptual logic of the C and N models in APSIM, which uses three conceptual soil C pools –

- BIOM (labile C-microbial biomass and microbial by-products - rapid turnover of days).
- HUM (stable C - slow turnover of months/years); and
- INERT- not specifically identified in the C pool diagram but considered not to participate in the modelled mineralisation/immobilisation processes (Probert et al. 1998).

The fresh C input pool is FOM (fresh organic matter) which comprises added organic amendments and on-site vegetative residues including decomposing root material. To account for the variation in the decomposability of the organic C in FOM, it has been sub-divided into three pools of different lability (and possibly different C:N ratios): carbohydrate-C, cellulose-C and lignin-C (Probert et al. 2005). These organic C forms must be characterised by analysis. Each pool and sub-pool have an allocated efficiency and decomposition rate, and when this is combined with measured (or inferred) C:N ratios, net N immobilisation as well as net mineralisation (ammonification) can be identified. MEDLI does not have this simple sophistication which allows flexibility in reflecting differing levels of C lability in FOM inputs.

Carbon flows between the pools are assumed to be first order, with the rate ($day^{-1}$) modified by soil water content and temperature and soil water content. Fluxes between the C pools drive the consequent N fluxes that are based on the C pool sizes and their respective C:N ratios. The C:N ratio of BIOM has an assigned value, while the C:N ratio of HUM is that measured in a sample of the soil layer being considered; FOM C:N ratio is measured and has an assigned modifier that captures the mineralisation/immobilisation characteristics. Mineralisation or immobilisation of mineral N is determined as the balance between the release of nitrogen during decomposition of FOM, BIOM and HUM, and the N required by the microbial biomass during microbial synthesis and humification. An inadequate supply of mineral N to satisfy the immobilisation demand results in a slowing of the decomposition.

Apart from the water, temperature, pH and C:N ratio response functions that drive mineralization, the Carbon model requires a number of other input parameters that partition carbon into its various pools. These are shown in Table 1 and presumably could be used as default values if the C model were to be used in MEDLI.

*Table 1. Maximum decay rates of carbohydrate, cellulose, and lignin pools in FOM are: rd_carb, 0.2 day-1; rd_cell, 0.05 day-1; rd_carb, 0.00095 day-1. Reproduced from Probert et al. (1998).*

| *Parameter* | *Value* | *Definition* |
|---|---|---|
| *mcn* | 8.0 | C:N ratio of **biom** pool |
| *ef_fom* | 0.4 | Efficiency of carbon retention when **fom** decomposes |
| *fr_fom_biom* | 0.9 | Proportion of retained carbon from **fom** synthesised into **biom** |
| *ef_biom* | 0.4 | Efficiency of carbon retention when **biom** decomposes |
| *fr_biom_biom* | 0.6 | Proportion of retained carbon from **biom** resynthesised into **biom** |
| *ef_hum* | 0.4 | Efficiency of carbon retention when **hum** decomposes |
| *ef_res* | 0.4 | Efficiency of carbon retention when residues decompose |
| *fr_res_biom* | 0.9 | Proportion of retained carbon from residues synthesised into **biom** |
| *rdbiom* | 0.0081 $day^{-1}$ | decomposition rate for **biom** |
| *rdhum* | 0.00015 $day^{-1}$ | decomposition rate for **hum** |

In comparison to APSIM, the N model used in MEDLI is shown conceptually in Figure 15 and there is no consideration of either $NO_3$ or $NH_4$ being immobilized in soil organic matter, whilst the organic N added in the effluent and that present in the native soil organic N store (defined by the user) are mineralised at different rates reflecting their assumed differences in lability (i.e. fresh organic matter vs humus type organic matter).

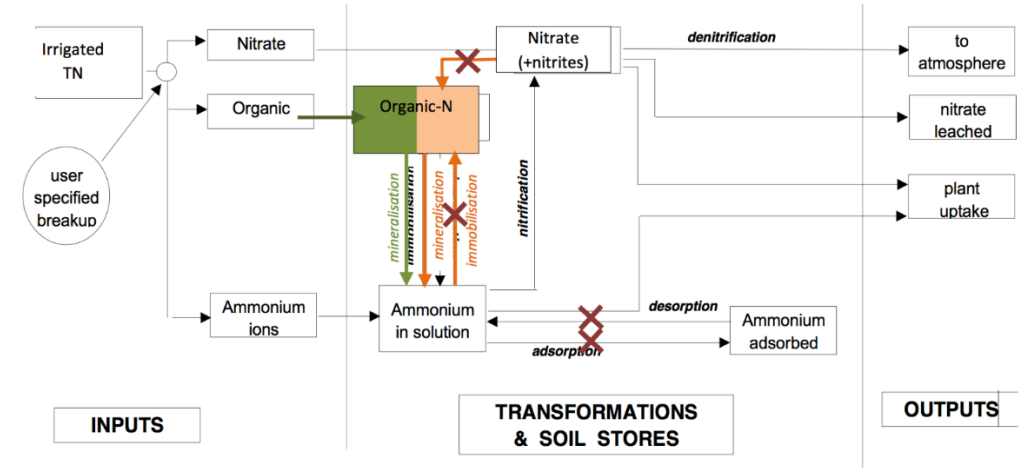



*Figure 15. Schematic of the N transformation processes considered in MEDLI.*

The processes of nitrification and denitrification are described in a similar way to that used in APSIM, but with the exception that the denitrification rate in MEDLI is not limited by the available carbon, but rather just its presence or absence. This could be a seriously incorrect assumption as MEDLI simulations at a Beaudesert effluent irrigation area showed that denitrification was very responsive to the **depth** of available carbon (normally assumed to be limited to the top 10 cm of soil). It is recommended that MEDLI considers a more sophisticated denitrification algorithm which could take the form (from APSIM):

$$R_{denit} = k_{denit}[NO_3]C_A f(T) f(\theta) f(pH)$$

Where $R_{denit}$ is the denitrification rate, $k_{denit}$ is the denitrification coefficient, with a default value of 0.0006, $[NO_3]$ is the amount of nitrate-N in the soil (mg/kg) and $C_A$ is the active carbon (mg/kg) defined as:

$$C_{A,i} = 0.0031FOM + 24.5$$

where FOM is the sum of the organic C (mg/kg) in the fresh organic matter's soil carbon pools.

Perhaps a better measure is the labile carbon content (Weil et al. 2003) to depth, as FOM is limited to the upper soil layers whilst soil water conditions suitable for denitrification occurs over the whole profile. The other three parameters capture the effects of temperature, soil water content, and pH on a 0 to 1 scale. MEDLI does not explicitly consider the pH effect, and denitrification need only be reduced if the pH of the receiving soil is lower than 5.5.

For high strength effluent, the N applied under conventional irrigation loading (say 5 to 6 ML/ha/yr) is such that N is often not a limitation for plant growth. Hence N loss mechanisms other than biomass sequestration need to be considered carefully. The three possible sinks are

- Sequestration by the root thatch
- Volatilization of ammonia
- Denitrification of nitrate-N

Perennial grass pastures such as kikuyu (*Pennisetum clandestinum*) develop a high organic carbon root thatch of dense root and plant residue material that resembles a peat layer. This layer can be several centimetres deep, exceed 15,000kg/ha, and is not normally included in surface soil samples. The presence of a root mat will also increase the sequestration of added effluent N (and P) via an increase in soil microbial biomass. This microbial sequestration is in addition to N sequestration in living root material. It is suggested that the MEDLI N (and P) module add algorithms for estimating N (and P) sequestration in the following pools:

- root material - estimated as a proportion of above-ground biomass with an assumed (or measured) concentration of 3%N and 0.3% P.
- microbial biomass in the root mat (thatch) - calculated by direct total N analysis of a root mat sample **and** measurement of root mat weight.
- microbial biomass in the surface soil (0-10 cm) - estimated by organic C analysis of the surface soil layer and adopting C:N and C:P ratios from the literature (about 12 and 156 respectively).

The loss of ammonia gas due to volatilisation of ammonium-N from the source effluent is only considered to occur during the irrigation event and assumed to equal some constant fraction of the NH4 concentration - say 15%. The chemistry of $NH_3/NH_4$ partitioning in TAN (total ammoniacal nitrogen) solutions is well understood and is determined primarily by the solution pH, as well as temperature and salinity (Emerson et al. 1975). At solution pH > 8.2, there is an exponential increase in $[(NH_3)aq/TAN]$ ratio and hence an increased opportunity for $NH_3$ loss . For example, at pH 9.0, the ratio is 36%, increasing to 60% at pH 9.5 (see Figure 16). These high pHs would rarely occur in domestic or agricultural effluent.

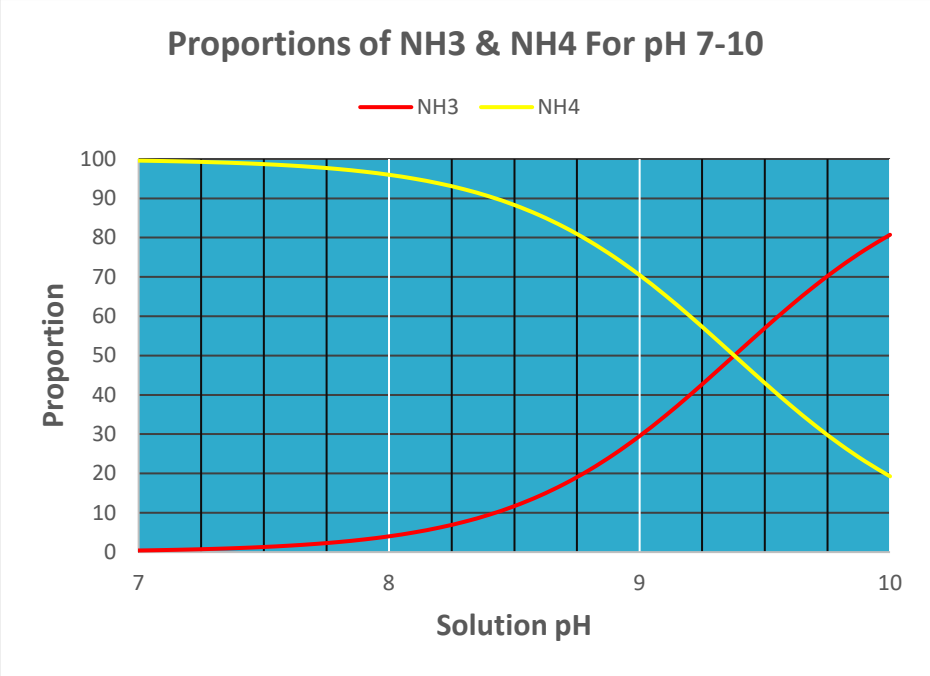



*Figure 16. The relationship between the fraction of NH3 and NH4 in a TAN solution (total ammoniacal nitrogen) as a function of its pH. Note that the sum of the fractions always equals 1. (Based on equations from Emerson et al. 1975).*

However, in addition to this chemical partitioning process, there appears to be a hydrodynamic process in spray irrigation where high pressure travelling irrigators (> 500kPa) cause TAN losses in excess of 50% (Natasha Smith - Gelita pers. comm.) due to evaporation/volatilization processes from the many fine droplets created. If the pressure drops below about 300kPa, the TAN losses reduce to <25%. It is very difficult to predict the size distribution of spray droplets (but see Kincaid et al. 1996) and the loss percentage will need to be established experimentally using catch cans acidified to prevent $NH_3$ loss. A typical loss pattern measured at Gelita using catch cans is shown in Figure 17.

Volatilization can also occur from urea fertilizer or cattle urine added to soil as its hydrolysis causes a temporary increase in soil pH to values favourable to the $NH_3$ form, and hence favourable to gaseous loss. Volatilisation is not currently included in MEDLI or APSIM. However, Vogeler et al. (2019) added a volatilisation routine to APSIM when simulating the effect of irrigation management on N losses from pasture. The routine is based on the mechanistic volatilisation model which considers the partitioning of ammonium-N in solution between [$NH_4^+$] and ($NH_3$)aq and Henry's Law to estimate ($NH_3$) gas. It is particularly relevant to $NH_3$ loses from cattle urine patches, but this land use (grazing) is not considered in MEDLI. It is **unlikely** that the extra complexity of adding a soil volatilization module to MEDLI is justified by the likely size of the $NH_3$ loss, given that the N applied is already in the hydrolysed form (i.e., as total ammoniacal nitrogen-TAN). A possible exception is applying high $NH_4$-N effluent to alkaline soils (Moody 2021).

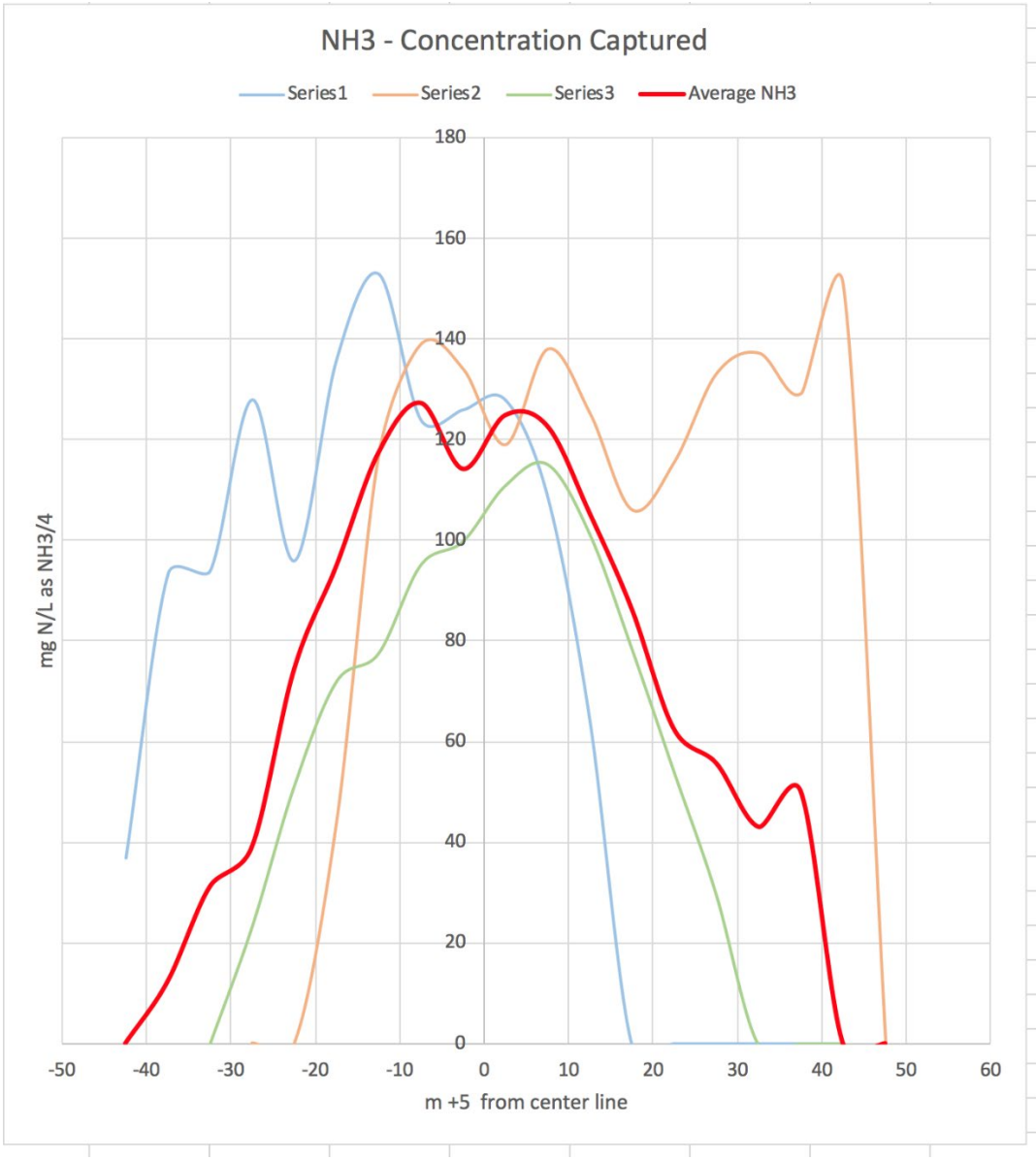



*Figure 17. Variation in NH4-N concentration (mg N/L) with distance (m) from the centre line of a Marani travelling irrigator. Effluent was captured in acidified catch containers. Three separate runs were undertaken with the mean results shown by the thick red line (Natasha Smith - Gelita pers. Comm….with permission).*

Denitrification is probably the most important loss pathway for N in effluent irrigated soils based on the $^{15}N$ mass balance experiments for fertilized pastures that were undertaken some decades ago by Henzell (1971), Catchpool (1975), Weier (1994), Weier et. al (1991,1993) and more recently by Rowlings et al. (2016). The overall data suggested that N recovery ratios were in the 40 to 60 % range with leaching and volatilization losses ruled out by the authors as major loss pathways. These experiments are particularly important because gaseous N loss is so difficult to measure directly, and its (seasonal) value is usually estimated by difference in (unlabelled) N mass balance experiments. The main requirement for denitrification is anaerobic conditions and a supply of labile carbon for the heterotrophic bacteria mediated reactions. In APSIM denitrification increases with [NO3-N] and labile organic C, whereas MEDLI uses a fixed denitrification value of 0.10×[NO3-N]. In DAIRYMOD, denitrification increases with increasing [NO3-N] to a maximum value of 0.22 mg N kg-1 soil. Using the denitrification algorithms compiled by Moody (2021) and a nitrate- N concentration of 100 mg N/kg, APSIM predicts a maximum N loss of 5mg N/kg soil /day, MEDLI 10 mg/kg/day, and DAIRYMOD 0.22 mgN/kg/day. For 10 cm of topsoil with a typical BD of 1.2g/cm3 the denitrification losses are **6, 12 and 0.25 kgN/ha/day respectively**. Given the maximum denitrification loss measured in high production dairy pastures in SEQ is about 4 kgN/ha/day (Frield et al. 2016) the

APSIM prediction seems reasonable, whilst the MEDLI value seems too high and the DAIRYMOD value far too low. Given that these maximum values set the upper limit for denitrification during a transient water logging event, it is **considered important to undertake a thorough literature review to settle on a well justified maximum value.** Other assumptions in the denitrification algorithms tend to reduce the predicted loss, in that labile C is often assumed to be limited to the top 10 cm or so of soil, which will drain to the DUL within a day or so. Hence the opportunity for denitrification is limited by both the assumed depth of labile C and the duration of waterlogged conditions. **The predicted denitrification response to less conservative conditions is worthy of investigation.**

Overall, MEDLI uses very similar algorithms as the mainstream N models such as APSIM to calculate ammonification, nitrification, and denitrification where an assumed maximum value is reduced by 0 to 1 scaling factors to capture the effects of temperature, soil water content and pH on the process. However, MEDLI does not contain a dynamic carbon model to mineralise the dead crop residue and partition it into various organic and inorganic pools, depending on the C:N ratio of the reaction products. This substantial increase in model complexity is probably not warranted for the *cut and cart* pasture management typical of effluent irrigated paddocks where most of the above ground biomass is removed. However there seems some value in establishing the basis of the difference between the APSIM and MEDLI 0-1 modifiers for ammonification, nitrification, and denitrification, and suggest revisions to MEDLI if necessary. It is unlikely that the quantum of $NH_3$ volatilization losses from effluent irrigated soils warrant the addition of another (complex) module in MEDLI. Volatilization losses during spray irrigation is an experimentally determined fraction of the TAN concentration in the effluent. The higher the nozzle pressure the higher the expected loss (Kincaid et al. 1996). Based on centre pivot results, a minimum value of 25% could be expected (Safley et al. 1992, Chastain 2019).

## 4.2. Phosphorus

During the development of MEDLI in the 1990s there was widespread concern about the export of terrigenous P on the water quality of inland rivers and some coastal estuaries (e.g., Peel Harvey in WA). Consequently, MEDLI incorporated a physically rigorous P model to estimate the leaching of water soluble (ortho phosphate) P below a given soil depth (>= rooting depth). When the P leaching front reached the threshold soil depth, the P storage capacity (kg/ha) of the soil profile was considered full, and the **sustainable P soil life** (the storage divided by the net annual loading of P in kg P/ha/yr) was reached. Subsequent research suggested that groundwater transport of P was a very unlikely export pathway as the regolith and aquifer material of most Australian landscapes have a strong propensity to adsorb and/or fix ortho phosphate P. Nevertheless, MEDLI adapted the P-soil interaction algorithms from the HSPF model (Johnson et al 1984) which were based on the P adsorption/desorption behaviour as quantified by the Freundlich isotherm equation which has the form

$$Ps = aP_{soln}{}^{b}$$

where Ps is the amount of sorbed P (mg/kg soil), and $P_{sol'n}$ is P concentration in the soil (or equilibrating) solution (mg/L).

The two curve-fitting coefficients, *a* and *b*, do not have specific physico-chemical meaning, but the product (*a*×*b)* has been termed the Buffer Index and has been used to characterise soil P buffer capacity.

When applied to MEDLI, the calculations follow the logic path (from Moody 2021):

- Partition incoming effluent P into solution P (Psol'n) and sorbed P (Ps).
- Route Psol'n between soil layers and partition the incoming P into solution P (Psol'n) and sorbed P (Ps) in each layer.
- Estimate the quantity of desorbed P (Pdes) in a soil layer when Psol'n decreases due to plant uptake or dilution by irrigation/rainfall.

- Adjust Psol'n and Ps in the soil layer as a consequence of the P desorption.

These calculations are based on *a* and *b* coefficients of the Freundlich equation in adsorption or desorption form, which must be measured for multiple depths for each soil of interest (or selected from the MEDLI library of soil properties). This is turn has created a significant issue for MEDLI users as the Freundlich isotherm measurements are both expensive (c. $700 per test) and available from relatively few soil chemistry laboratories.

Moody (2021) has suggested an alternative method to calculate the soil solution P concentration in MEDLI based on two routine single point soil measurements:

- the **Colwell extractable P** (a measure of biologically available P) and
- the **Phosphorus Buffering Index** (PBI - a single point measurement that characterises the soils' capacity to moderate changes in soil solution P concentration when P is either added or removed from the soil - Burkitt et al. 2002).

The flowchart is shown in Figure 18 and comprises the following assumptions and predictive relationships:

- Colwell-P is assumed to be an estimate of sorbed P (Ps)
- Partitioning of incoming effluent P into solution P (Psol'n) and freshly sorbed P (Ps) is based on a published linear regression equation between the Colwell P:PBI ratio and the soil solution P concentration (see Figure 1-2 from Moody)
- A number of functional equations (based on Colwell P and PBI values) which have been developed to describe the soil solution concentration Psol'n immediately after effluent application (sorption), and after the diluting effects of a rainfall event (desorption)

Similar to the HSPF algorithms used in MEDLI, the Moody approach calculates the **soil solution P concentration** that determines bioavailability to crops, and also the movement of P in runoff and drainage by diffusion and mass flow. Moody goes on to say the alternative model:

- Needs only measurement of Colwell P and PBI for each soil layer of interest, and
- Measurement of dissolved reactive P (DRP) and dissolved organic P concentrations in the incoming effluent
- Assumes dissolved organic P in the incoming effluent is treated as DRP from the viewpoint of P sorption reactions
- Takes no account of the slow fixation reactions which reduce the potential for P desorption because of mineral lattice incorporation vs surface adsorption

**The approach suggested by Moody seems to be simple to implement in MEDLI and is worthy of the effort to compare its output predictions with that of the existing Freundlich algorithms used in MEDLI, provided matching soil properties can be ensured.**

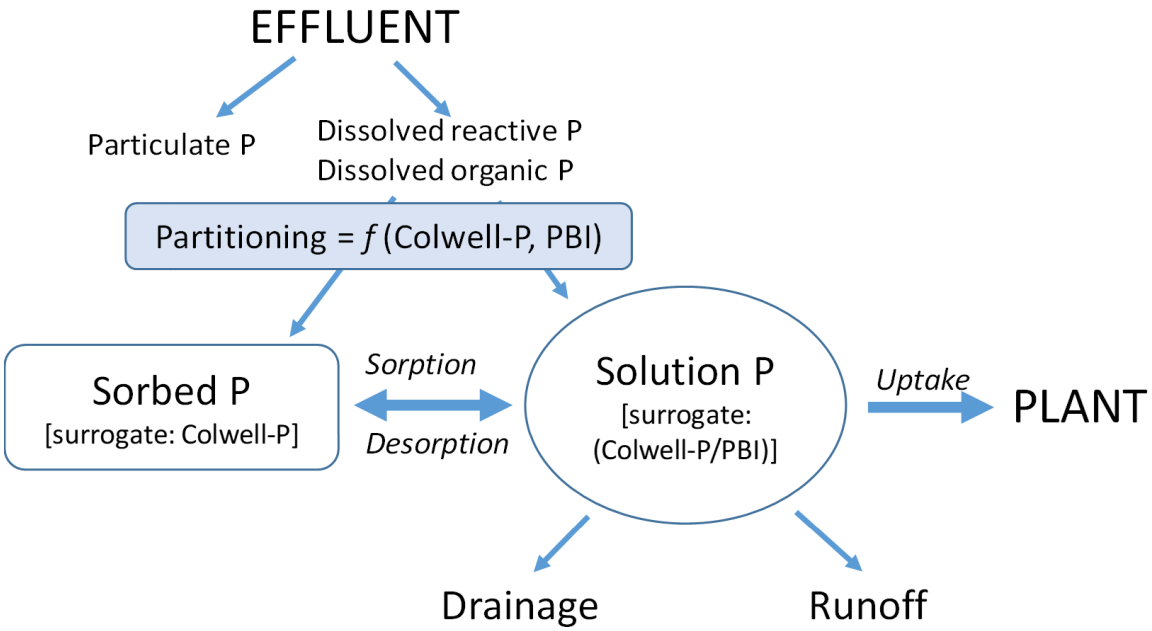



*Figure 18. Flowchart of the phosphorus pools and processes and the relevant surrogate measurements and algorithms to calculate the soil solution P concentration following application of effluent (from Moody 2021).*

Finally, we note that Moody also reviewed the P modules in the DAIRYMOD and APSIM models with the latter being quite sophisticated to take into account the interchange of P between the surface organic residue and the inorganic P. In both cases, Moody concludes that the APSIM and DAIRYMOD P modules have little to offer in terms of informing or revising the P module in MEDLI. The focus of the APSIM and DAIRYMOD P components is primarily on assessing the adequacy of soil, fertiliser, and other sources of P for crop growth; unlike MEDLI, there is no focus on assessing the potential environmental risk of oversupply of bioavailable P, and in this respect, MEDLI is unique.

## 4.3. Phosphorus in Runoff

As sediment loss from permanent irrigated pasture is likely to be very small, the most likely export pathway is via soluble P, also called Dissolved Reactive Phosphorus (DRP). Moody (2021) reports on studies that show that for P applications up to 80 kg P/ha/yr, the likely loss is ≤1 kg P/ha/yr. Although this load is small, the corresponding concentrations in the runoff often exceeded the ANZECC water quality guidelines (≤100 µg P/L), several-fold. Moody considered it is therefore imperative that dilution of the runoff from fertilised pastures occurs before it enters a watercourse, and thus the water quality impacts of the drainage system from paddock to farm boundary come into play.

Other field studies have shown that the longer the number of rain-free days post P fertilization of pasture, the lower the total P export, so management of P application in relation to timing of runoff events appears to be the main strategy for mitigating P runoff losses. This would be very difficult to achieve in effluent irrigated pasture since regular irrigation is critical in managing the effluent volume in the balancing storage.

A more useful approach would be to relate soil solution P concentration in the topsoil to DRP concentrations in the runoff. Burkitt et al. (2010) established a linear or curvilinear relationship (depending on the extraction method to estimate solution concentration) for rainfall simulator studies. But others caution that these are likely to be underestimates of field behaviour because of the lack of equilibration time between soil surface and runoff due to short flow path and high velocity. Later analysis by Moody (2011) showed that the ratio (Colwell-P to PBI) is the appropriate surrogate for soil solution P concentration, and he gave the predictive relationship:

$$Solution\ P = 0.279 * (Colwell\text{-}P/PBI_{Colwell}) + 0.059$$

where Colwell-P and $PBI_{Colwell}$ are the values of the source soil.

It would be expected that P in the top few centimetres of soil would be best correlated with DRP in the runoff. However, Moody (2021) argues that field and small plot studies show that agronomic (0 –10 cm) soil P testing in pastoral soils is sufficient for estimating the potential for losses of P in runoff, and that there is no need to collect shallow soil samples especially for this purpose.

Given that soil solution P can be estimated from routine soil chemistry measurement, the challenge in applying this concept to MEDLI is knowing the soil solution P - runoff DRP relationship. **The relationships developed by Burkitt et al. (2010) (but not reported in Moody 2021) could be a good starting point.**

An alternative method of estimating dissolved P concentration in runoff is described in the HowLeaky manual (Queensland Government, 2019), a model frequently used to estimate nutrient export from catchments draining into the Great Barrier Reef. Briefly the algorithms are:

$$Phos\_Conc\_Dissolve\_mg\_per\_L = \frac{-100.0 + 30 \times phos\_saturation\_index}{1000}$$

$$phos\_saturation\_index = \frac{Colwell\text{-}P \times p\_enrich}{p\_\max\ \_sorption} \times 100$$

$$p\_\max\ \_sorption = 1447 \times (1 - e^{-0.001 * PBI})$$

Apart from the **P enrichment ratio** (used to account for the preferential transport of P-rich fine material from hillslopes) the input parameters needed to evaluate the above equations are the Colwell P and the PBI value for the top 10cm of soil. For irrigated pasture, it is unlikely that significant sediment will be transported in the runoff and hence the enrichment ratio could be taken as unity. If this assumption is not correct (because of different plant types) then it can be calculated from:

$$EnrichmentRatio = Min(10, Max(1{,}15 - 0.33 \times ClayPercentage))$$

Where *ClayPercentage* is the percentage clay in the topsoil.

The range of the function is limited to 1 ($ClayPercentage$ >45) to 10 ($ClayPercentage$ <15). The method is based on data from soils in Queensland that ranged from 26 to 65% clay, and so is best suited to clay soils. The enrichment ratios are high (≥5) for soils less than 30% clay.

It is uncertain how well validated these algorithms are, and this point should be investigated further before their incorporation into MEDLI. A good starting point would be the evaluation of the equations (including that of Moody 2011) for a range of Colwell-P/PBI values to see how the predicted DRP mg/L values compare with the values measured in runoff from irrigation paddocks, or their receiving waters.

## 4.4. Nitrogen in Runoff

Because N tends to be at a much higher concentration than P in effluent, it would be expected that dissolved level of inorganic N could be “quite high” in runoff from effluent irrigated pastures. HowLeaky suggests three options to predict this concentration.

**The first** is the Victorian DPI methodology (described in the HowLeaky technical manual-2019) which uses the algorithm:

$$N\_conc_{runoff} = N\_conc_{soil} \times k \times (1 - e^{-cv \times runoff})$$

where $N\_conc_{runoff}$ is the Nitrate concentration in the runoff (mg/L); $N\_conc_{soil}$ is the soil nitrate concentration (mg N/kg) in the surface soil layer (notionally 0-2cm); $cv$ is a parameter that describes the curvature of change in soil and water (ratio) at increasing runoff values (initial guess is 0.2); $Runoff$ is daily runoff in mm, and k is an empirical soil water/runoff mixing factor with a suggested value of 0.5.

The soil nitrate concentration in the surface layer (0-2 cm) $N\_conc_{soil}$ (mg N/kg) is derived from the measured nitrate load ($N\ load_{so}$ kg N/ha) in this surface layer and uses the equation:

$$N\_conc_{soil} = \frac{a \times 100 \times N\_load_{soil}}{d \times p}$$

Where $\rho$ is the soil bulk density (t m$^{-3}$); $d$ is depth of surface soil layer (in mm, i.e., 20 mm); and $\alpha$ is a conversion factor that can be used also for calibration.

Although not mentioned by the authors, it's possible that the 0-10 cm soil nitrate concentration (mg/kg) could be used, as per the findings for similar dissolved P runoff calculations (described above).

**The other 2 approaches** (Rattray et al. 2016 and Frazer et al. 2017) calculate dissolved inorganic nitrogen (DIN= $NO_3$-N plus $NH_4$-N) in runoff ($N\_conc_{runoff}$) in response to a fertiliser application. The method inputs a sequence of fertiliser application rates and dates and calculates nitrate concentration in the runoff (mg N/L) from the equation:

$$N\_conc_{runoff} = \frac{lastnappliedrate}{a} \times cumrain^{-b}$$

Where $lastnappliedrate$ was the most recent application rate from the input time-series; $a$ and $b$ are the "Power Fit Alpha and Beta values" from the input parameters based on DIN runoff data from a banana paddock (see Rattray et al. 2016); and $cumrain$ is the effective rainfall and irrigation until a runoff event occurs. (The logic behind using the inverse of cumulative effective rainfall presumably reflects $NO_3$ leaching into deeper soil layers)

The Frazer approach is similar to the Rattray approach in that it uses a time series of applied N fertilizer, a soil water /runoff mixing factor (k), a nitrogen loss/mm runoff factor, and a daily loss proportion, DL (but the meaning of DL is not explained).

When choosing which approach to try in MEDLI, the algorithm with the maximum amount of physically measurable inputs and the fewer empirical matching coefficients seems preferable. **Hence it is recommended that the Victorian DPI approach be considered for further investigation** as runoff and soil nitrate-N concentration are inputs (both calculated daily in MEDLI), the **k** mixing factor has a physical meaning as it describes the dilution of the soil solution with runoff water, but the meaning of the **cv** parameter is confusing. Similar to the Drainage Functions (i.e., **TTi** and **ti**) the shape of the $N\_conc_{runoff}$ response surface should be explored with a range of physically sensible inputs and wherever possible, assessed against measured runoff data, especially those from high production pastures.

# 5. Pond Chemistry

The pond module in MEDLI was developed from the intensive livestock industry where the effluent is high in suspended solids, and TAN dominates the N species. Consequently, sedimentation of solids is considered a major process and is assumed to provide a substantial sink for organic P and organic N. Subsequent loss of N is assumed to occur via $NH_3$ volatilization using a fixed coefficient. P not settled in the first (anaerobic) pond was considered to move undiminished in the soluble form into all subsequent ponds, and hence onto the irrigation area. Nitrogen on the other hand was assumed to be dominated by $NH_4$ and hence continued to be volatilized from all subsequent ponds using the same "transfer coefficient".

Mike Johns was requested to provide a report that particularly focused on nitrogen and phosphorus transformations and removals in ponds and how the modelling of the removal of these nutrients in ponds could be improved.

The Johns and Butler report (Johns and Butler, 2021) reviewed the assumptions and default values in MEDLI Pond Chemistry module and identified aspects that are either questionable, out of date, generally not applicable to non-piggery applications, or where recent research has provided an improved understanding of the field and/or generated superior approaches that can be realistically embedded in MEDLI. Where the approach used (in MEDLI) was sound, and there had been little or no change in the underlying science, they were classified as "Strong". Where the approach adopted was vulnerable to error, especially when applied to STPs or food production facilities, they were classified as "Vulnerable". These vulnerable aspects were prioritised in the subsequent technical literature review.

Three major vulnerable aspects were identified for particular focus:

- In the Nitrogen Mass Balance, the treatment of ammonia and its volatilisation from ponds.
- In the Phosphorus Mass Balance, the assumptions used in the partitioning of phosphorus between the solid and dissolved states.
- The estimation of sludge deposition and partitioning of nutrients in ponds.

Johns and Butler (2021) also noted that achieving the stringent requirements for sustainable effluent irrigation systems in Australia has led to a reduction in the number of "traditional" pond systems that are featured in MEDLI. For many agri-industry sites, relevant changes include the adoption of Covered Anaerobic lagoons, Biological Nutrient Removal systems (BNR), membrane bioreactors (MBR), chemical dosing for P reduction, and low permeability pond liners. Clearly these changes in the MEDLI "marketplace" seriously impact the utility of the MEDLI pond module, especially for the larger treatment systems which are more likely to install the more complex treatment technologies. The changes significantly complicate nitrogen transformations occurring during treatment. For example, oxidised nitrogen species were rare in "traditional" pond systems but may predominate in the treated effluent of newer technologies. Also, ammonia volatilisation may be significantly reduced in covered lagoons relative to open anaerobic ponds with long retention times.

## 5.1. Nitrogen Mass Balance

MEDLI assumes that the only forms of nitrogen of consequence in the ponds are organic (ON) and ammonia nitrogen. It predicts the concentration and mass of these forms in the pond effluent by applying a proportionality constant, rather than using a nitrogen species mass balance. Oxidised forms of nitrogen are ignored.

In the opinion of Johns and Butler (2021), the primary weaknesses of the **nitrogen mass balance** approach in MEDLI are:

- Settling of nitrogen-containing solids is assumed in the anaerobic pond only.
- A single "proportionality constant" is assumed sufficient to model ammonia concentrations and volatilization rate in the ponds. MEDLI assumes that the TN is comprised of 70 to 80% ammonia which, whilst typically true after anaerobic treatment, is not generally true for all wastewater ponds and effluent types. The MEDLI volatilization rate also ignores seasonal

impacts, pH, temperature and mixing which can be profound, especially in final storage lagoons with long retention times. For a daily time-step model, this simplification is prone to considerable error in the mass of nitrogen irrigated.

- The models assume no nitrogen loss due to biological uptake and subsequent sedimentation of the resulting biomass, or from nitrification/denitrification reactions catalysed by bacteria in the pond.

In their literature review of N removal from waste stabilization ponds, Johns and Butler (2021) concluded:

- Algal growth and subsequent sedimentation and simultaneous nitrification/denitrification are the most significant total nitrogen removal pathways in ponds
- The major ammonium removal pathway in facultative ponds (also known as waste stabilization ponds) is now considered to be biomass (algal and bacterial) growth.
- Measured volatilisation accounts for < 5% of total ammonia removal
- Algal growth inhibition occurs at high organic, ammonia and sulphate concentrations which explains the negligible algal growth in anaerobic ponds

Johns and Butler (2021) also reviewed models for predicting N removal from waste stabilisation ponds for treating sewage, and recommended the Pano and Middlebrooks (1982) equation which has the form (for temperatures up to 20°C):

$$\frac{C_e}{C_i} = 1/\left[1 + \frac{A}{Q}(0.0038 + 0.000134T) * e^{\{(1.041+0.044T)(pH-6.6)\}}\right]$$

Where:

Ce and Ci= ammonia-N concentration (mg/L) of *effluent* and *influent*, respectively

Q= average flow rate into pond ($m^3/d$)

A= pond surface area ($m^2$)

T= pond water temperature ($^oC$)

For temperatures > 20°C, a different form of the equation is used (See Johns and Butler 2021, p14). Johns and Butler (2021) argue the Pano and Middlebrooks equation provides a reasonably good average prediction of **ammonia** removal from ponds despite its development on the assumption of *ammonia volatilization* dominance (which is clearly incorrect for facultative and maturation ponds). The reason is that the model essentially describes N removal as a first order reaction in a completely mixed reactor (pond) system which reasonably describes (in a lumped fashion) most of the N removal or transformation mechanisms at work (e.g. incorporation into biomass, nitrification/denitrification) for similar pH and temperature ranges.

The use of ammonia N as the input parameter for the Pano and Middlebrooks might be considered a major disadvantage in modelling TN removal but Johns and Butler (2021) observes that ammonia N tends to represent the bulk of the soluble N present (except where ammonia effluent levels are very low) since concentrations of oxidized nitrogen in waste stabilisation pond effluents is typically negligible. Given that much of the non-ammonia TN in pond effluents is organic N incorporated into microbial or algal cells and is principally particulate nitrogen, it is likely to be partitioned into the sludge or slowly mineralised if applied in the irrigation water.

If TN removal is an important outcome for the irrigation scheme, then Johns and Butler (2021) suggests the Reed et al. (1995) equation could be uses, viz:

$$C_e = C_i e^{-K_T\left(t+60.6(pH-6.6)\right)}$$

Where:

Ce,I = TN concentration of *effluent* and *influent* respectively

KT = rate constant (1/d) at temperature T (°C) with the relationship to temperature expressed as:

$$K_T = K_{20}\theta^{(T-20)}$$

K20 = rate constant value at 20°C = 0.0064/d

Θ = temperature constant, 1.039

A = pond surface area

T = pond water temperature (°C)

t = hydraulic retention time (d)

Note that the pond water temperature can be obtained from the widely used Mancini & Barnhart equation given in Shilton (2005).

There is an important caveat with the above findings, in that almost all recent literature addresses STP waste stabilisation ponds characterised by low TN levels (50 mg/L or less). For industrial or intensive animal effluents where TN levels may be 200 - 400 mg/L (for meat processing plants) or even higher for intensive agriculture, some of the conclusions above may not be appropriate. For example, ammonia volatilization losses from high N (500 mg N/L) land fill leachate in a tropical climate have been measured at rates orders of magnitude higher than that in sewage-based systems.

Many of the above objections can be removed if MEDLI were to adopt dynamic biokinetic models (see Ho et al. 2019) that describe the N transformation processes in detail based on Monod kinetics with Arrhenius temperature adjustments, and nitrification inhibition by pH and DO. For example, the Dynamic Rational Model (Mayo and Abbas 2014) considers dynamic mass balances of ammonia, organic and nitrate nitrogen and captures six N loss/transformation pathways including mineralisation, nitrification, denitrification, microbial uptake (algae and bacteria), permanent sedimentation and ammonia volatilisation. Alternatively, the Activated Sludge Model #3 has been modified to include algal growth & ammonia volatilization which are important in open treatment lagoons (Gehring et al. 2010).

The advantages of these models over the empirical models such as Pano and Middlebrooks is that they allow discrimination between the various N removal mechanisms based on equation sets for each mechanism. However, Johns and Butler (2021) **recommends against** their further consideration in MEDLI because of their complexity (due to the large equation set and the number of associated model parameters that need to be quantified) and the absence of convincing validation in full scale waste stabilisation pond systems. In contrast, the simpler Pano and Middlebrooks model outcomes has been widely supported by studies on full-scale systems across the world.

Overall, Johns and Butler (2021) recommendations for N modelling in MEDLI include:

- MEDLI incorporates a sedimentation loss of particulate nitrogen in the first pond but assume none in subsequent ponds. Like the approach of Mayo & Abbas (2014), a simple linear function is assumed based on a Net Settling Fraction (Fr-N). This approach has merit, but the challenge is what this value should be. The Pano and Middlebrooks approach works only with the soluble N fraction – an acknowledged weakness. There remains no simple solution.

- MEDLI allows a Net Settling Fraction (Fr-N) for only the first (anaerobic) pond in a series. An alternate option would be to allow for this term to be available in all ponds, with the value decreasing down the pond series.
- The current MEDLI approach is based on the now disputed view that ammonia volatilisation is a predominant N removal mechanism. The equation used to estimate volatilisation is extremely empirical – even by pond modelling standards – and appears to have little dependence on factors critical to volatilisation such as water temperature, pH, retention time and wind velocity.
- There is benefit in adopting the Pano & Middlebrooks (1982) model approach to replace the existing ammonia volatilisation equations in MEDLI. The model has been well validated with pond systems and provides a superior estimation of soluble nitrogen (ammonia) losses to the existing MEDLI equation. Although its focus on ammonia ignores other soluble nitrogen species, Johns and Butler (2021) argue that ammonia is the principal soluble form of nitrogen in most waste stabilisation pond, and agro-industrial effluents with soluble biodegradable organic nitrogen species rapidly mineralise in ponds. The implementation of this model would strengthen estimation of soluble nitrogen removal in MEDLI.
- A challenge for adoption of the Pano & Middlebrooks model, however, is estimating the seasonal pond pH, which is impacted by algal growth. It is likely that that the user will need to input a seasonal pH curve for the pond system based on historical behaviour for the most accurate results
- Nitrogen loss by sedimentation of the influent particulate organic nitrogen and the N sequestered in the particulate biomass (algae and bacteria) remains an intractable issue. This is of concern as biomass sedimentation appears to be a major mechanism of N removal. Overall, the existing approach in MEDLI which uses a simple net settling fraction (Fr-N) seems warranted, provided the value is *reasonable and not overstated*.
- MEDLI needs to focus improvements in nitrogen estimation for STP waste stabilisation pond systems where traditional ponds remain in widespread use. In contrast, medium to large agro-industrial wastewater plants treating high nitrogen loads and concentrations have adopted intensive BNR systems where effluent of a known nitrogen concentration is produced. These concentrations can be inputted into MEDLI as the effluent composition from the final pond.

## 5.2. Phosphorus Mass Balance

MEDLI calculates the Total Phosphorus mass balance in the pond using the same two-compartment model approach as that used for nitrogen. One compartment defines the soluble (non-settling) fraction and the second compartment the solid (settling) TP fraction. Only the anaerobic pond has a settling fraction, Fr-P. Speciation of phosphorus forms is neglected, since biological activity usually rapidly converts organic forms of phosphorus into the inorganic phosphate form.

In the view of Johns and Butler (2021), the major weaknesses of the phosphorus mass balance approach used in MEDLI are:

- Settling of solids is assumed only in the anaerobic pond.
- MEDLI's default assumption that 90% of TP entering the pond settles into the sludge is not appropriate for STP and agri-industrial effluents. It almost certainly underestimates TP loads to the irrigation area if this default is selected in these situations.

In most wastewater pond systems, phosphorus is removed by biomass assimilation and subsequent settlement (Ashworth & Skinner, 2011) and by phosphate precipitation reactions promoted by alkaline pH conditions in the ponds (Shilton, 2005). Although quite variable, phosphorus reduction is unlikely to exceed 50% without chemical addition. These reductions are typically much less in agri-industrial systems where initial TP levels are much higher than in sewage.

The predominance of the removal mechanisms remains unclear. Shilton (2005) reports that precipitation results in the largest fraction of phosphorus removed, whilst other studies (Vendramelli et al. 2016) reported that phosphorus sequestration by pond biomass appeared to be the greatest

contribution in facultative sewage ponds. Calculation of phosphorus removal by precipitation requires measurement of cations such as iron, calcium, and magnesium (in the water column and sludge), and pond pH and temperature, which vary seasonally.

The modelling of phosphorus removal in waste stabilisation ponds is almost non-existent with the options of an empirical regression equation (Gomez et al. 2000) or an empirical phenomenological equation (Vijay and Yuan 2017) with tries to capture the main chemo-physical processes (precipitation & biomass sequestration). Given the Gomez equation takes no consideration of the effects of factors such as temperature, hydraulic retention time, pH, etc. on P removal, its application to other (non-European) areas is problematic.

The Vijay and Yuan approach involves a 3-term phenomenological equation where the first term accounts for P loss due to *assimilation into biomass*, and the second and third terms account for P *precipitated* through reactions with trivalent aluminium and iron, assuming a pond pH in the range 8 – 10. Assimilation is estimated as a linear function of the biomass volatile suspended solids (VSS) concentration/growth and the pond retention time. The equation was developed for sewage effluent in Canada.

$$P_o = P_i\left(1 - \frac{e^{(A*0.053)}}{4}\right) - \frac{K_{sp}(AlPO_4)}{Al_i} - \frac{K_{sp}(FePO_4)}{Fe_i}$$

And:

$$A = VSS * G * VPC * t$$

Where:

$P_{o,I}$ = phosphate concentration *out* and *in* (mg/L)

A = assimilated phosphate (mg/L)

VSS = volatile suspended solids (mg/L)

G = 0.17, VSS growth rate ($d^{-1}$)

VPC = 0.0275, biomass P/C ratio (based on generalised cell formulae of algae and bacteria)

t = average hydraulic retention time of pond (d)

$K_{sp}$ = solubility products of the respective precipitation reactions

Johns and Butler (2021) argue that, using a typical VSS of 100 mg/L, the equation predicts over 40% removal (for an initial P of 30 mg/L) even with precipitation ignored, and in the absence of anything better, the results have some merit for estimating effluent phosphate concentrations for Australian conditions. However, they do caution that there is no compensation for temperature which can be expected to have a significant effect on VSS growth. More importantly, the pond data set used to estimate model parameters was the same as that used to validate the model.

Overall, Johns and Butler's recommendations for P modelling in MEDLI include:

- The current MEDLI approach to estimate P removal in ponds is simple and brutal. All P removal is credited to the first (anaerobic) pond through use of *Fr-P* – the net settling fraction. The default value is 90%, which will substantially over-estimates P removal for STP waste stabilisation and agro-industrial ponds.
- The Vijay & Yuan model offers a relatively elegant, simple, and reasonable equation set for use in the pond chemistry module. This model looks particularly suited for STP waste stabilisation ponds of any type. Adjusting the "G" factor for temperature in the manner used by many existing kinetic models in wastewater design could allow for climatic differences. In addition, the maximum P removal could be capped at 50% to reflect published

measurements. However, the model was designed for operation between pH 8-10; a waste stabilisation pond operating at pH 7 might have much less P precipitation than one at pH 8.

- The Vijay and Yuan model would eliminate the requirement for a settling fraction. MEDLI would assume that the P in the settled biomass is removed as sediment from the base of the pond.
- MEDLI should focus improvements in phosphorus removal for STP waste stabilisation pond systems where traditional ponds remain in widespread use
- Medium to large agri-industrial wastewater plants treating high phosphorus load (and concentration) usually install intensive BNR and/or chemical precipitation systems to arrive at the required compliance P level. These compliance level concentrations are relatively constant and can be inputted into MEDLI as the effluent composition of the final pond.

## 5.3. Anaerobic Pond Module

The review has had little to say on anaerobic ponds other than to reiterate that $NH_3$ volatilization is probably overestimated using the MEDLI algorithm and that the Pano & Middlebrook equation should be considered for this pond, although the underlaying assumption of the loss processes is wrong. This seems a questionable recommendation as **algal growth inhibition** occurs at high organic, ammonia and sulphate concentrations (Gehring et al. 2010, Ashworth and Skinner 2011) which explains the negligible algal growth in anaerobic ponds (in addition to poor light penetration). Rather it is more likely that some fraction of the organic N and P (not explicitly specified in MEDLI) is the major loss pathway. The issue of defining a reasonable value for this fraction (especially sewage effluent) remains unresolved.

# 6. Conclusions

## 6.1. Soil Hydrology

The Curve Number-cascading bucket-Ritchie evaporation approach used in MEDLI is very similar to the approach taken by the majority of the 18 daily time-step one-dimensional hydrology models that were reviewed in detail. This is not surprising, as the majority of the algorithms in these models came from the EPIC and CERES-Maize stable.

Alternatives to this approach usually involve numerical solution to the non-linear Richards equation, which in turn require inputs of the difficult-to-measure soil hydraulic functions K- $\boldsymbol{\theta}$ and $\boldsymbol{\psi} - \boldsymbol{\theta}$.

The soil evaporation algorithm in MEDLI has been identified as needing modification to the dead cover scaling factor, and the residue load (kg/ha) approach used in HowLeaky seems an appropriate solution.

Recommendations on using better science to describe the infiltration, deep drainage and solute leaching processes in MEDLI has been hampered by the complexity of the soil physics involved. However, some recommendations have been made to explore the Green & Ampt infiltration equation, the K- $\boldsymbol{\theta}$ function to better inform the parameters in the existing soil water redistribution algorithm, and the Burns equation to describe the mass of solute leached for a given amount of deep drainage. More rigorous analysis requires the input of a specialist soil physicist, and a recommendation has been made to engage a suitable contractor by commission rather than by open tender (see Cook 2021).

The deep drainage algorithm used in MEDLI was explored in detail by plotting the time response of drainage rate and cumulative deep drainage with changes in the value of the scaling factor ti. It was reassuring to find that the responses followed those expected from soils of different textures (e.g., sand to clay loam), but it was suggested that the value of ti could be better chosen given knowledge of a soil's K- $\boldsymbol{\theta}$ function.

The issue of model validation has been a reoccurring theme throughout the review, and this applies especially to irrigated soils where deep drainage is one of the most important outputs to assess scheme sustainability. More investigation (desk and field studies) is warranted to confirm that MEDLI adequately captures the runoff and deep drainage behaviour of irrigated soils. A possible avenue is comparing MEDLI deep drainage estimates with those from the SALF model (Shaw & Kitchen 2019) for a range of soils with matching data. Where this has been attempted (e.g., Beaudesert), the lack of agreement between the two estimates is of concern.

## 6.2. Nutrients

The Nitrogen module in MEDLI uses Michaelis–Menten type equations to predict the rates of mineralization, nitrification and denitrification which are adjusted by 0-1 scaling factors to take into account reductions (from a defined maximum rate) due to suboptimal values of temperature, soil water status and pH. This is very similar to the approach used by the more sophisticated N models in say APSIM and DAIRYMOD, but the actual functions, and sometimes the maximum rates, vary between models. The paucity of validation data for irrigated situations indicate there is no compelling reason to change the functions used in MEDLI. The exception is the denitrification process where the maximum values vary over an order of magnitude, and it appears that the APSIM value (about 6 kg N/ha/day) most closely reflects field measured values in high production dairy pastures (Frield et al 2016). Given that denitrification is one of the two most important sinks for applied N in effluent irrigated pasture (the other is biomass uptake) it is recommended that MEDLI adopt this value. It is also recommended that a more detailed literature search on maximum denitrification rate be undertaken to confirm or modify the 6 kg/ha/day figure.

Denitrification requires a labile carbon source as well as anaerobic conditions. In MEDLI there is no allowance for the relative availability of C; rather it operates on a C presence/absence rule and is usually confined to the surface 10 cm. This is likely to limit the number of days denitrification which can occur in a year since the surface soil will reach the DUL sooner than deeper layers. Recent MEDLI modelling of effluent irrigated pasture in SEQ revealed a very large increase in denitrification if C were assumed to occur over the full rooting depth (of 60 cm). Hence it is recommended that MEDLI

incorporate into its denitrification algorithm, a labile carbon scaling factor similar to that used in APSIM. And that measured labile carbon values be inputted for the whole soil profile (i.e., >> 10 cm).

Volatilization of N from soil is unlikely to be significant for effluent irrigation as the N is already applied in the hydrolysed form as NH4/NH3. APSIM does not consider this process except for a special adaption for NH3 loss from urine patches. However, volatilization losses from the spray irrigation can be substantial (e.g., c. 50% of TAN) depending on the pH (> 8) and the nozzle operating pressure (e.g. > 500kPa). There is no easy way to predict these ammonia losses except by experimental measurements using simple, acidified catch cans. But a default value of 15 to 20% would seem appropriate for lower pressure centre pivots.

Unlike more sophisticated N models such as the one used in APSIM, MEDLI does not contain a Carbon cycle module which allows for the mineralization and immobilization of N in fresh organic matter (FOM). Moody (2021) argues that having soil C dynamics driving the N processes is mechanistically correct, is intuitively logical, and could be incorporated into MEDLI reasonably easily following the APSIM or DAIRYMOD exemplars. However, as MEDLI is often applied to cut and cart pasture, the opportunity for significant residue levels after harvest is unlikely. Hence the extra complexity of a dynamic C module in MEDLI is unlikely to have a significant effect on the predicted surplus N available for leaching. The quantum of N leaching loss is one of the key assessment criteria for assessing environmental sustainability.

The P model in MEDLI is based on the Freundlich adsorption isotherm which is used to estimate the soil solution concentration at any soil depth, especially that at the bottom of the rooting depth, or at the bottom the assumed soil profile depth. The input data is both expensive to measure and difficult to find a soil chemistry laboratory, whilst the risk of P leaching to groundwater is remote except in very sandy soils whose groundwater is well connected to the receiving surface waters (e.g., WA). Its continued use in MEDLI is not recommended except for cases of special landscape vulnerability. Moody (2021) has presented an alternative model based on the ratio of Colwell-P to PBI - both easily measured, single point measurements. Similar to the Freundlich based algorithms used in MEDLI, the Moody approach calculates the soil solution P concentration that determines bioavailability to crops, and also the movement of P in runoff and drainage by diffusion and mass flow. The approach suggested by Moody (2021) seems to be simple to implement in MEDLI and is worthy of the effort to compare its output predictions with that of the existing Freundlich algorithms used in MEDLI, provided matching soil properties can be ensured. This ratio approach also underpins the risk assessment of P export from sugar cane farms in Great Barrier Reef catchments.

The major P export pathway of environmental concern is via attachment to sediment or in a dissolved form moving with the surface runoff. Given the high surface cover associated with irrigated permanent pasture, erosion is highly unlikely to be a significant factor and can be ignored for most situations of interest to MEDLI. However, for the exceptions, the sediment erosion/enrichment algorithms of HowLeaky could be adapted for use in MEDLI.

For dissolved P in runoff, there are two options. This first option is the soil solution P predicted by the new Moody algorithm (based on Colwell-P and PBI) which needs to be translated into runoff concentrations. Empirical soil solution P - Runoff dissolved P functions based on rainfall simulator results by Burkitt et al (2010) could be a first approximation. The second option is to use the algorithms for dissolved P described in HowLeaky. It is uncertain how well validated these algorithms are, and this point should be investigated further before their incorporation into MEDLI. A good starting point would be the evaluation of the equations (including that of Moody 2011) for a range of Colwell-P/PBI values to see how the predicted DRP mg/L values compare with the values measured in runoff from irrigation paddocks, or their receiving waters. But perhaps the larger question is whether the quantum of this P export pathway is worth the modelling effort (in MEDLI), given Moody's review (Moody 2021) reported that P losses from fertilized permanent pasture were usually < 1kg/ha/yr.

Because N tends to be at a much higher concentration (and more soluble) than P in both soil and effluent, it would be expected that dissolved level of inorganic N could be "quite high" in runoff from effluent irrigated pastures. HowLeaky suggests three options to predict this concentration, with the first option using a measured soil nitrate concentration, a mixing factor to allow for dilution by surface runoff, and another factor that allows for the change in the mixing factor as the runoff event proceeds.

The algorithm was based on results from a Victorian DPI study of permanent pasture and seems easy to implement in MEDLI especially if the nitrate-N in the top 10cm can be used instead of the 0-2cm value recommended in HowLeaky. Its validation is unknown. The other two approaches are based on using the time series of fertilizer application (kg/ha), the cumulative rainfall from the last fertilizer addition to when runoff occurs, and two fitting parameters based on N runoff experiments in North Queensland. Their usefulness for incorporation into MEDLI is unlikely.

## 6.3. Pond Chemistry

The pond chemistry review (by Johns and Butler 2021) argued that the current module used in MEDLI is really only fit for piggery effluent and even then, the partitioning factors for settling are too high, as is the N volatilization loss. The equation used to estimate volatilisation is extremely empirical – even by pond modelling standards – and appears to have little dependence on factors critical to volatilisation such as water temperature, pH, retention time and wind velocity.

The literature suggests that volatilization contributes < 5% $NH_3$-N loss unless the effluent is very high strength (say 500mg/L) and the climate is tropical. Rather, the main N removal pathways are algal growth and its sedimentation, and associated nitrification/denitrification reactions.

Use of the Pano & Middlebrooks (1982) empirical equation is supported for use in MEDLI to calculate the removal of soluble N. Although it is based (incorrectly) on $NH_3$ loss via volatilization, its form captures N removal as a first order reaction. Moreover, use of $NH_3$-N as the input variable is not a great drawback as it comprises the bulk of the **soluble N** in ponds.

If TN is the important variable to calculate, then the Reed et al. (1995) equation could be considered, but this needs an Arrhenius type temperature correction factor to be added.

Nitrogen loss by sedimentation of the influent particulate organic nitrogen and the N sequestered in the particulate biomass (algae and bacteria) remains an intractable issue. The net settling fraction (Fr-N) approach has merit, but the challenge is what this value should be. The value should be "reasonable and not overstated".

The current MEDLI approach to estimate P removal in ponds is simple and brutal. All P loss is credited to the first (anaerobic) pond through use of the net settling fraction (Fr-P). The default value is 90%, which will substantially over-estimates P removal for sewage ponds and agri-industrial ponds.

However, the removal process of P in ponds is uncertain, with experts' views split between biomass sequestration and settling, and natural precipitation reactions.

There are very few predictive equations for P removal from ponds, but Johns and Butler (2021) recommend that the Vijay and Yuan (2017) model should be considered. This is a three-term phenomenological equation where the first term accounts for P loss due to assimilation into biomass, and the other terms account for P precipitation reactions. Although developed in Canada on sewage effluent, Johns and Butler suggest it can be used in other climates provided a temperate correction is made (Johns and Butler suggest a method) and it provides plausible P removal % even when the precipitation terms are ignored. However, predicted losses should be capped at 50%.

Overall, Johns and Butler (2021) believe that MEDLI should focus improvements on nitrogen and phosphorus removal for sewage waste stabilisation pond systems where traditional ponds remain in widespread use. Medium to large agri-industrial wastewater plants treating high nutrient loads (and concentrations) usually install intensive BNR and/or chemical precipitation systems to arrive at the required compliance P level. The output concentrations are relatively constant and can be inputted into MEDLI as the effluent composition of the final pond.

# 7. Review Methodology Learnings

A critical literature review of subjects as complex as soil hydrology, nutrient processes, and pond chemistry in a 10 to 15 day per person contract allocation is particularly challenging, given that key papers first need to be located, then sourced, followed by their detailed analysis. It is likely that only experts in the fields will have the experience to achieve a critical and informative review in the time allocated. These experts are probably best chosen by invitation rather than by open tender.

It is important to have a scoping report as the first Milestone of a model review contract in order to describe the research methodology and identify major science gaps

In undertaking a review of the science underpinning models, there is a compromise between the number of models accessed and reviewed, and the review of the basic science that underpins the algorithms. In case of hydrology, the science options for rainfall infiltration, soil water redistribution, and solute leaching are voluminous. However, it is considered that changes of significance are more likely to found in the science rather than in the algorithms of another model, given most models reviewed (in a given field) were likely to share much of the underlying logic. Subject matter experts are more likely to be familiar with the science, and hence are better able to make informed choices. That is, science expertise is likely to be more useful than modelling expertise.

The most competent reviewers of science gaps in models are developers/users who actively publish in the scientific literature - the most active seem to be the NZ practitioners who have the added advantages of grazed landscapes that have high N loads, soils with substantial deep drainage, and significant denitrification due to high rainfall. These are the conditions most likely to occur in Australian effluent irrigation schemes

In the MEDLI review, external modelling experts were polled to advise on a list of important hydrology models and the journals they were likely to be published in - including review papers that described a comparison of models

Contractors undertaking a science review need good literature search and review skills, as well as ready access to manuscript search tools (e.g., SCOPUS) and to the manuscripts of interests. For example, our SCOPUS searches identified over 7000 titles/abstracts of interests - with expert selection reducing this to about **800** manuscripts. This is a substantial resource now available via the Elsevier reference manager tool, MENDELEY (https://www.elsevier.com/en-au/solutions/mendeley).

It was important to share literature selections between contractors. This was achieved using the group share option in MENDELEY. It was set up by DES library at ESP. In fact, the current review task would have been difficult to achieve without the fulsome support of DES library staff.

It is also important to get regular informal feedback on research direction from the commissioning client, rather than wait for a critique on the submitted report(s). This helps ensure limited resources are not spent pursing “low relevance” directions.

The validation of many models seems to be partial or non-existent, especially for the difficult to measure processes such as denitrification, deep drainage, and solute leaching. Predicted yields, soil nitrogen stores, runoff and erosion are exceptions to this statement. If credible validation of current models is not available, the justification to make them more bio-physically complex is questionable.

There is a strong case to undertake a more detailed review of the validation of current models focusing on those processes which are of most interest to the commissioning client. Such processes are deep drainage, denitrification, solute leaching, followed by erosion loss and sediment enrichment and dissolved nutrients in overland flow.

Many of the processes considered in daily time step 1-D hydrology models are described using simple algorithms which take the place of complex basic equations developed in the soil physics literature. These complex equations are usually based on a solution /manipulation/extension of the Richards and/or the convective dispersion equations. Without a thorough understanding of the physics of infiltration, deep drainage, and solute leaching, it is difficult to assess whether the simplified algorithms developed by modellers are physically plausible, unless they have been confirmed by experimental measurement. As an alternative, it suggests that the current algorithms used to predict these three main processes (infiltration, drainage, leaching) be critiqued by a well-qualified, quantitative soil physicist- an expertise that was missing from the MEDLI Science Review team.

# 8. References

Adams, JE, Arkin GF, and Ritchie JT, (1976). Influence of row spacing and straw mulch on first stage drying. Soil Science Society Amer. Journal 40 436-442.

Addiscott, TM, (1977). A simple computer model for leaching in structured soils. *J. Soil Sci*. **28,** 554–563.

Addiscott, M and Wagenet, RJ, (1985). Concepts of solute leaching in soils: a review of modelling approaches. *Journal of soil Science* **36**, 411-424.

Allen, RG, Pereira, LS, Raes, D, Smith, M, & Ab, W (1998). Irrigation and Drainage Paper No. 56, FAO, 300pp. https://doi.org/10.1016/j.eja.2010.12.001.

Ashworth, J & Skinner, M, (2011). *Waste Stabilisation Pond Design Manual,* Northern Territory, Australia: Power and Water Corporation.

Asseng, S, Fillery, IRP, Anderson, GC, Dolling, PJ, Dunin, FX, and Keating, BA (1998). Use of the APSIM wheat model to predict yield drainage and nitrate leaching for a deep sand. *Aust J Agric Research* **49** 363-377.

Balwinder-Singh, Eberbach PL, and Humphreys, E (2014). Simulation of the evaporation of soil water beneath a wheat crop canopy. *Agricultural Water Management*, **135** 19–26.

Biggar, JW, and Nielsen, DR, (1976). Spatial variability of the leaching characteristics of a field soil. *Water Resour. Res*., **12**, 78-84, 1976.

Bond, JJ, and Willis, WO, (1970). Soil water evaporation: first stage drying as influenced by surface residue and evaporation potential. *Soil Science Society Amer. Journal* **34** 924-928.

Buckthought, L, (2013). The interactive effects of nitrogen fertilizer and animal urine on nitrogen efficiency and losses in New Zealand dairy farming systems. PhD Thesis Lincoln University, NZ.

Burkitt LL, Dougherty WJ, Carlson SM, Donaghy DJ (2010). Effect of variable soil phosphorus on phosphorus concentrations in simulated surface runoff under intensive dairy pastures. *Australian Journal of Soil Research* **48**, 231-237.

Burkitt LL, Moody PW, Gourley CJP, Hannah MC (2002). A simple phosphorus buffering index for Australian soils. *Australian Journal of Soil Research* **40**, 497-513.

Burns IG, (1975). An equation to predict the leaching of surface-applied nitrate. *Journal of Agricultural Science* **85**,443--454.

Burns, IG (1976). Equations to predict the leaching of nitrate uniformly incorporated to a known depth or uniformly distributed throughout a soil profile. *The Journal of Agricultural* Science **86**, 305-313.

Burns, IG, Greenwood, J, (1982). Estimation of the year-to-year variations in nitrate leaching in different soils and regions of England and Wales. *Agriculture and Environment* ***7,*** 35-45.

Campbell GS, (1974). A simple method for determining unsaturated conductivity from moisture retention data. *Soil Science* **117** 311-314.

Campbell, GS, (1985). Soil physics with basic. Elsevier, New York, New York, USA.

Catchpoole, V, (1975). Pathways for losses of fertilizer nitrogen from a Rhodes grass pasture in south-eastern Queensland. *Australian Journal of Agricultural Research* **26**, 259-268.

Catchpoole, VR, Oxenham, DJ, Harper, LA, (1983). Transformation and recovery of urea applied to a grass pasture in south-eastern Queensland. *Aust. J. Exp. Agric*. **23**, 80–86.

Chastain JP (2019). Ammonia volatilization losses during irrigation of liquid animal manure *Sustainability,* **11**, 6168; doi:10.3390/su1121616.

Cichota, R, Snow, V, Vogeler, I, Wheeler, D, and Shepherd, MA, (2012). Describing N leaching from urine patches deposited at different times of year with a transfer function *Soil Research* **50** 694-707.

Cichota, R, Brown, H, Snow, VO, Wheeler, DM, Hedderley, D, Zyskowski, R and Thomas, S, (2010). A nitrogen balance model for environmental accountability in cropping systems. New Zealand Journal of Crop and Horticultural Science.38(3). https://www.tandfonline.com/doi/full/10.1080/01140671.2010.498401.

Cichota, R, Snow, VO, Vogeler, I, Wheeler, DM. and Shepherd, MA. (2012). Describing N leaching from urine patches deposited at different times of the year with a transfer function. *Soil Research* **50** 694-707.

Cichota, R, Snow, VO, Vogeler, I, (2013). Modelling nitrogen leaching from over- lapping urine patches. *Environ. Model. Software*. **41**, 15-26.

Cichota, R, Vogeler, I, Snow, VO, Webb, TH, (2013). Ensemble pedotransfer functions to derive hydraulic properties for New Zealand soils. *Soil Research,* **51**, 94-111.

Clothier, BE, Heng, LK, Magesan, GN, and Vogeler, I, (1995). The measured mobile-water content of an unsaturated soil as a function of hydraulic regime. *Australian Journal of Soil Research* **33** 397-414.

Clothier, B.E, Kirkham, M.B, and McLean, J.E. (1992). In situ measurement of the effective transfer volume for solute moving through soil. *Soil Science Society Amer. Journal* **56** 733-736.

Cook, FJ and Cresswell, HP (2007). Estimation of soil hydraulic properties. Chapter 84 in *Soil Sampling and methods of Analysis.* Eds Carter, MR and Gregorich, EG. Canadian Society Soil Science. Taylor & Francis

Cook FJ (2021). MEDLI science review: Modelling of Water and Solute Transport in MEDLI. Report to the Queensland Water Modelling Network, Department of Environment and Science by Freeman Cook & Associates.

Dikinya, O, (2005). Comparison of instantaneous profile method and inverse modelling for the prediction of effective soil hydraulic properties. *Aust J Soil Research.* **43,** 599-606.

Dillon, PJ, (1989). An analytical model of contaminant transport from diffuse sources in saturated porous media. *Water Resources Research*, *25*(6), 1208–1218.

Donigian, AS, Bicknell, BR, & Imhoff, JC, (1995). Hydrological Simulation Program - Fortran (HSPF). In VP. Singh (Ed.), Computer models of watershed hydrology (pp. 395–442). Highlands Ranch, Colorado: Water Resources Publications.

Du, X, Feng, H, Helmers, MJ, Qi, Z, (2017). Comparing simulated nitrate-nitrogen concentration in subsurface drainage using Drainmod-N II and RZWQM2. *Irrig. Drain*. **66,** 238–251.

Emerson, K, Lund, RE, Thurston, RV, and Russo, RC, (1975). Aqueous ammonia equilibrium calculations: effect of pH and temperature. *J. Fish. Res. Board Can*. **32**: 2379-2383.

Foley, J and Fainges, J, (2014). Soil evaporation-how much water is lost from northern crop systems and how agronomic models accurately represent this loss? *GRDC Goondiwindi Update, Goondiwindi, Qld, Australia.*

Foley, J and Whish, J. (2015). Measuring soil evaporation across soils of the northern cropping zone. *GRDC Final Report Project # ERM00002.*

Fraser G, Rohde K, Silburn DM, (2017). Fertiliser management effects on dissolved inorganic nitrogen in runoff from Australian sugarcane farms. Environmental Monitoring and Assessment 189:409. DOI 10.1007/s10661-017-6115-z.

Freebairn, DM and Wockner, GH. (1986). A study of soil erosion on Vertisols of the eastern Darling Downs, Queensland. II The effect of soil, rainfall and flow conditions on suspended sediment losses. *Australian Journal of Soil Research*, 24, 159-172.

Friedl, J, Scheer, C, Rowlings, D, Mcintosh, H, Strazzabosco, A, Warner, D and Grace P, (2016). Denitrification losses from an intensively managed sub-tropical pasture-impact of soil moisture on the partitioning of N2 and N2O emissions. *Soil Biology & Biochemistry* **92** 58-66.

Gardner WR, and Hillel DI, (1962) The relation of external evaporative conditions to the drying of soils. *Journal of Geophysical Research* **67** 4319-4325.

Gehring, T, Silva, JD, Kehl, O, Castilhos, Jr, AB, Costa, RHR, Uhlenhut, F, Alex, J, Horn, H, Wichern, M, (2010). Modelling waste stabilization ponds with an extended version of ASM3. *Water Science and Technology,* Volume 61, pp. 713-720.

Génermont S, Cellier P (1997). A mechanistic model for estimating ammonia volatilization from slurry applied to bare soil. *Agricultural & Forest Meteorology* **88**, 145-16.

Ghahramani, A, Freebairn, DM, Sena, D, Cutajar, JL, Silburn, DM, (2019) A pragmatic parameterisation and calibration approach to model hydrology and water quality of agricultural landscapes and catchments. *Environmental Modelling & Software* (*accepted for publication)*

Gijsman, AJ, Jagtap, SS, Jones, JW, (2002). Wading through a swamp of complete confusion: how to choose a method for estimating soil water retention parameters for crop models. *Eur. J. Agron.* **18,** 77–106.

Godwin, DC, and Jones, CA, (1991) Nitrogen dynamics in soil-plant systems. Chapter 13 in: Modelling Plant and Soil Systems. Agronomy Monograph no. 31.

Gomez, E, Paing, J, Casellas, C, and Picot, B, (2000). Characterisation of phosphorus in sediments from waste stabilization ponds. *Water Science and Technology,* 42(10-11), pp. 257-264.

Harrison MT, De Antoni Migliorati M, Doughterty D, Grace P, Eckard RJ (2018) 'Modelling biomass, soil water content and mineral nitrogen in dairy pastures: a comparison of DairyMod and APSIM', paper presented at the Australasian Dairy Science Symposium, 21-23 November 2018, Palmerston North, New Zealand.

Henzell, EF, (1971). Recovery of nitrogen from four fertilizers applied to Rhodes grass in small plots. *Australian Journal of Experimental Agriculture & Animal Husbandry* **11**: 420-430.

Ho, L, Alvarado, A, Larriva, J, and Pompeu, CGP, (2019). An integrated mechanistic modeling of a facultative pond: Parameter estimation and uncertainty analysis. *Water Research,* Volume 151, pp. 170- 182.

Huth, NI, Bristow, KL, and Verburg, K (2012). SWIM 3: Model use, calibration, and validation. *Transactions of the ASABE*, **55** 1303–1313.

Johns M and Butler B (2021). MEDLI science review: Pond chemistry module. Report to the Queensland Water Modelling Network, Department of Environment and Science by Johns Environmental Group Pty Ltd, Brisbane.

Johnson IR, Chapman DF, Snow VO, Eckard RJ, Parsons AJ, Lambert MG, Cullen BR (2008). DairyMod and EcoMod: biophysical pasture-simulation models for Australia and New Zealand. *Australian Journal of Experimental Agriculture* **48,** 621-631.

Johnson RC, Imhoff JC, Kittle JL, Donigan AS (1984). Hydrological Simulation Program- Fortran (HSPF): User Manual for Release 8.0. Environmental Research laboratory, US Environmental Protection Agency, Athens, Georgia.

Jones, CA, and Kiniry, JR, (Eds.) (1986). CERES-Maize Texas A&M University Press, College Station, 194 pp

Jury, WA, Sposito, G and White, RE, (1986). Aa transport function model of solute transport through soil. 1. Fundamental concepts. *Water Resources Research.* 22, 243-247.

Jury, WA, and Roth, K, (1990). Transfer Functions and Solute Movement through Soil: Theory and Applications. (Birkhauser Verlag; Basel.)

Jury, WA, (1982). Simulation of solute transport using a transfer function model. *Water Resources Research* **18** 363-368.

Jury, WA, Stolzy, LH, and Shouse, P, (1982). A field test of the transfer function model for predicting solute transport. *Water Resources Research* **18** 369-375.

Jury, WA, Sposito, G. and White, RE, (1986). A transfer function model of solute transport through soil. 1. Fundamental concepts. *Water Resources Research*, **22**, 243-247.

Kincaid, DC, Solomon KH and Oliphant, JC, (1996). Drop size distributions for irrigation sprinklers. *Transactions of the ASAE*. **3,** 839-845.

Knisel, WG, (ed) (1980). CREAMS: A field-scale model for chemicals, runoff, and erosion from agricultural management systems. USDA, Conservation Research Report No. 26, 640 pp.

Knisel, WG, (1980). CREAMS: A Field-Scale Model for Chemicals, Runoff and Erosion from Agricultural Management Systems. United States Department of Agriculture, Conservation Research Report 26, 640 pp.

Ladson, AR (2021). MEDLI science review: Hydrology – model and process. Report to the Queensland Water Modelling Network, Department of Environment and Science by Moroka Pty Ltd.

Littleboy, M, Silburn, DM, Freebairn, DM, Woodruff, DR. and Hammer, GL, (1989). PERFECT: A computer simulation model of Productivity Erosion Runoff Functions to evaluate conservation techniques. Queensland Department of Primary Industries. Bulletin QB89005

Littleboy M, Silburn, DM, Freebairn, DM, Woodruff, DR, Hammer GL, and Leslie JK (1992). Impact of soil erosion on production in cropping systems. 1 development and validation of a simulation model *Aust J Soil Research* **30** 757-774

Littleboy, M, Cogle, A, Smith, G, Yule, D, Rao, Kpc, (1996). Soil management and production of Alfisols in the semi-arid tropics. I. Modelling the effects of soil management on runoff and erosion *Aust J Soil Research* **34** 91-102

Littleboy, M, Freebairn, DM, Silburn, DM, Woodruff, DR and Hammer, GL, (1999). PERFECT Version 3.0. A computer simulation model of productivity erosion runoff functions to evaluate conservation techniques.

Magesan, GN, Scotter, DR and White, RE (1999). The utility of Burns equation to describe solute movement through soil under various boundary and initial conditions. *European Journal of Soil Science* **50** 649-656.

Mayo, A. and Abbas, M, (2014). Removal mechanisms of nitrogen in waste stabilization ponds. *Physics and Chemistry of the Earth,* Volume 72-75, pp. 77-82.

McMahon, TA, Peel, MC, Lowe, L, Srikanthan, R, and McVicar, TR, (2013). Estimating actual, potential, reference crop and pan evaporation using standard meteorological data: a pragmatic synthesis. *Hydrol. Earth Syst. Sci, 17*(1331–1363).

Mein RG, and Larson, CL, (1973). Modelling infiltration during a steady rain. Water Resour. Res. **9,** 384-394.

Menzies NW, Skilton JA, and Guppy CN (1999). Phosphorus storage on effluent irrigated land. *Journal of Environmental Quality* **28**, 750-754.

Moody PW, (2011). Environmental risk indicators for soil phosphorus status. *Soil Research* **49**,247-252.

Moody, PW, (2021). MEDLI science review: Methodologies used by biophysical models for simulating soil nutrient pools and processes in pasture systems - Carbon, nitrogen and phosphorus. Report to the Queensland Water Modelling Network, Department of Environment and Science.

Nielsen, R, and Biggar, JW, (1962). Miscible displacement. **3.** Theoretical considerations. *Soil Science Society of America Proceedings* **26**, 216-221.

Owens, JS, Silburn, DM, McKeon, GM, Carroll, C, Willcocks, J and deVoil, R, (2003). Cover runoff equations to improve simulation of runoff in pasture growth models *Aust Journal Soil Research,* **41** 1467 1488.

Pano, A, and Middlebrooks, E, (1982). Ammonia nitrogen removal in facultative wastewater stabilization ponds. *Water Pollution Control Federation,* 54(4), pp. 344-351.

Patil, NG and Singh, SK, (2016). Pedotransfer functions for estimating soil hydraulic properties: a review. *Pedosphere* **26** 417-430

Philip, JR, (1957). Evaporation and moisture and heat fields in the soil. Journal of Meteorology 14:354-366.

Ponce, VM, and Hawkins, RH, (1996). Runoff curve number: has it reached maturity. *Journal of Hydrologic Engineering.* 1(1), 11-19.

Probert ME (2004). A capability in APSIM to model phosphorus responses in crops. In 'Modelling nutrient management in tropical cropping systems' pp 92-100. (Eds Delve RJ, Probert ME) ACIAR Proceedings No. 114, 138pp.

Probert ME, Delve RJ, Kimanic SK, Dimes JP, (2005). Modelling nitrogen mineralization from manures: representing quality aspects by varying C:N ratio of sub-pools. *Soil Biology & Biochemistry* **37,** 279–287.

Probert ME, Dimes JP, Keating BA, Dalal RC, Strong WM (1998). APSIM's Water and Nitrogen Modules and Simulation of the Dynamics of Water and Nitrogen in Fallow Systems. *Agricultural Systems* **56,** 1-28.

Queensland Government, (2019). HowLeaky Model V5 Technical Documentation: Version 1.09. Department of Natural Resources, Mines and Energy and the Department of Environment and Science. https://science.des.qld.gov.au/__data/assets/pdf_file/0018/100467/HowLeaky-manual.pdf (Accessed June 2021).

Ratliff, LF, Ritchie JT, and Cassel, DK (1983). Field-measured limits of soil water availability as related to laboratory-measured properties. *Soil Science Society of America Proceedings* **47**:770-775.

Rattray, D, Shaw, M, Silburn, DM, (2016). Modelling Reductions of Pollutant Loads Due to Improved Management Practice in the Great Barrier Reef Catchments Paddock Modelling for Bananas, Technical Report. Report Cards 2014 and 2015. Queensland Department of Natural Resources and Mines, Toowoomba, Queensland.

Rawls, WJ, Brakensiek, DL, Saxton, KE, (1982). Estimation of soil water properties. *Trans. ASAE* **25** ,1316–1320.

Reed, SC, Crites, RW, and Middlebrooks, JE. (1995). Natural Systems for wastewater management & treatment. McGraw Hill.

Ritchie, JT, (1972). A model for predicting evaporation from a row crop with incomplete cover. *Water Resources Research*, 8, 1204-1213.

Ritchie, JT, and Crum, J, (1989). Converting soil survey characterisation data into IBSNAT crop model input. In. "Land Qualities in Space and Time". Proceedings of a symposium by International Society of Soil Science, Wageningen, the Netherlands. 22-26 August 1988. J. Bourma and AK. Bregt (Eds.). pp 155-167.

Rowlings DW, Scheer C, Liu S, Grace PR (2016). Annual nitrogen dynamics and urea fertilizer recoveries from a dairy pasture using $^{15}N$; effect of nitrification inhibitor DMPP and reduced application rates. *Agriculture Ecosystems and Environment* **216**, 216-225.

Safley, LM, Barker, JC, and Westerman, PW, (1992). Loss of nitrogen during sprinkler irrigation of swine lagoon effluent, *Bioresources Technology* **40** 7-15.

Salvucci, GD, (1997). Soil and moisture independent estimation of stage-two evaporation from potential evaporation and albedo or surface temperature. *Water Resources Research*, **33** 111–122.

Scotter, DR, White, RE, and Dyson, JS, (1993). The Burns leaching equation. *Journal of Soil Science,* **44**, 25-33.

Sharpley, AN and Williams, JR. (Eds.) (1990). EPIC - Erosion/Productivity Impact Calculator: 1. Model documentation. USDA. Agriculture Technical Bulletin. No. 1768. 235 pp.

Shaw, R and Kitchen, J, (2019). SALF2 - Salinity and Leaching Fraction calculator v1-1-0 Available from salf2calculator@gmail.com.

Shilton, A, 2005. *Pond Treatment Technology.* London: IWA Publishing.

Silburn, DM, and Freebairn, DM, (1992). Evaluation of the CREAMS model, 3. Simulation of the hydrology of Vertisols *Aust J Soil Research* **30** 547-564

Silburn, DM, Carroll, C, Ciesiolka, CAA, deVoil, RC, and Burger, P, (2011). Hillslope runoff and erosion on duplex soils in grazing lands in semi-arid Queensland. 1. Influences of cover, slope and soil. *Soil Research* **49** 105-117.

Snow, V, Bond, W, Myers, B, Theiveyanathan, S, Smith, C, and Benyon, RG, (1999). Modelling the water balance of effluent irrigated trees *Agric Water Management* **39** 47-67.

Stewart, LK, Charlesworth, PB, Bristow, KL, and Thorburn, PJ, (2006). Estimating deep drainage and nitrate leaching from the root zone under sugarcane using APSIM-SWIM. *Agricultural Water Management*, *81*(3), 315–334.

Stirzaker, R, Biggs, H, Roux, D, and Cilliers, P, (2010). Requisite simplicities to help negotiate complex problems. *Ambio* **39**, 600–607.

Towner, D, (1983). A theoretical examination of Burns' (1975) equation for predicting the leaching of nitrate fertilizer applied to a soil surface. *Journal of Agricultural Science* **100,** 293-298.

Van Bavel, CHM, Stirk, GB, Brust, KJ (1968). Hydraulic properties of clay loamy soil and the field measurement of water uptake by roots. I. Interpretation of water content and pressure profiles. *Soil Science Society of America Proceedings.* **32**, 310–317.

Vendramelli, R, Vijay, S, and Yuan, Q, (2016). Phosphorus removal mechanisms in a facultative wastewater stabilization pond. *Water Air Soil Pollut,* 227(417).

Verberg, K, Bond, W, Hirth, J, Ridley, AM, (2007). Lucerne in crop rotations on the Riverine Plains: 3. Model evaluation and simulation analyses *Aust J Agric Research* **58** 1129-1141.

Verburg, K, (1995). Methodology in soil water- solute balance modelling: an evaluation of APSIM-SoilWat and SWIMv2 models. CSIRO Division of Soils Technical Report No. 131.

Vereecken, H, Weynants, M, Javaux, M, Pachepsky, Y, Schaap, MG and van Genuchten MTh, (2010). Using pedotransfer functions to estimate the van Genuchten- Mualem soil hydraulic properties: a review. *Vadose Zone Journal* **9** 795-820

Vibart, R, Vogeler, I, Cichota, R and Horne, D, (2015). A comparison of APSIM and OVERSEER predictions of nitrogen leaching from a well-drained soil under a dairy farm. 28th Annual FLRC Workshop. Farmed Landscapes Research Centre. Massey University. Palmerston North, New Zealand.

Vijay, S and Yuan, Q, (2017). Simplified empirical model for phosphorus removal in a facultative wastewater lagoon. *Journal of Environmental Management,* Volume 201, pp. 1-5.

Vogeler I, Giltrap D, Cichota R. (2013). Comparison of APSIM and DNDC simulations of nitrogen transformations and $N_2O$ emissions. *Science of the Total Environment* **465,** 147–155.

Vogeler, I, Lucci, G, and Shepherd, M (2016). An assessment of the effects of fertilizer nitrogen management on nitrate leaching risk from grazed dairy pasture. *Journal Agric* Science. **154,** 407-424

Vogeler I, Thomas S, and van der Weerden T, (2019). Effect of irrigation management on pasture yield and nitrogen losses. *Agricultural Water Management* **216**, 60-69.

Wang, Y, Shao, MA, Liu, Z, (2012). Pedotransfer functions for predicting soil hydraulic properties of the Chinese Loess Plateau. *Soil Sci.* **17,** 424–432.

Watson, KK, (1966). An instantaneous profile method for determining the hydraulic conductivity of unsaturated porous media. *Water Resources Research* **2,** 709-715.

Weier, KL, (1994). Nitrogen use and losses in agriculture in subtropical Australia. *Fertilizer Research.* 39, 245–257.

Weier KL, Macrae IC, and Myers RJK (1991). Seasonal variation in denitrification in a clay soil under a cultivated crop and a permanent pasture. *Soil Biol & Biochem* **23**:629–635.

Weier KL, Macrae IC, and Myers RJK (1993). Denitrification in a clay soil under pasture and annual crop—estimation of potential losses using intact soil cores. *Soil Biol & Biochem* **25**:991–997.

Weier, KL, Macrae, IC, Myers, RJK, (1993). Denitrification in a clay soil under pasture and annual crop: losses from $^{15}N$-labelled nitrate in the subsoil in the field using $C_2H_2$ inhibition. *Soil Biology and Biochemistry* **25**, 999-1004.

Weil, RR, Islam, KR, Stine, MA, Gruver, JB, Samson-Liebig, SE, (2003). Estimating active carbon for soil quality assessment: a simplified method for laboratory and field use. *American Journal of Alternative Agriculture* **18**, 3-17.

Wheeler DM, Ledgard SF, Monaghan RM, McDowell RW, de Klein CAM (2006). OVERSEER nutrient budget model—what it is, what it does. In 'Implementing sustainable nutrient management strategies in agriculture.' Occasional Report No. 19. (Eds LD Curries, JA Hanly) pp. 231–236. (Fertilizer and Lime Research Centre, Massey University: Palmerston North, NZ).

White, I, Sully, MJ, and Perroux, KM (1992). Measurement of surface soil hydraulic properties using disc permeameters, tension infiltrometers and other techniques. in *Advances in measurement of soil physical properties* SSSA Special Pub # 30

Zhang, Y and Schaap, MG (2017). Weighted recalibration of the Rosetta pedotransfer model with improved estimates of hydraulic parameter distributions and summary statistics. *J Hydrology* **547,** 39-53

# Appendix A. Summary description of a representative range of one-dimensional hydrology models including their algorithm structure, time step and spatial scale

A summary of the capability of 18 models is provided below in Table A1. There are 25 columns of data in total which are laid out across 4 tables.

*Table A1: Summary of modelling approaches*

| No | Model | Full Name | Brief description | Infiltration/Runoff | Curve number soil water deficit | Temporal modelling approach | Time step | Spatial scale |
|---|---|---|---|---|---|---|---|---|
| 1 | AGNPS | Agricultural Non-Point Source. | Analyse nonpoint-source pollution and prioritise water quality problems. Runoff, sediment, nutrients and chemical oxygen demand are simulated for each cell and routed to the outlet. | Curve number (event based).<br><br>Peak flow rate calculated as in CREAMS | Curve number based on land use, soil type and soil moisture. (Curve number is a model input. There is no soil moisture accounting) | Event based | 1 minute | Watershed scale. Distributed. 2D (grid) cell size 0.4 to 16 ha. |
| 2 | ANSWERS | Areal Nonpoint Source Watershed Environmental Simulation | Model the quality and quantity of water and the effect of management interventions | Interception and surface ponding are removed from rainfall. Infiltration is modelled as a function of soil moisture. Runoff is any unaccounted for rainfall | Does not use curve numbers | Event based | 1 minute | Model size from a few ha to 300,000 ha" |
| 3 | APSIM | Agricultural Production System Simulator | Simulates biophysical processes in farming systems with a focus on the influence of climate risk on economic and ecological outcomes to management interventions. | Two options.<br>1. Curve number approach as in CREAMS, PERFECT etc. (No runoff is assumed from irrigation applications).<br>2. Rainfall/evaporation at the soil surface specified as a boundary condition to the Richards equation | 1. As in PERFECT i.e. current soil water content effects the s parameter.<br>2. As per SWIM i.e. specification of boundary conditions, soil roughness and the way roughness changes through time and with cumulative rainfall | Continuous | SOILWAT uses a daily time step. SWIM uses an adaptive time | Distributed (square grid over a landscape). Small watershed scale i.e. larger than field scale |
| 4 | CERES | Crop Estimation through Resource and Environment Synthesis | Model purpose is to provide:<br>- assistance with farm decision making<br>- Risk analysis for strategic planning<br>- Within-year management decisions<br>- Large area yield forecasting both foreign and domestic<br>- Policy analysis<br>- Definition of research needs | Infiltration is the difference between daily precipitation and runoff. Runoff is calculated using a modified SCS-Curve number approach (similar to other models) (Williams et al., 1991).<br>All irrigation is assumed to infiltrate | Similar to EPIC i.e.. s (retention parameter) is a function of soil water content as a fraction of available water (field capacity - wilting point). Relationship takes account of the distribution of water in the soil profile | Run for any length of time before the crop sowing date, then for the growing season of the crop. | Daily | 1D model, Field scale |

| No | Model | Full Name | Brief description | Infiltration/Runoff | Curve number soil water deficit | Temporal modelling approach | Time step | Spatial scale |
|---|---|---|---|---|---|---|---|---|
| 5 | CREAMS | Chemicals, Runoff, and Erosion from Agricultural Management Systems | CREAMS is a physically based, daily simulation model that estimates runoff, erosion, and sediment transport, to determine the yield of plant nutrients and pesticide, and sediment from field-sized areas. | Two options.<br>1. When daily rainfall is available, runoff is estimated using a curve number approach. (Williams and LaSeur, 1976)<br>2. If sub-daily data are available, an infiltration model (based on Green and Ampt) is used.<br><br>Uses an empirical equation to predict peak runoff based on runoff volume, catchment area, channel slope, and length-width ratio. Irrigation was added to CREAMS in 1983 (Del Vecchio et al., 1983). | Depth averaged retention parameter based on weighing of soil moisture in 7 soil layers. Soil moisture is characterized as ratio of actual/upper limit. Weighting factors are a function of the ratio of soil depth to root zone depth. | Continuous | Daily time step for evaporation and soil water movement between storms and shorter time increments, depending on available rainfall records, during storms | Field scale (1D)<br>Management unit having<br>1. single land use<br>2. relatively homogeneous soils<br>3. Spatially uniform rainfall<br>4. Single management practices.<br>Mixed land uses are subdivided, predictions are made for each sub-area and then combined, |
| 6 | EPIC | Erosion Productivity Impact Calculator | EPIC simulates erosion and plant growth to determine the effect of erosion on yield. Includes economic assessments | Curve number to calculate runoff volume. Rational method to calculate peak flow (stochastic approach used to estimate sub-daily peaks) | s (retention parameter) is a function of soil water content as a fraction of available water (field capacity - wilting point). Relationship takes account of the distribution of water in the soil profile | Continuous. Capable of simulating 100s of years | Daily | 1 ha area, up to 10 soil layers |
| 7 | GLEAMS | Groundwater Loading Effects of Agricultural Management Systems | Model developed for field-size areas to evaluate the effects of agricultural management systems on the movement of agricultural chemicals within and through the plant root zone | Curve number approach as in CREAMS | Same as CREAMS | Continuous | Daily | Field scale (see description for CREAMS) |
| 8 | GRASP | Grass Production | Model of climate-soil-plant-animal-management of pastures in northern Australia | Rainfall is partitioned into infiltration and runoff on the basis of surface cover, rainfall intensity and soil water deficit (Scanlon et al., 1996). Sub-daily rainfall intensity is derived from daily rainfall. Does not model infiltration in cracking soils | Not used | Continuous. Some procedures are calculated annually, e.g. pasture burning | Daily | 1D model representing a point in the landscape. Has been adapted to 2D in programs such as AussieGRASS |

| No | Model | Full Name | Brief description | Infiltration/Runoff | Curve number soil water deficit | Temporal modelling approach | Time step | Spatial scale |
|---|---|---|---|---|---|---|---|---|
| 9 | HowLeaky | | Designed to assess the impacts of different land uses, soil conditions, management practices and climate types on water balances and water quality | Curve number based. Infiltration is water left over after runoff. Can model infiltration into cracking soils. | Effective rain = rainfall plus un-infiltrated irrigation<br>CN2(bare) = curve number (rainfall v runoff response) for average antecedent moisture conditions and for bare and untilled soils. CN2 is modified to account for crop cover, surface residue cover and surface roughness.<br>Applied CN is a function of soil water deficit and Smax (maximum retention under dry antecedent conditions).<br>Allows modified approach to calculating Smax (Robinson 2011) | Continuous | Daily | Field scale (1D) |
| 10 | HSPF | Hydrologic Simulation Program Fortran | Watershed hydrology and water quality model for conventional and toxic organic pollution. Can model pervious and impervious areas. Models waterway and hillslope processes. HSPF is based on a set of modules in a hierarchical structure. | Precipitation is supplied by the user which can then be intercepted by vegetation and detained on the surface. Remainder is partitioned between runoff, infiltration, interflow and remaining in storage | not used | Continuous (few min to > 100 years) | Sub-hourly to daily time step. Commonly hourly. | Watershed scale. A few ha to large watersheds (160,000 km2). Catchments are divided into areas providing homogeneous hydrologic and water quality response. Models streamflow as well as hillslope processes |
| 11 | HYDRUS-1D | | Software package for simulating the one-dimensional movement of water, heat and multiple solutes in variably saturated media | Can model ponding at the soil surface with or without runoff. Behaviour at top and bottom boundaries is specified as boundary conditions.<br>Dirichlet boundary condition - ponded infiltration (1D vertical water flow).<br>Neuman boundary condition - specification of flux of water entering or leaving a system.<br>Atmospheric boundary condition require specification of precipitation and evaporation | Not used | "Daily variations in evaporation, transpiration and precipitation rates". Meteorological variables can be generated | Adaptive time step depending on the speed of convergence | 1D, field scale |
| 12 | LEACHM | Leaching Estimation And Chemistry Model | Process based model of water and solute movement, transformations, plant uptake and chemical reactions in the unsaturated zone | Specification of the upper boundary condition determines the partition between runoff and infiltration | Not used | Intended for use during a growing season | Adaptive time step depending on the speed of convergence | 1D, field scale |

| No | Model | Full Name | Brief description | Infiltration/Runoff | Curve number soil water deficit | Temporal modelling approach | Time step | Spatial scale |
|---|---|---|---|---|---|---|---|---|
| 13 | OVERSEER | | OVERSEER is a strategic management tool that supports optimal nutrient use on form for increased profitability and managing within environmental limits. Simulates off-farm losses of nutrients and greenhouse gases | Daily rainfall greater than a threshold amount generates runoff, the remainder infiltrates. Threshold rainfall is a function of soil moisture (variable), and clay content, slope and a drainage factor.<br>Wheeler, 2018a | Does not use curve numbers | - 2 year modelling period for pastoral, cut and carry and fruit.<br>- 3 year cycle for crops | Daily time step for the hydrology model. Monthly loads for N, annual loads for other nutrients | Paddock or farm scale (1D) |
| 14 | PERFECT | Productivity Erosion Runoff Functions to Evaluate Conservation Techniques | PERFECT is a biophysical model that simulates the plant soil water management dynamics in an agricultural system to predict runoff, soil loss, soil water, drainage, crop growth and yield | Curve number based. Infiltration is water left over after runoff. Can model infiltration into cracking soils. | CN2(bare) = curve number (rainfall v runoff response) for average antecedent moisture conditions and for bare and untilled soils.<br>CN2(bare) is modified for the effects of cover and roughness (which is a function of tillage type and rainfall since tillage). The S parameter is modified based on soil water content. | Continuous | Daily time step | Field scale (1D) |
| 15 | RUSLE | Revised Universal Soil Loss Equation | The RUSLE is an erosion model predicting long time average annual soil loss resulting from raindrop splash and runoff | Not used | Not used | Lumped | Annual average | Field scale (1D) |
| 16 | SWAT | Soil and Water Assessment Tool | Predict the effects of alternative land use management practice on water, sediment, crop growth, nutrient cycling, and pesticides | SCS-Curve number or Green & Ampt to determine runoff volume. Rational formula or TR-55 to determine peak flow rate. | s, the retention parameter, is a function of soil moisture (fraction of field capacity) | Continuous | Usually daily but can use sub-daily to yearly time step (Yuan et al., 2020; Borah & Bera, 2003). | Small watersheds (10 $km^2$) to continental scale (Europe). Catchments are divided into sub-basins and into Hydrological Response Units (HRUs). HRUs are homogeneous in terms of land use, soils, and topography. |

| No | Model | Full Name | Brief description | Infiltration/Runoff | Curve number soil water deficit | Temporal modelling approach | Time step | Spatial scale |
|---|---|---|---|---|---|---|---|---|
| 17 | SWIM | Soil Water Infiltration and Movement | Simulates runoff, infiltration, redistribution, solute transport and redistribution of solutes, plant uptake and transpiration, soil evaporation, deep drainage and leaching | Rainfall and/or irrigation provided as inputs. Infiltration behaviour is specified as a boundary condition. Commonly runoff is an empirical function of ponding depth. Can model sealing and crusting soils and their time dependence | Not used | Continuous | Adaptive time step. Small stepping during conditions of rapid change. SWIM will linearly interpolate cumulative climate inputs e.g., PET and rainfall. | Can be used at very small scales e.g., laboratory columns. Can be used at management scales as part of APSIM |
| 18 | WEPP | Water Erosion Prediction Project | Continuous simulation program to predict soil loss and sediment deposition from overland flow on hill slopes and concentrated flow in small channels | Interception by vegetation is related to above ground biomass.<br>Infiltration estimated by modified Green-Ampt Mein-Larson model (Chu, 1978) which takes, as an input, soil moisture from the upper soil layer. | Curve number is not used | Continuous | Time step depends on the module. Hydraulic calculations use an adaptive time step. WEPP uses stochastically generated weather data so the time step is not constrained by observational data | Tens of metres for hillslope profiles and hundreds of metres for small watersheds. Uses overland flow elements (OFE) which have homogeneous properties and a uniform response. |

*Table A1: Summary of modelling approaches (continued)*

| No | Model | Potential ET | Soil evaporation | Soil water redistribution | Transpiration | Transpiration-soil water storage relationship | Erosion | Sediment enrichment |
|---|---|---|---|---|---|---|---|---|
| 1 | AGNPS | Not used | Not modelled | Not modelled | Not modelled | Not modelled | Models Nonpoint sediment sources and can include point sources (gullies, feedlots)<br>Soil loss calculated using a modification of the USLE. Sediment is routed between cells. Transport capacity based on flow velocity and shear stress.<br>Uses 5 particle sizes: clay, silt, small aggregates, large aggregates and sand. | Enrichment ratio based on sediment yield and soil texture |
| 2 | ANSWERS | Not used | Not modelled | Subsurface drainage only occurs when soil water content is greater than field capacity. Tracking soil water distribution is not a focus of this event model. | Not modelled | Not modelled | Modification of the USLE to include rill and inter-rill (a) rainfall detachment (Meyer and Wishmeier, 1969), and (b) overland flow detachment (Foster, 1976). Rate of sediment movement is a function of rainfall detachment, flow detachment, and available transport capacity of overland flow. Channel erosion is assumed to be negligible but channel deposition is modelled. | Not modelled |

| No | Model | Potential ET | Soil evaporation | Soil water redistribution | Transpiration | Transpiration-soil water storage relationship | Erosion | Sediment enrichment |
|---|---|---|---|---|---|---|---|---|
| 3 | APSIM | Priestly-Taylor or Penman-Monteith | 1. Ritchie two stage model, including effect of surface residue and crop cover on runoff and potential evaporation.<br>2. Evaporation demand as a boundary condition when solving the Richards equation | Two submodels, SOILWAT and APSIM-SWIM.<br>SOILWAT is a cascading soil layer model (up to 10 layers) similar to that in CERES and PERFECT. Can model perched water tables and unsaturated flow.<br>APSIM-SWIM is based on the numerical solution to the Richards Equation (see the description of SWIM) | The transpiration approach is not well explained in documentation but likely that SOILWAT uses similar routines to PERFECT<br>In SWIM, transpiration is modelled by root exploration and extraction potential | 1. As in PERFECT<br>2. Root demand as a sink term in Richards equation | Erosion modelling combines sediment concentration with runoff volume calculated by the SOILWAT module and takes account of surface residue from crop modules and/or the RESIDUE module. There are two options for obtaining sediment concentration:<br>1. The approach developed by Rose (1985) which allows separate calculation of bed and suspended load.<br>2. A modification of the USLE to calculate daily sediment concentration rather than annual soil loss. A similar approach was used in PERFECT | Empirical, power function, based on the total soil loss (t/ha) |
| 4 | CERES | Priestley-Taylor (1972) | Ritchie (1972) model.<br>Soil evaporation potential rate is PET modified by LAI.<br>Two stage evap.<br>Stage 1 at potential rate until the cumulative evaporation exceeds U (the upper limit of stage 1 drying).<br>Stage 2 at CONA.<br>Modification of Ritchie (1972) to reduce soil evaporation when the soil water content in the upper soil layer reaches a low threshold. Evaporation can remove soil to air dry, assumed to be half the lower limit (LL) of the upper layer. (LL is -15 bar water content) (Ritchie, 1998) | Soils modelled as a series of 7 to 10 layers, 200 to 300 mm deep. Drainage is a function of the water content above the drained upper limit (DUL). Drainage coefficient is the fraction of water (between DUL and field saturation) that can drain on each day. A single drainage coefficient is specified for the entire profile. Upward flow of water in the top 4 soil layers is calculated based on soil evaporation. Soil water can move by diffusion (Rose, 1968) | Transpiration is the minimum of the potential rate, or a rate calculated from the capacity of the root system | Root water uptake (and hence transpiration) is reduced to zero when soil water reduces to the soil lower limit (-15 bar). | Not modelled | Not modelled |

| No | Model | Potential ET | Soil evaporation | Soil water redistribution | Transpiration | Transpiration-soil water storage relationship | Erosion | Sediment enrichment |
|---|---|---|---|---|---|---|---|---|
| 5 | CREAMS | Priestley-Taylor (1972) | Ritchie (1972) model.<br>Soil evaporation potential rate is PET modified by LAI.<br>Two stage evaporation to defined wilting point<br>Stage 1 at potential rate) until the cumulative evaporation exceeds U (the upper limit of stage 1 drying).<br>Stage 2 at CONA<br>No decrease in stage 2 rate as soil dries. | Soil movement between layers. Drainage occurs when soil water content is greater than field capacity. The amount of drainage is a function of Ksat and the difference between current soil water content and field capacity. The capacity for the next soil layer to hold the drained water is also considered. Unsaturated water flow is ignored | Potential transpiration = PET adjusted for LAI if LAI is < 3. | Actual transpiration is reduced below potential when soil water storages is less than 25% of field capacity.<br>Transpiration continues down to soil water content of - 15 bar (wilting point).<br>Water demand by vegetation varies by soil depth. | USLE plus sediment transport capacity of overland flow, channel erosion and deposition and storage of sediment in dams | Enrichment ratio based on an empirical relationship with sediment load.<br>Er = A(SED)^B<br>SED = kg/ha of sediment<br>A = 7.4<br>B = 0.2 |
| 6 | EPIC | Priestly-Taylor (1972) or Penman. Later version used Penman-Monteith (Mearns et al., 1999) | Potential soil evaporation = PET adjusted for LAI. Actual evaporation calculated from exponential functions of soil depth and water content. | Storage routing approach to modelling soil percolation. Flow from a soil layer occurs when soil water content exceeds field capacity. Movement is limited by the available capacity of the lower soil layer. Models lateral flow | Potential transpiration = PET adjusted for LAI if LAI is < 3. Transpiration demand is distributed between soil layers | Actual transpiration is reduced below potential when soil water storages is less than 25% of plant available water. Exponential reduction to ~0 when soil dries to wilting point (Jones and Kiniry, 1986) | Water erosion based on USLE (Three versions of USLE are offered). Also simulates wind erosion. | Sediment enrichment ratio is a function of the sediment delivery ratio (DR). DR is estimated from the ratio of peak runoff rate and peak rainfall excess rate. Sediment enrichment ratio varies logarithmically between 1 and 1/DR. Sediment enrichment ratio approaches 1 for high sediment concentrations |
| 7 | GLEAMS | Same as CREAMS | Same as CREAMS | Seven computational soil layers. Soil properties can vary by layer. Storage-routing technique used to simulate layer-to-layer percolation is the same as CREAMS | Same as CREAMS | Same as CREAMS | Improvement in calculation of sediment particle characteristics compared to CREAMS (Foster et al., 1985) | Similar to CREAMS but with improved estimates based on changes to parameterization of sediment particle characteristics of detached soil |

| No | Model | Potential ET | Soil evaporation | Soil water redistribution | Transpiration | Transpiration-soil water storage relationship | Erosion | Sediment enrichment |
|---|---|---|---|---|---|---|---|---|
| 8 | GRASP | Pan | Transpiration is calculated first then soil evap. Total evapotranspiration cannot exceed potential.<br>Soil evaporation is based on a potential rate (pan), adjusted for soil cover and tree density. Actual soil evaporation is potential adjusted for available water | Based on an updated version of the WATSUP soil water balance model (Rickert and McKeon, 2000; McKeon et al., 1982). Soil water updated daily on the basis of infiltration and drainage when a soil layer is above field capacity. Three layers plus a 4th below 100 cm which is only available for trees. All water above field capacity is drained from each layer to the layer below in one day. Does not model run-on, lateral drainage, upward movement of soil moisture, or unsaturated flow. | Separate calculation of transpiration from grass and trees. Trees remove water first. Actual transpiration based on potential rate adjusted for available water. Wilting point is a property of vegetation rather than soil. GRASP does not simulate root growth | Transpiration is a function of the ratio of available soil moisture (actual soil water - wilting point soil water) to capacity (field capacity - wilting point) | Not modelled | Not modelled |
| 9 | HowLeaky | Pan | Ritchie<br>Two stage evaporation to defined wilting point<br>Stage 1 at potential rate (modified by crop residue) until the cumulative evaporation exceeds U (the upper limit of stage 1 drying).<br>Stage 2 at CONA<br>No decrease in stage 2 rate as soil dries.<br>Potential soil evaporation is a function of green cover and/or crop cover.<br><br>Section 1.6 states that potential soil evaporation is based on unsatisfied evaporative demand i.e., difference between potential evapotranspiration and transpiration. However, Section 4.1 suggests it is potential transpiration that is based on unsatisfied evaporative demand. That is, it is not clear which if soil evaporation, or transpiration is calculated first | Cascading bucket (similar to PERFACT and CREAMS) | Potential rate:<br>PET x green cover, or<br>PET x LAI<br>Also includes a simple Crop-factor model that lumps evaporation and transpiration into a single evapotranspiration output.<br>Potential rate is based on unsatisfied evaporative demand i.e. difference between potential evapotranspiration and soil evaporation. | Function of soil water for each layer. Based on the ratio of plant available water and drained upper limit. | Modified USLE function of:<br>runoff volume<br>cover<br>soil erodibility<br>management practice<br>topography | Empirical functions for calculating enrichment of total P in sediment and concentration of soluble P in runoff.<br>Uses Phosphorus buffering index test (PBI) to modify soil P concentration in runoff |
| 10 | HSPF | Input by user. Typically Pan values are used with an adjustment factor | Potential rate is adjusted for cover and soil moisture (ratio of available to max available) | Interflow outflow, percolation, and groundwater outflow using empirical relations.<br>Based on the LANDS subprogram of the Stanford Watershed Model | Potential rate adjusted for vegetation type, depth of rooting, density of vegetation cover, stage of plant growth and moisture characteristics | Depends on ratio of actual available soil moisture to max available soil moisture | Rainfall splash detachment and wash off. Transport capacity is a function of water storage and outflow. Scour based on stream power (Borah & Bera, 2003) | Referred to as "potency" factors. Separate user supplied factors are required for washed off sediment and scoured sediment |

| No | Model | Potential ET | Soil evaporation | Soil water redistribution | Transpiration | Transpiration-soil water storage relationship | Erosion | Sediment enrichment |
|---|---|---|---|---|---|---|---|---|
| 11 | HYDRUS-1D | Penman-Monteith or Hargreaves equations | Evaporative demand is set as a boundary condition at the soil surface | Numerical solution of Richards Equation for variably saturated water flow and the advection-dispersion equations for heat and solute transport. Can take account of matric and macropore flow and model vapour transport. Flow and transport can occur in the vertical, horizontal any other direction | Transpiration is modelled by root water uptake which is specified as a sink term in the differential equations | Sink term as part of the Richards equation to model water uptake by roots | Not modelled | Not modelled |
| 12 | LEACHM | PET input by the user as weekly totals | PET partitioned into potential transpiration and potential soil evaporation based on the crop cover fraction. | Finite difference solution to Richards equation | Calculated as a sink term that is a function of hydraulic conductivity, effective crown water potential, root resistance, soil water matric potential, fraction of active roots in the depth segment | Richards equations with root uptake as a sink term | Not modelled | Not modelled |
| 13 | OVERSEER | PET required as an input, documentation doesn't specify any specific requirements | Soil evaporation (and transpiration) is set to zero when soil moisture reaches wilting point. PET is allocated between soil evaporation and transpiration depending on vegetation cover. | Calculations use 100 mm soil layers. Profile depth is 600 mm for pastoral blocks and 1500 mm for Lucerne and crops | Transpiration = PET x cover x dryness<br>cover = monthly crop cover (0,1)<br>dryness approaches zero as profile soil water content approaches wilting point. | Transpiration (and soil evaporation) is set to zero when soil moisture reaches wilting point. | Not modelled | Not modelled |
| 14 | PERFECT | Pan | Two stage evaporation. Drying is initially at potential rate to a user defined limited. Followed by slower stage 2 drying. Evaporation will remove soil water from the two upper profile layers and drying continues below wilting point to the user specified air dry limit (layer 1) and in layer 2 to halfway between wilting point and the air-dry limit. Stage 1 drying recommences after infiltration but is limited be amount of infiltration. This differs from the original Ritchie (1972) algorithm.<br>Potential rate is based on Pan adjusted using a function that depends on crop cover, LAI and crop residue. | Cascading bucket (similar to CREAMS) | Based on potential, allocated to each soil layer and then adjusted for the available soil moisture in each layer | Transpiration can only dry a profile layer to its defined wilting point | Modified USLE function of:<br>runoff volume<br>cover<br>soil erodibility<br>management practice<br>topography. Uses a modified LS (length slope) factor from the RUSLE (Freebairn and Wockner, 1986).<br>Calculates daily sediment concentration rather than annual sediment load. Also models the impact of soil erosion on crop yield (Littleboy et al., 1992) | Not used |

| No | Model | Potential ET | Soil evaporation | Soil water redistribution | Transpiration | Transpiration-soil water storage relationship | Erosion | Sediment enrichment |
|---|---|---|---|---|---|---|---|---|
| 15 | RUSLE | Not used | Not used | Not used | Not used | Not used | Annual average soil loss is a function of the same six factors as the USLE but based on more data, better computational procedures, and more sophisticated relationships. | Not used |
| 16 | SWAT | Hargreaves, Priestley-Taylor or Penman-Monteith | Uses the method of Ritchie (1972) | Lateral subsurface flow using kinematic storage model (Sloan et al., 1983), and groundwater flow using empirical relations. | Potential ET is a linear function of potential ET and leaf area index. Actual ET depends on available soil moisture | Rate depends on the fraction of field capacity down to wilting point. | Modified USLE (Williams and Berndt (1976). Sediment yield expressed in terms of runoff volume, peak flow and USLE factors. | Uses a sediment enrichment ratio as part of the calculation of N and P export |
| 17 | SWIM | Evaporative demand needs to be supplied by the user. This becomes a sink term when solving the Richards eqn. | Soil evaporation is a sink term when solving the Richards eqn. Uses the method of Campbell (1985). Evaporation is a function of the relative humidity of the atmosphere and the relative humidity at the soil surface which is a function of its water content. | Numerical solution of Richards Equation and the advection-dispersion equation. Flow is one dimensional. Lateral flow is not calculated | The PET supplied by the user must incorporate the effect of stomatal and aerodynamic resistance. SWIM can model transpiration from 4 vegetation types. Vegetation is behaviour is assumed fixed and known in advance as SWIM does not model plant growth | Actual transpiration rate depends on soils ability to supply water as determined by the solution to the Richards equation | Not modelled | Not modelled |
| 18 | WEPP | Penman (Penman, 1963; Jensen, 1974) where data are available (daily radiation, temp, wind, dew point temp or relative humidity). Priestly-Taylor (1972) when only solar radiation and temperature data are available. | Potential soil Evaporation is a function of potential ET and LAI. Uses the Ritchie (1972) 2 stage model. Upper limit of stage 1 soil evaporation is calculated from soil texture as is the rate of stage 2 evaporation. Soil evaporation is limited by available water. | Storage routing through soil layers. WEPP can also simulate subsurface lateral flow and flow to drainage tiles and ditches. Water content exceeding field capacity drains to the next layer. Saturated hydraulic conductivity is calculated from soil texture, organic matter and porosity. It seems that unsaturated soil water movement is not considered. | Potential transpiration is the difference between PET and Soil Evap. Potential transpiration is distributed between layers based on root zone depth. Actual transpiration is limited by plant water stress which depends on soil water content | In soil where moisture is less than critical (the moisture content where plants become stressed) actual transpiration is based on the ratio of available moisture content to critical water content, otherwise, transpiration is at the potential rate | Hydrology component of WEPP calculates peak runoff rate, runoff duration, effective rainfall intensity, and effective rainfall duration. Soil detachment by rainfall is calculated. Hydrologic variables are input to a hydraulic model to calculate flow shear stress and sediment transport capacity. Transport is calculated on hillslopes, rills and channels. | Not used |

*Table A1: Summary of modelling approaches (continued)*

| No | Model | P export | N export | Required soil hydraulic properties | Deep drainage | Solute leaching | Nitrate leaching |
|---|---|---|---|---|---|---|---|
| 1 | AGNPS | P export is modelled from surface runoff. Approach adapted from CREAMS | N export is modelled from surface runoff. Approach adapted from CREAMS | SCS curve number<br>Average land slope (%)<br>Soil erodibility factor<br>Soil texture | Not modelled | Chemical transport includes soluble and sediment adsorbed phases | Not modelled |
| 2 | ANSWERS | Not modelled | Not modelled | Surface storage coefficient<br>Steady state infiltration rate<br>Total porosity<br>Field capacity<br>Antecedent soil moisture<br>USLE "K"<br>Infiltration rate descriptors:(Infiltration control zone depth,<br>Coefficient describing how the infiltration rate decreases as soil moisture content increases) | Not modelled | Not modelled | Not modelled |
| 3 | APSIM | includes the modules MANURE that models the release of P and SOILP that models transformation of P | Comprehensive processes for modelling N that in mineralisation of crop residues in the soil by the SOILN module, decomposition of crop residues at the soil surface by the RESIDUE module. Tracking of three pools of organic matter. This was in response to weakness in the CERES model and to improve modelling of N input from legumes and the changing rate of organic matter decomposition with soil depth. SOILN also models urea hydrolysis, nitrification and denitrification. | For SOILWAT: lower limit, drained upper limit, air-dry water content and saturated water contents and thickness of each soil layer.<br>For APSIM-SWIM: moisture characteristic and hydraulic conductivity relationship for each layer | For SOILWAT deep drainage is based on water moving below the lowest soil layer. Unsaturated flow cannot lead to deep drainage. For APSIM-SWIM a range of boundary conditions can be specified at the base of the soil profile | 1. Solutes move with saturated and unsaturated flow. Incoming and existing solutes are fully mixed to determine the concentration of water leaving a soil layer<br>2. Combination of Richard's equation and advection dispersion equation | Estimates of N leaching are based on concentration of N in water moving beyond the soil profile. APSIM has been used to estimate N leaching from cropping systems including wheat and sugarcane (Asseng et al., 1997; Verburg et al., 1996) |

| No | Model | P export | N export | Required soil hydraulic properties | Deep drainage | Solute leaching | Nitrate leaching |
|---|---|---|---|---|---|---|---|
| 4 | CERES | Not modelled | N is modelled as a limiting plant nutrient (via an N balance) rather than modelling N export as a pollutant. CERES models include a submodel, CERES-N. | Soil properties<br>- Curve number<br>- Drainage coefficient<br>- Runoff coefficient<br>- Evaporation coefficient<br>- Soil surface albedo<br>- Lower limit of plant available water<br>- Field drainage upper limit<br>- Rooting preference coefficients (weighting factors) for each layer (0-1) (depend on Soil type but generally decrease with depth). A value of 1 indicates soil hospitable to root growth<br>- Field saturated Soil water content<br>- Limit of first stage soil evaporation<br>See Ritchie, 1998 | Drainage from the entire soil profile the drainage from the lowest layer | Not usually modelled, but CERES was modified to predict pesticide leaching for a particular application (Gerakis and Ritchie, 1998) | Not modelled |
| 5 | CREAMS | Models adsorbed phosphorus, solute phosphorus. Soluble P are leached from crop residue but does not more through the soil. | Models mineralisation, nitrification and denitrification, plant uptake and leaching by soil water movement out of the root zone. Enrichment ratios are used to estimate the portion of N transported with sediment | Soil profile is assumed to have constant hydraulic properties.<br>Required parameters are:<br>Saturated hydraulic conductivity<br>Portion of plant-available storage filled at field capacity<br>Soil porosity<br>Immobile soil water content.<br>Stage 1 soil evaporation parameter<br>Soil density<br>Depth of root zone<br>Effective capillary tension<br>Sand, silt and clay components | Water moving below the root zone. Estimated from averages and cumulative data rather than providing daily values | Pesticide component simulates foliar interception, degradation, washoff, as well as soil processes of adsorption, desorption and degradation in soil. Soluble and sediment attached components are modelled. Sediment enrichment ratios are used | N is leached from crop residues into soil by the fraction of rainfall that does not runoff.<br>N leached from soil is based on an N balance that takes account of N inputs, N uptake by plants, denitrification, mineralisation (organic N to nitrate). Leached N is deep drainage x concentration in root zone. |
| 6 | EPIC | Models soluble P loss in surface runoff. Assumes P conc in sediment is 175 times that in water. Attached P = sediment yield x concentration of P in soil x enrichment ratio. | For the top layer (10 mm of soil). Loss is a function of concentration x sum of (runoff, percolation and lateral subsurface flow). N can move upwards in water movement in response to evaporation and is supplied by rain. Similar approach in lower layers except there is no runoff.<br>Uses a mass balance to track N. Particulate N based on sediment yield, N concentration in sediment and an enrichment ratio. Models denitrification as a function of temperature and water content. Models N mineralisation and immobilization | Soil albedo<br>Number of soil layers<br>Initial soil water content-fraction of field capacity<br>Min depth to water table<br>Max depth to water table<br>Initial depth to water table<br>Bulk density of each soil layer<br>Oven dry bulk density of each layer<br>Wilting point of each layer<br>Field capacity of each layer<br>Sand content of each layer<br>Silt content of each layer<br>Organic N concentration of each layer | Uses a water balance model to movement of the water table. Based on 30 day running sums of rainfall, runoff and potential evap. (The documentation says potential, but it seems it should be actual) | No modelling of solutes separately from N and P | N leaching is calculated from water leaving the lowest soil profile x N concentration |

| No | Model | P export | N export | Required soil hydraulic properties | Deep drainage | Solute leaching | Nitrate leaching |
|---|---|---|---|---|---|---|---|
| 7 | GLEAMS | Same as CREAMS | Same as CREAMS | Porosity<br>Water retention characteristics<br>Organic matter content | Daily values from water balance. An improvement from CREAMS was calculation of daily drainage values. | Focus on pesticides.<br>Similar modelling approach to CREAMS.<br>Expanded the available modelled pesticide application approaches.<br>Improved pesticide degradation modelling.<br>GLEAMS was tested using Bromide as a surrogate for a very mobile pesticide. | Same as CREAMS |
| 8 | GRASP | Not modelled | N is modelled as a plant nutrient, but the focus is not on N export. GRASP does not model the complete N cycle or transformations | Soil depth<br>Moisture holding characteristics at air-dry, wilting point and field capacity throughout the soil profile | Based on drainage below the bottom of the lowest soil layer | Not a focus of the GRASP model | Not a focus of the GRASP model |
| 9 | HowLeaky | Calculates dissolved, particulate, total P and bioavailable P.<br>P enrichment ratio accounts for P-rich fine material from hillslopes | Separate models for:<br>1. Dissolved N in runoff<br>2. Dissolved N in leaching<br>3. Particulate N in runoff<br>Simple approach<br>Does not use a nitrate volume balance or routing.<br>Uses the method of Rattray or Fraser to calculate dissolved N in runoff after fertilizer application. | 1. Number of horizons<br>2. Layer depth (mm)<br>3. Air dry moisture (% vol)<br>4. Wilting point (% vol)<br>5. Field capacity (% vol)<br>6. Sat. water content (% vol)<br>7. Max drainage from layer (mm/day)<br>8. Bulk density ($g/cm^3$)<br>9. Stage 2 evap CONA ($mm\ day^{-0.5}$)<br>10. Stage 1 evap limit U (mm)<br>11. Runoff curve num (CN) (bare soil)<br>12. CN reduction 100% cover<br>CN reduction - tillage<br>13. Rainfall to 0 roughness (mm) (cumulative rainfall required to remove surface roughness)<br>14. USLE K factor<br>15. USLE P factor<br>16 Field slope (%)<br>17. Slope length (m)<br>18. Rill/interrill ratio (0-1)<br>19. Soil cracking<br>20. Max crack infiltration (mm)<br>21. Sediment delivery ratio | Cascading bucket. Loss from lowest profile layer is deep drainage. Rate is capped to a maximum (mm/day) | Routing approach:<br>Initial solute concentration across soils layer and in rainfall and irrigation water.<br>Mixing coefficient used to route solute through soil when rainfall or irrigation leads to drainage.<br>(This approach is not used for N) | Simple approach to calculating dissolved N leaching load.<br>Requires information on N concentration in soil profile to be input possibly from other biophysical models.<br>Does not use volume balance or routing.<br>Load is concentration in deepest soil layer x drainage x efficiency. |

| No | Model | P export | N export | Required soil hydraulic properties | Deep drainage | Solute leaching | Nitrate leaching |
|---|---|---|---|---|---|---|---|
| 10 | HSPF | The PHOS module models transport, plant uptake, adsorption/desorption, immobilisation and mineralisation of P. Export includes P attached to sediment. P leaching is modelled. | Modules NITR and NITRX simulates N transport and soil reactions and tracks nitrate, ammonia and organic N, denitrification mineralisation, immobilization, fixation, volatilization of Ammonia and partitioning between particulate and soluble. N reactions are modelled separately for each soil layer. Export Includes N attached to sediment and leached N. | 1. Coefficient and exponent in the soil detachment equation<br>2. Coefficient and exponent in the sediment wash-off equation<br>3. Potency factors (enrichment ratios) for scour and wash-off<br>4. Soil layer storage capacities (field capacities and lower limits)<br>5. Parameters for infiltration equation<br>6. Fraction of groundwater inflow that is lost<br>7. Density of deep-rooted vegetation | Models transfer of water to groundwater (which reappears as baseflow) or lost to deep percolation. Can include lateral inflow to groundwater storage or interflow. | Includes modules to simulate nonreactive tracers. | Can model N leaving as deep drainage. Also allows adjustment factors if leaching estimates are too large. |
| 11 | HYDRUS-1D | Not modelled | N is treated as a solute. Capable of simulating transformation of N through urea, ammonium, nitrite, nitrate, nitrogen gas and nitrous oxide. Export is calculated from advection, diffusion and gaseous transport | Horizontal and vertical saturated hydraulic conductivity<br>Location of any impervious layers<br>Locations of transitions between soil layers<br>Soil characteristic curve<br>Soils can be non-uniform | Lower boundary condition can be specified. | Solute transport equations model advection-dispersion in liquid phase and diffusion in gaseous phase. Includes modelling of solute reaction and degradation and transfer between liquid and gaseous phases. Multiple solutes can be modelled and can react and interact | Leaching is handled through the advection diffusion equation responding to specified boundary conditions for the bottom of the soil layer |
| 12 | LEACHM | Not mentioned in documentation | Simulates the transformation and flux of N between three N pools including mineral, NH-4 and NO-3. Mineralisation, nitrification, denitrification and volatilisation are modelled. | Profile depth<br>Lower boundary condition<br>Soil bulk density<br>Saturated hydraulic conductivity<br>Root flow resistance<br>Upper boundary condition<br>Molecular diffusion coefficient<br>Dispersivity<br>Segment thickness | A boundary condition can be specified for the bottom of the soil layer which will allow calculation of deep drainage | Advection-dispersion equation. Volatilisation and transformations can be modelled | Comprehensive modelling of N sources, sinks and transformations. Leaching calculated as N concentration of drainage below the soil profile |
| 13 | OVERSEER | Not modelled | N balance for the soil profile including inputs from rain, irrigation and fertilizer, mineralised soil organic matter and crop residue, outputs via volatilization and denitrification, plant update and leaching.<br>Considers N export via leaching.<br>Long term average annual values are produced by the model. | Soil water content at:<br>- wilting point<br>- field capacity<br>- saturation<br>- bulk density<br>- saturated conductivity<br>- profile drainage class (Good - Very Poor)<br>- soil texture group (Light, medium, heavy)<br>maximum root depth<br>Wheeler, 2018b | Drainage occurs when soil water exceeds field capacity. Maximum drainage rate is limited by saturated hydraulic conductivity | Not modelled (other than N) | Nitrate leading is defined as N percolating below 1.5 m depth (Cichota et al., 2010) |

| No | Model | P export | N export | Required soil hydraulic properties | Deep drainage | Solute leaching | Nitrate leaching |
|---|---|---|---|---|---|---|---|
| 14 | PERFECT | Not modelled | Not modelled | Information for up to 10 soil layers<br>Lower soil water limit (-15 bar)<br>Upper soil water limit (field capacity)<br>Saturated water content<br>Bulk density<br>Curve number<br>Soil erodibility (K factor)<br>Soil evaporation factors CONA and U | Uses an algorithm from CREAMS/GLEAMS (Leonard et al., 1987)<br>Cascading bucket. Loss from lowest profile layer is deep drainage.<br>No restriction on water movement below the modelled soil layers. | Not modelled | Not modelled |
| 15 | RUSLE | Not modelled | Not modelled | Surface roughness<br>Soil moisture<br>Root mass in the upper 100 mm of the soil profile | Not modelled | Not modelled | Not modelled |
| 16 | SWAT | P is partitioned into sediment bound and soluble fractions. Export includes application of enrichment ratio | Simulates N forms and transformations including nitrification, volatilisation, denitrification, plant uptake, N in residue. Calculates the amount of Nitrate in runoff, lateral flow, and leaching (blow the lowest layer). N in runoff includes sediment attached N and application of enrichment ratio | Information for soil layers<br>Lower soil water limit (-15 bar)<br>Upper soil water limit (field capacity)<br>Saturated water content<br>Bulk density<br>Curve number | Drainage below the lowest soil layer can be partitioned to groundwater recharge and deep drainage | Pesticides are modelled in a similar way to GLEAMS and includes application efficiency, volatilisation, half-life in soil, wash off fraction. Leaching estimates based on percolation from soil layers | Leaching is based on loss of N from lower soil layers in deep drainage |
| 17 | SWIM | P export attached to particles is not modelled. Could model P as a solute | N can be modelled as a solute. N modelling has been undertaken at management scales using APSIM-SWIM e.g., Verberg et al. (1996). | Soil water retention curve for soil layers<br>Boundary conditions at soil surface<br>Boundary conditions at bottom of soil<br>Initial conditions in terms of water content or matric potentials<br>Root radius<br>Root conductance | A time dependent boundary condition needs to be supplied by the user for the bottom boundary condition as one of four options:<br>1. variable matric potential gradient<br>2. Variable potential<br>3. Zero flux<br>4. Seepage with variable threshold suction.<br>Option 2 can be used to specify a fluctuating water table | Uses the advection-dispersion differential equation. Solute initial and boundary conditions are specified along with source/sink terms | Can model N as a solute. Has been used to model nitrogen export and leaching under effluent irrigation (Snow, 1995; Snow, 1996; Snow and Bond, 1996) |
| 18 | WEPP | Not modelled | Not modelled | Random roughness<br>Orientated roughness<br>Bulk density<br>Hydraulic conductivity<br>Interrill erodibility<br>Rill erodibility<br>Critical shear stress | Water moving below the root zone is lost and is not tracked | Not modelled | Not modelled |

*Table A1: Summary of modelling approaches (continued)*

| No | Model | Limitations | Comments | References |
|---|---|---|---|---|
| 1 | AGNPS | AGNPS is an event based. This limitation was overcome with the release of AnnAGNPS | AGNPS v5 was released in 2018 | Young et al. (1989)<br>https://www.nrcs.usda.gov/wps/portal/nrcs/detailfull/<br>?ss=16&navtype=BROWSEBYSUBJECT&<br>cid=stelprdb1042468&<br>navid=140100000000000&pnavid=1400000000000000&<br>position=Not%20Yet%20Determined.Html&<br>ttype=detailfull&<br>pname=AGNPS%20Home%20Page%20\|%20NRCS |
| 2 | ANSWERS | Event based so water movement that is important at larger temporal scales is not modelled e.g., soil evaporation and transpiration | It appears that ANSWERS (the event-based model) is no longer being updated.<br>ANSWERS-Continuous has been developed and incorporates elements of GLEAMS and EPIC. | Beasley et al., 1987; 1988 |
| 3 | APSIM | Seems a comprehensive and flexible model that has been thoroughly test. The ability to include plug in modules makes the model highly adaptable | "Plug ins" can be developed to model components of farming systems as required | Keating et al., 2003<br>Documentation at https://www.apsim.info/<br>SOILWAT module https://www.apsim.info/documentation/model-documentation/soil-modules-documentation/soilwat/ |
| 4 | CERES | The focus of CERES is on crop yield rather than erosion, deep drainage, or export of N, P and solutes. APSIM builds on an improves many of the CERES algorithms | There are a variety of CERES model that apply to different crops e.g., wheat, rice, maize, barley, grain sorghum, pearl millet.<br>Basso et al. (2016) provides a review of CERES model performance against measured values, including assessment of the simulation of soil water and ET.<br>Contributors to CERES included Henry Nix (ANU) | Ritchie and Otter, 1985; Ritchie and Godwin, D. (nd) CERES Wheat 2.0 https://nowlin.css.msu.edu/wheat_book/ (accessed 19 Jan 2020) |
| 5 | CREAMS | Deep drainage is modelled by difference rather than explicitly. However, there are some validation data that show results are reasonable at annual time scales.<br>Field scale model rather than watershed scale.<br>Does not include N fixation by legumes. | CREAMS was built quickly which required adoption of existing models. The approach used in CREAMS has been highly influential with components widely adopted in other models. | Knisel, 1980 |
| 6 | EPIC | 1D model. Applicable to a small area. | Enrichment ratio function seem very approximate but in important for correct estimation of N and P loads.<br>As well as the Erosion Productivity Impact Calculator, there is an Environmental Policy Integrated Climate Model which is called EPIC | Sharpley and Williams (1990); Williams et al., 1984 |
| 7 | GLEAMS | Does not consider the recycling of solute (bromide, pesticides) back into the soil from plant residues.<br>Not intended to accurately predict absolute quantities but intended to show relative differences as responses to management actions | Modification of CREAMS to better represent movement of water within and through the root zone and improve long-term simulation.<br>Computational structure altered to output daily values. In contrast to CREAMS, GLEAMS allows for non-uniform soil characteristics.<br>Future versions will model crop residue and its effect on erosion | Leonard et al., 1987 |

| No | Model | Limitations | Comments | References |
|---|---|---|---|---|
| 8 | GRASP | Does not model the complete N cycle. Does not model run-on or lateral drainage<br>The focus of the model is not on N or P export, N leaching or deep drainage. | CEDAR is a clean recoding of the GRASP | CEDAR GRASP manual 2019 |
| 9 | HowLeaky | 1. Event processes, which occur over < 1 day may be poorly represented. For example, erosion caused by a short duration intense storm.<br>2. One dimensional. Only applicable for field-sized areas with gentle slopes and with homogeneous soils, vegetation, topography and climate. Does have an option to calculate lateral flow on steep slopes. | PERFECT algorithms are available in HowLeaky by setting model options.<br>An option to model infiltration in cracking soils is available. Doesn't have a sophisticated approach to modelling N so N export and leakage may not be as accurate of other models e.g., APSIM | HowLeaky Model V5 Technical documentation Version 1.06 |
| 10 | HSPF | Calibration is challenging requiring experience and expertise. There is a lack of documentation on parameter estimation. Data requirements are extensive (Yuan et al., 2020). | The modular nature of HSPF means it should be straightforward to modify for specific applications. Focus on watersheds rather than hillslopes or fields. | EPA, USGS; WinHSPF 3.0; Public; https://www.epa.gov/ceam/basinsdownload-andinstallation<br>Donigian et al. (1995) |
| 11 | HYDRUS-1D | Complicated, likely to have lengthy run times (but computers are getting faster all the time). Would need to have experienced users to set up and operate the model | Hydrus 1D is available for free. Hydrus 2D/3D are available commercially. The ability to model multiple solutes and their interactions could be important for some problems | Simunek et al. (2009) |
| 12 | LEACHM | Not effective in evaluating impacts of management practices on ground water loadings | If the complexity of using Richards equation is warranted, it may be better to use a model such as SWIM, APSIM-SWIM or HYDRUS which seem to be more flexible | Hutson and Wagenet (1995) |
| 13 | OVERSEER | 1. Doesn't consider N in surface runoff or bound to particles. | The monthly time step for some results may be an issue in some cases | OVERSEER Nutrient budgets technical manual for the Engine (Version 6.3.0) www.overseer.org.nz |
| 14 | PERFECT | 1. Processes which occur over < 1 day may be poorly represented. For example, erosion caused by a short duration intense storm.<br>2. One dimensional. Only applicable for field-sized areas with gentle slopes and with homogeneous soils, topography and climate.<br>3. Deep drainage is lost instantaneously. PERFECT does not consider any restrictions to water movement below the soil. | Many of the algorithms in PERFECT were adopted in later models e.g. How Leaky | Littleboy et al., (1999) |
| 15 | RUSLE | The RSULE is restricted to estimating average soil loss | Prediction relationships developed from US data. | Renard et al. (1997) |
| 16 | SWAT | 1. Not appropriate to model events (Yuan et al. 2020)<br>2. Does not consider the effect of season on vegetation growth (Qi et al. 2017) | SWAT is regularly updated, has an active user community and over 1300 relevant articles have been published | USDA-ARS; SWAT2012; Public; https://swat.tamu.edu/<br>Yuan et al. 2020 |

| No | Model | Limitations | Comments | References |
|---|---|---|---|---|
| 17 | SWIM | 1. Complex model with extensive data requirements<br>2. Does not model soil movement | SWIM was developed as a research tool but has recently been incorporated into APSIM (APSIM-SWIM) so can be used to address management problems.<br>The link with APSIM also allows improved modelling of plant growth and transpiration | Verberg et al., (1996) |
| 18 | WEPP | Does not model N or solutes | Uses weather generation rather than requiring input of climate data.<br>Can model irrigation | Flanagan and Nearing (1995) |

# Appendix B. Soil Evaporation

Most of the hydrology models use the 2-stage Ritchie model which requires specification of two parameters, U and CONA; the first parameter (U) describes the amount of water (mm) that can be lost from the soil under energy limited conditions, whilst the second parameter CONA describes the rate of evaporation determined by the supply capacity of the soil. As this is essentially a diffusive process its rate is proportional to inverse of the square root of time. Hence CONA has units of $mm/t^{0.5}$.

U varies with soil texture (3 to 8 mm) with higher values associated with higher clay contents. CONA on the other hand tends to be less variable with soil texture (about 4 to 5 $mm/t^{0.5}$) but is responsive to lower seasonal evaporative demand (Foley et al. 2014) reducing from say 5 to 3 $mm/t^{0.5}$ in winter. Overall, the Ritchie model has been well validated for a range of textures (Foley and Wish 2015) and there seems to be no compelling evidence to adopt the more physically rigorous SWIM module that is an option in APSIM (Foley and Fainges 2014).

However, Ladson's review (Ladson 2021) notes that Salvucci (1997) makes a distinction in diffusive loss stage for two different soil types:

- Low permeability soils where unsaturated hydraulic conductivity is much less than the potential soil evaporation rate
- High permeability soils where the unsaturated hydraulic conductivity is much greater than the potential soil evaporation rate.

For low permeability soils, the cumulated evaporation is proportional to the square root of time (rate proportional to $t^{-1/2}$), which is the approach used in MEDLI. For high permeability soils, the cumulative evaporation is proportional to log (time) (rate is proportional to $t^{-1}$) . For both soil types the initial rate of stage 2 evaporation starts at a rate proportional to $t^{1/2}$ but then slows for high permeability soil (Figure B1). Brutsaert (2014) also shows that cumulative stage 2 soil evaporation is not always proportional to square root of time, and references a number of papers that present empirical data suggesting an exponential decay in evaporation rate provides a better fit to the data.

It's unlikely this difference will be important in effluent irrigated soils, but may be important in dryland conditions. Users of MEDLI often model dryland conditions to set a benchmark for deep drainage loss (mm/yr). Hence it seems that a more rigorous review of the experimental soil evaporation literature may be warranted for scientific completeness.

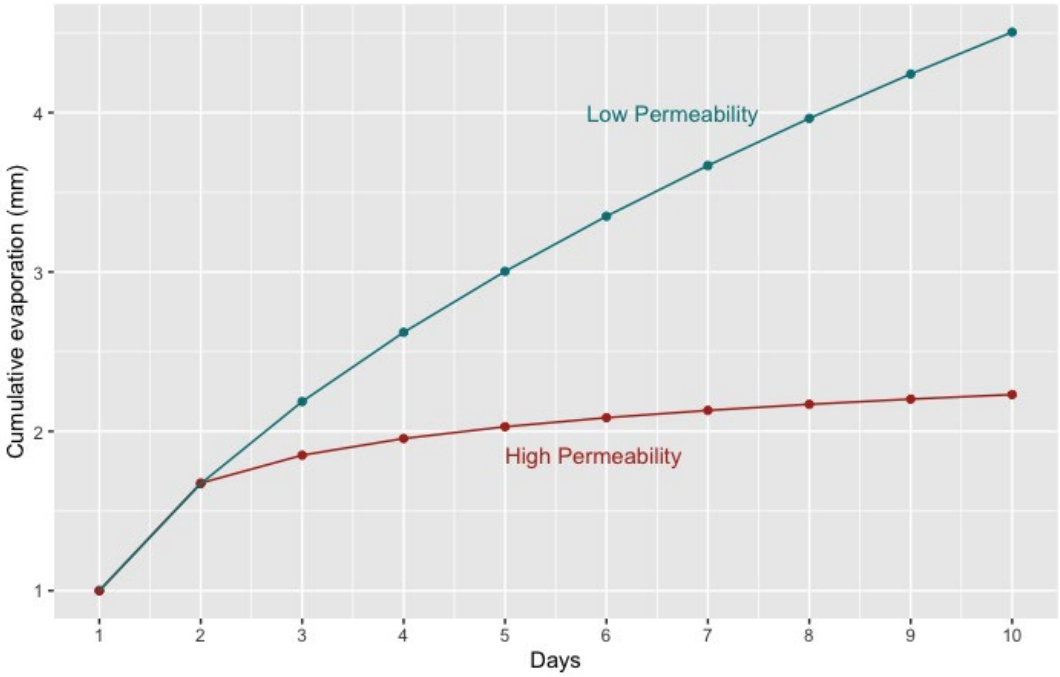



*Figure B1 Cumulative evaporation for high and low permeability soils according to Salvucci (1997)*

MEDLI assumes that if soil cover is 100%, then soil evaporation is zero. This implies that dead stubble cover **1 mm** thick is as effective at reducing evaporation as say **10 mm** of dead cover. This conclusion is not supported by experimental evidence where evaporation from wet soil with different stubble loads (kg/ha) was tracked as a function of drying time (Bond and Willis 1970). In fact, APSIM uses this finding to adjust their evaporation algorithm, whereas HowLeaky uses the expression:

$$e^{-0.22 \times total\_crop\_residue}$$

to accommodate stubble loads (t/ha) in addition to fractional green cover effects on soil evaporation. MEDLI needs to consider this modification. However, as Ladson points out (Ladson 2021), crop residue will also store & release water, and the more often the wetting frequency, the more important will be the magnitude of this evaporation loss. Hence reduced soil evaporation will be partially offset by stubble evaporation.

MEDLI has assumed that potential soil evaporation reduced linearly as the combination of green cover and surface dead cover increases. Hence at 100% green + dead cover, potential soil evaporation is zero. See eqn 5.10 and 7.64 from MEDLI manual, and the response function plotted in Figure B2. Note that green and dead cover values are additive.

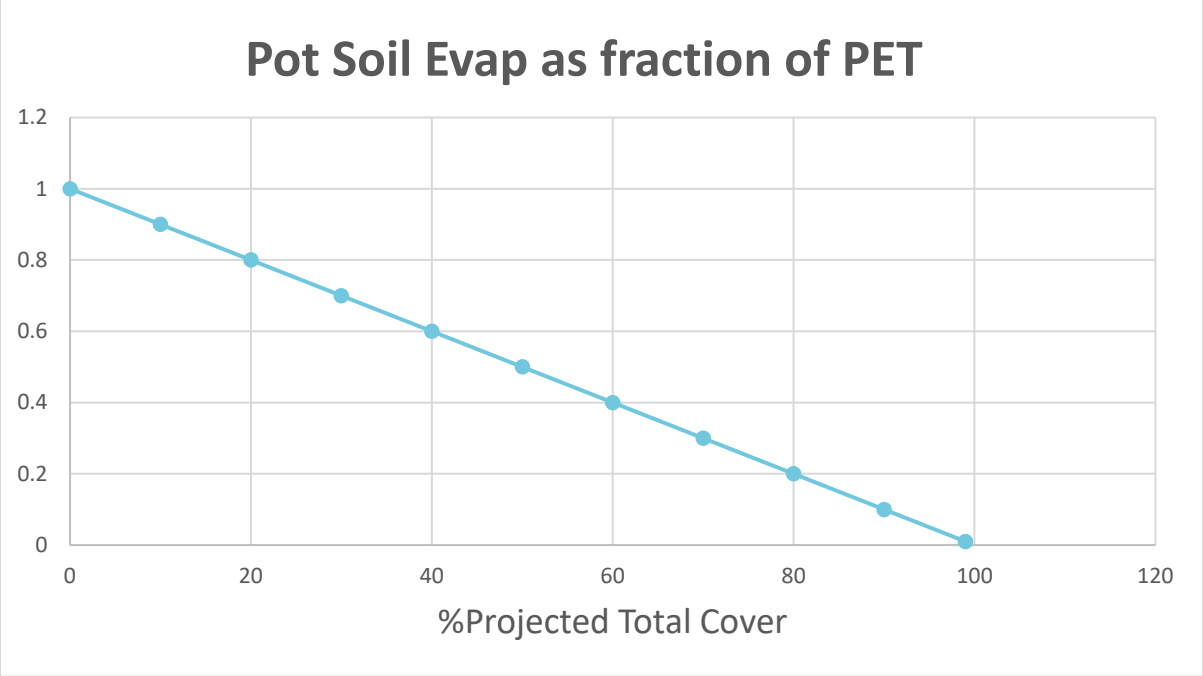



***Figure B2.*** *The Cover-Evaporation Response Function used in MEDLI. Note that total cover includes green and surface residue (dead) cover.*

$$E_{pot} = pan \times pancoeff \times \left(\frac{100 - TotCover}{100}\right)$$ .....Equation 5.10

where:

$E_{pot}$ = Potential soil evaporation (mm)
pan = Pan evaporation (mm)
pancoeff = Coefficient to account for crop effects
TotCover = Total projected green and dead crop cover (%). For further details, see Section 7.4 Use of Green and Dead Cover for Estimating Soil Evaporation.

$PotEvap_i = Pan_i * Pancoef * (1\text{-}TotCover_i)$ .....Equation 7.64

where:

$PotEvap_i$ = potential evaporation for day *i* (mm).
$Pan_i$ = daily Class A pan evaporation on day *i* (mm) *(input value)*
Pancoef = pan coefficient which adjusts the Class A pan value to that expected for a Class A pan surrounded by the plant environment *(input value)*.
$TotCover_i$ = proportion of the land area that is with plant cover (dead or green) and hence, is not subject to soil evaporation on day *i*.

As this function completely ignores the effect of the mass (kg/ha) / thickness (mm) of dead (stubble) cover, it is likely that MEDLI **underestimates** the amount of soil evaporation for mown pasture where part of the soil surface is exposed to solar radiation after each harvest.

In the CEDAR GRASP model, (McKeon et al. 1982, Rickert et al. 2000, Day et al. 2019) the effects of green and dead cover are combined in a multiplicative manner as follows:

$$Effective\_surface\_cover = 1 - (1 - trans\_cover) \times (1 - dead\_cover)$$

Where:

trans_cover is the proportional effect of total biomass on reducing soil evaporation

dead_cover is the proportional effects of standing dead material and litter on reducing soil evaporation.

We have evaluated this equation for various combinations of green and dead cover and the results are shown in Table B1.

*Table B1. Combination of green and dead cover in GRASP to generate Effective Cover fraction value (EffCover) and the subsequent reduction in potential soil evaporation (expressed as a fraction).*

| Trans_Cover | Dead_Cover | Eff Cover | %Pot SE |
|---|---|---|---|
| 0 | 0.5 | 0.5 | 50% |
| 0.1 | 0.5 | 0.55 | 45% |
| 0.2 | 0.5 | 0.6 | 40% |
| 0.3 | 0.5 | 0.65 | 35% |
| 0.4 | 0.5 | 0.7 | 30% |
| 0.5 | 0.5 | 0.75 | 25% |
| 0.6 | 0.4 | 0.76 | 24% |
| 0.7 | 0.3 | **0.79** | **21%** |
| 0.8 | 0.2 | 0.84 | 16% |
| 0.9 | 0.1 | 0.91 | 9% |
| 1 | 0 | 1 | 0% |

The potential soil evaporation is calculated from the expression:

$$\text{Potential\_soil\_evap} = \text{PET}\ (1 - \text{Effective\_Surface\_Cover})$$

and is shown in Table B1 as a fraction of potential soil evaporation (% Pot SE).

For an effective cover fraction of say 0.79, the potential soil evaporation is 21% of its maximum potential value for the day. We note that 0.79 corresponded to a combination of 0.7 green cover and 0.3 dead cover, which in MEDLI, would equal 100% Effective Cover, and hence zero soil evaporation. Consequently, when MEDLI is used to model effluent irrigated pasture, soil evaporation losses could be underestimated, and hence soil water deficit and therefore irrigation demand will be underestimated.

There is a compelling body of evidence to support the view that the amount of surface residue (either mass or depth) can have a substantial effect on soil evaporation rate. Figure B3 shows the results of laboratory studies by Bond & Willis (1970) which explored the effect of increasing amounts of (wheat) stubble on the time course of evaporation. Clearly 2 t/ha of stubble substantially reduce evaporation loss over a 10- or 15-day period compared with a completely bare soil. We note that Figure B3 is used in APSIM to reduce soil evaporation with increasing stubble mass over the fallow period. Similarly, Steiner (1989) measured the effect of **depth of stubble** thickness on relative evaporation rate and her results are shown in Figure B4**.** It can be seen that even a thickness as small as 2.5 mm can have a substantial effect on relative evaporation rate (giving an E/Epot of about 0.4). Klocke et al. (2009) also reported that that a "deep" residue depth with 100% surface cover reduced soil evaporation rate by > 50% although the data was not amenable to develop a cover/mass response function.

In contrast, the HowLeaky team (Queensland Government 2019) used soil evaporation data from a row spacing/mulch field experiment in the USA (Adams et al. 1976) to develop a cover/evaporation response function which took the form:

$$potential\_soil\_evaporation = potential\_soil\_evaporation \times e^{\frac{0.22 \times total\_crop\_residue}{1000}}$$

noting crop residue is measured in tonnes/ha and the potential soil evaporation for **nil residue** is:

$$potential\_soil\_evaporation = pan\_evap \times (1 - total\_cover \times 0.87)$$

where total cover only includes the green cover. The scalar of 0.87 is taken from a similar routine used in the APSIM model based on the row crop results reported in Adams et al. (1976).

An example of the crop residue response function is shown in Figure B5 where a residue load of say c 2.5 t/ha corresponds to an adjustment factor of about 0.6.

**Overall, we conclude that the MEDLI model should consider using the cover/evaporation adjustments algorithms from HowLeaky** (Queensland Government 2019)**.**

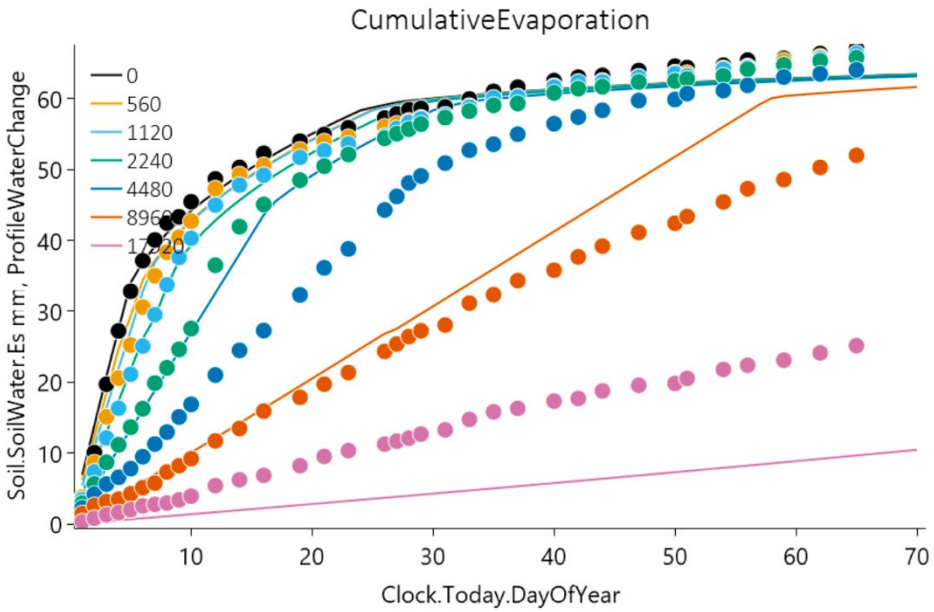



*Figure B3. Effect of residue mass on the time tend of evaporation from laboratory soil columns (Bond and Willis 1970). (Graph from ASPSIM manual. Note that the numbers refer to residue values in kg/ha.)*

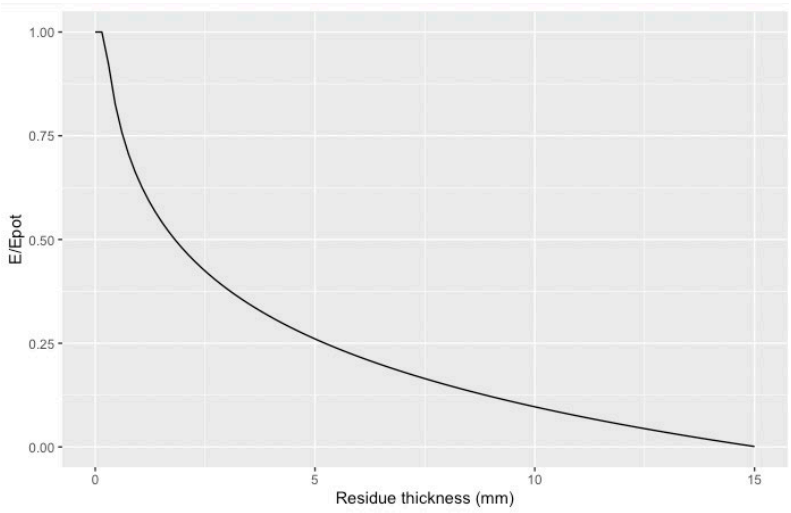



*Figure B4. The effect of residue thickness on soil evaporation expressed as a fraction of potential evaporation (Steiner 1989 as reported in Ladson 2021).*

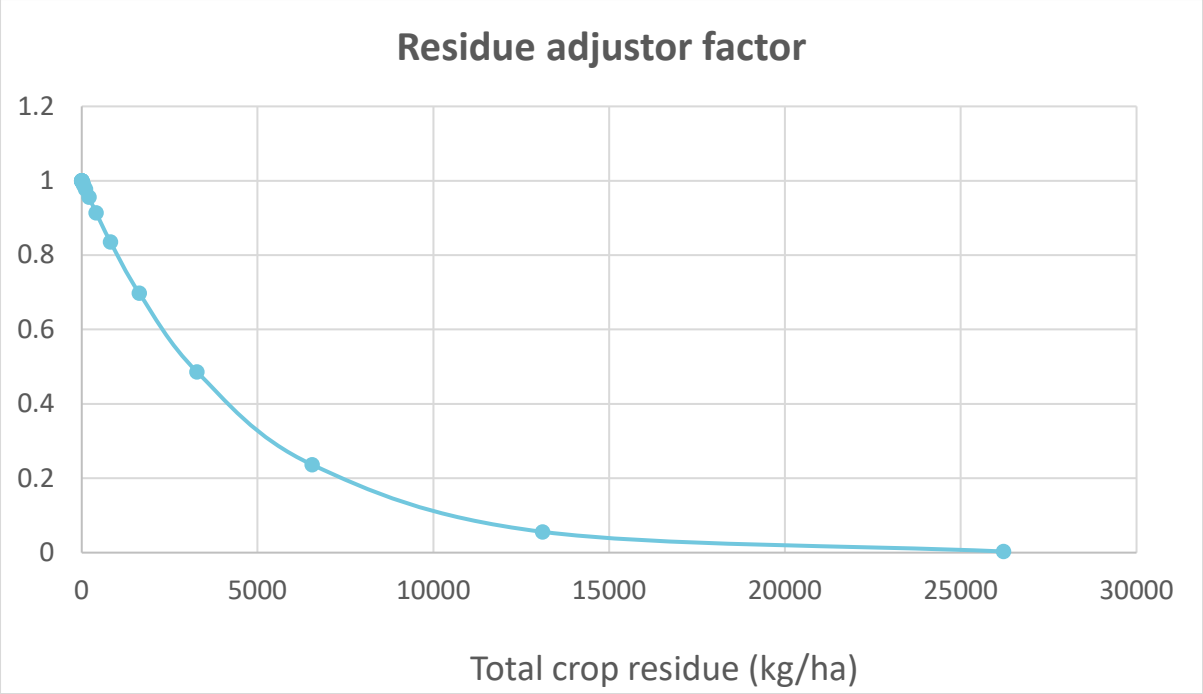



*Figure B5. The effect of mass of crop residue on the soil evaporation adjustor factor. For zero residue, the factor equals one meaning soil evaporation can occur at the potential rate (from HowLeaky manual, Queensland Government, 2019).*

## References

Adams, JE, Arkin GF and Ritchie JT, (1976). Influence of row spacing and straw mulch on first stage drying. *Soil Science Society Amer. Journal* **40** 436-442.

Bond, JJ, and Willis, WO, (1970). Soil water evaporation: first stage drying as influenced by surface residue and evaporation potential. *Soil Science Society Amer. Journal* **34** 924-928.

Brutsaert, W, (2014). Daily evaporation from drying soil: universal parameterisation with similarity. *Water Resources Research* **50** 3206–3215

Day, K, McKeon, G, and Carter, J, (2019). Cedar Grasp Technical Manual. Department of Environment and Science.

Foley, J, and Fainges, J, (2014). Soil evaporation-how much water is lost from northern crop systems and how agronomic models accurately represent this loss? *GRDC Goondiwindi Update, Goondiwindi, Qld, Australia*

Foley, J, and Whish, J, (2015). Measuring soil evaporation across soils of the northern cropping zone. *GRDC Final Report Project # ERM00002.*

Klocke, NL, Currie, RS, and Aiken, RM, (2009). Soil water evaporation and crop residues. *Transactions - American Society of Agricultural and Biological Engineers*, *52*(1), 103–110.

Ladson, AR (2021). MEDLI science review: Hydrology – model and process. Report to the Queensland Water Modelling Network, Department of Environment and Science by Moroka Pty Ltd.

McKeon, GM., Rickert, KG., Ash, AJ., Cooksley, DG. and Scattini, WJ, (1982). Pasture production model. *Proceedings of the Australian Society of Animal Production* 14:201-204.

Queensland Government, (2019). HowLeaky Model V5 Technical Documentation: Version 1.09. Department of Natural Resources, Mines and Energy and the Department of Environment

and Science. https://science.des.qld.gov.au/__data/assets/pdf_file/0018/100467/HowLeaky-manual.pdf (Accessed June 2021).

Rickert, KG, Stuth, JW, and McKeon, GM, (2000). Modelling pasture and animal production. *In*: *'Field and Laboratory Methods for Grassland and Animal Production Research'*. (Eds L 't Mannetje and RM Jones.) pp. 29–66. (CABI Publishing: New York.)

Salvucci, GD, (1997). Soil and moisture independent estimation of stage-two evaporation from potential evaporation and albedo or surface temperature. *Water Resources Research*, **33** 111–122.

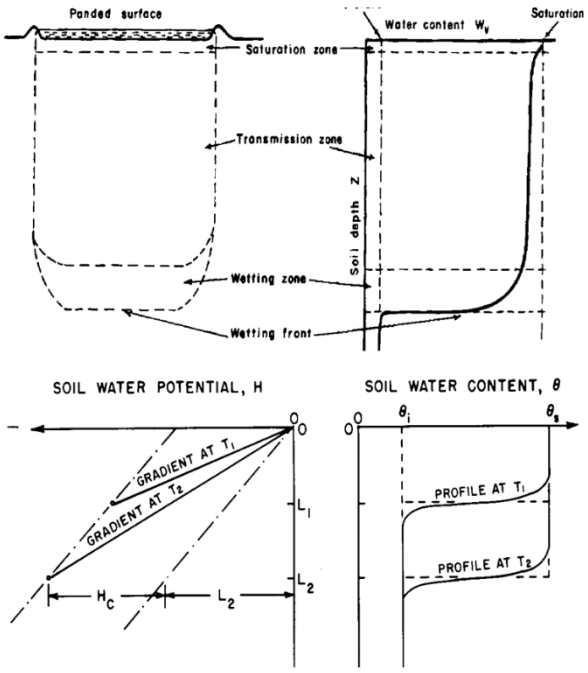
Steiner, JL, (1989). Tillage and surface residue effects on evaporation from soils. Soil Science Society of America Journal 53:911-916.

# Appendix C. Green & Ampt Infiltration Equation

Although Curve Number is well embedded as the infiltration model of choice in most of the one-dimensional hydrology models, the more physically based Green & Ampt approach is frequently mentioned in hydrology textbooks and engineering lecture courses. The model was originally conceived by Green & Ampt in 1911 and has the following assumption for ponded water infiltration (note the graphic & explanatory text were taken from University of Connecticut lecture series on Vadose *Zone Hydrology/Soil Physics*, 2004)

**Basic Assumptions of the Green-Ampt Approximation:**

- A distinct wetting front exists such that the water content behind it ($\theta_0$) remains constant, and abruptly changes to initial water content ($\theta_i$) ahead of the wetting front
- The soil in the transmission zone has constant properties ($\theta_0$, $K_0$, and $\psi_0$)
- The matric potential at the wetting front is constant and equals $\psi_f$




Using Darcy's Law and some integral calculus, it can be shown that ponded infiltration behaviour can be described by the following equation, where $\mathbf{L_f}$ is the depth of the wetting front, $\Delta\mathbf{H}$ is the water potential gradient between the ponded soil surface and the wetting front at matric potential, $\boldsymbol{\psi}_f$ , and $\Delta\boldsymbol{\theta}$ is the change in soil water content between the transmission zone water content, $\boldsymbol{\theta}$**o,** and the initial water content, $\boldsymbol{\theta}$i:

Cumulative Infiltration at any time t = $$L_f - \Delta h \ln\left[1 + \frac{L_f}{\Delta h}\right] = \frac{K_0\, t}{\Delta\theta}$$

In reality, the infiltration algorithm of MEDLI applies to rainfall events that occur between irrigation events as MEDLI assumes all the irrigation water applied infiltrates the soil. However, with rainfall, the infiltration rate reduces with time due to a reduction in the soil hydraulic gradient until surface ponding occurs (provided the rainfall rate > Ks). Thereafter infiltration occurs at an ever-decreasing rate which is less than the rainfall rate, whereas before ponding, all the rainfall infiltrates the soil. Hence estimating time of ponding **(Tp)** is a very important (variable) parameter to calculate in the G-A model. The follow conceptual graphic (Figure B1) shows the development of a wetting profile in a soil subjected to a steady rainfall rate, noting $\boldsymbol{\theta}$**o** and $\boldsymbol{\theta}$**s** have the same meaning as previously.

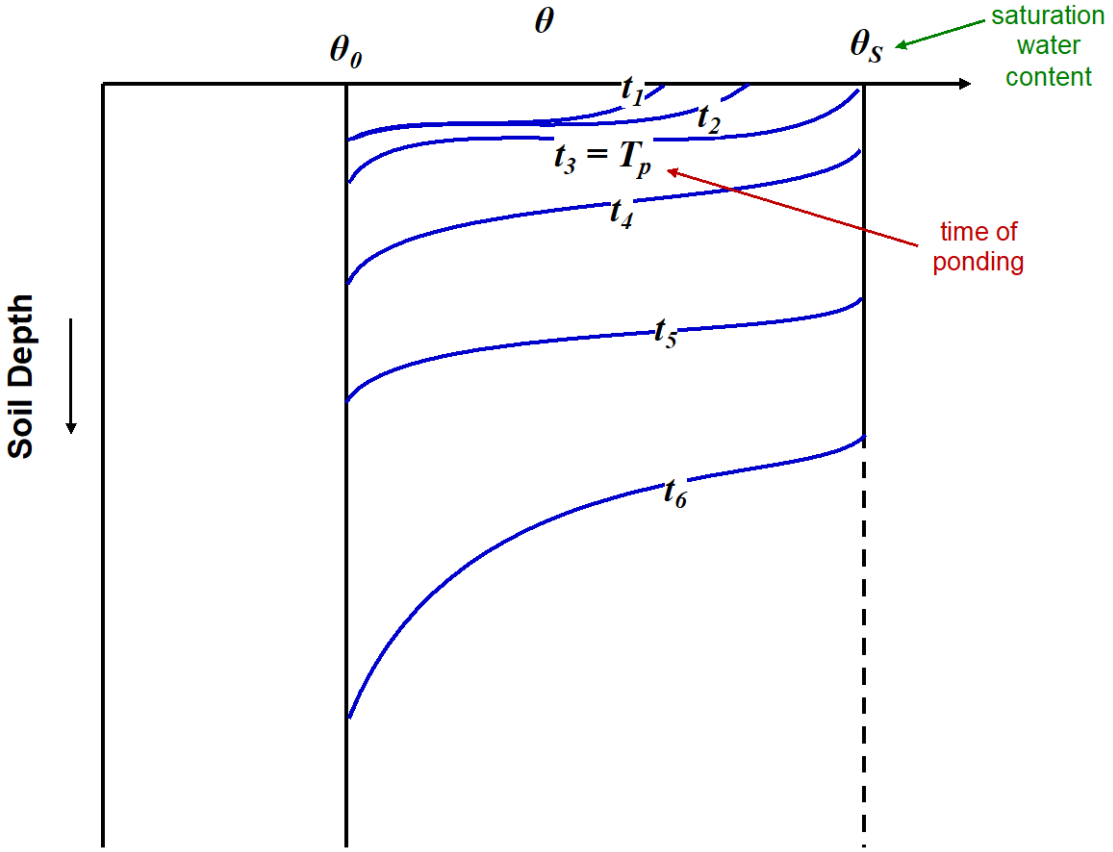



*Figure C1. The development of the soil wetting front in an idealised soil subjected to a steady rainfall input which exceeds the saturated hydraulic conductivity of the soil. (From S. Dingman - Physical Hydrology 2015)*

In 1973, Mein and Larson developed the G-A theory into something practical that could be used to describe/predict the infiltration of steady rainfall into a soil - the process shown in Figure C1. The following equations come from their work, and these & the companion descriptive text, are taken from a hydrology course at Cornell University (Physical *Hydrology for Ecosystems-BEE 3710, Cornell Uni 2011)*

In its simplest form the Green and Ampt equation for infiltration rate, *f*, can be written as:

$$f = -K_s \frac{dh}{dz} \qquad \frac{dh}{dz} = \text{hydraulic gradient} \qquad [\text{cm}^3\ \text{s}^{-1}\ \text{cm}^{-2}] \qquad \text{...Eq. B1a}$$

$$f = -K_s \frac{h_f - h_o}{Z_f} \qquad [\text{cm}^3\ \text{s}^{-1}\ \text{cm}^{-2}] \qquad \text{...Eq. B1b}$$

assume no ponding, $h_o = 0$

$$f = K_s \frac{|\psi_f| + Z_f}{Z_f} \qquad [\text{cm}^3\ \text{s}^{-1}\ \text{cm}^{-2}] \qquad \text{...Eq. B1c}$$

The subscript "f" refers to the wetting front and "o" refers to the soil surface, e.g., $h_f$ is the hydraulic head at the wetting front (sum of matric forces at the wetting front and the weight of the water above), and $h_o$ is the hydraulic head at the surface (zero, unless there is water ponded on the surface). $\psi_f$ =

matric pressure at the wetting front [cm of water], $K_s$ = saturated hydraulic conductivity [cm/hr]. The depth of the wetting front can be related to the cumulative amount of infiltrated water, F [cm], by:

$$F = Z_f(\theta_s - \theta_i) \qquad [\text{cm}^3\ \text{s}^{-1}\ \text{cm}^{-2}] \qquad \text{...Eq. B2}$$

where $\theta_S$ = saturated moisture content and $\theta_i$ = initial moisture content before infiltration began.

Rearranging Eq. B2 to solve for $Z_f$ and substituting it into Eq. B1c, the infiltration rate, $f(t)$, becomes:

$$f(t) = K_s + K_s\frac{|\psi_f|(\theta_s - \theta_i)}{F} \qquad \text{for } t > t_p \qquad [\text{cm}^3\ \text{s}^{-1}\ \text{cm}^{-2}] \qquad \text{...Eq. B3a}$$

$$f(t) = P \qquad \text{for } t \le t_p \qquad [\text{cm}^3\ \text{s}^{-1}\ \text{cm}^{-2}] \qquad \text{...Eq. B3b}$$

where: $P$ = rainfall rate (cm $\text{hr}^{-1}$) and $t_p$ is the time (hr) when water begins to pond on the surface

Unfortunately, Eq. B3a does not have time as a variable but instead uses $F$, the cumulative amount of water that has infiltrated. Recognizing that $f = dF/dt$, Eq. 3 can be solved to get the following expression for $F(t)$:

$$t = t_p + \frac{1}{K_s}\left[F - F_p + |\psi_f|(\theta_s - \theta_i)\ln\left(\frac{|\psi_f|(\theta_s - \theta_i) + F_p}{|\psi_f|(\theta_s - \theta_i) + F}\right)\right] \qquad \text{...Eq. B4}$$

where $F_p$ = the amount of water that infiltrates before water begins to pond at the surface [cm] and $t_p$ = the time it takes to have water begin to pond at the surface [hr].

The following are expressions of these quantities:

From Eq. B3a and B3b:

$$F_p = \frac{|\psi_f| K_s(\theta_s - \theta_i)}{P - K_s} \qquad t = t_p \text{ and } P > K_s \qquad \text{...Eq. B5}$$

Integrate B3b:

$$t_p = \frac{F_p}{P} \qquad \text{...Eq. B6}$$

To determine the amount of infiltration from a rainstorm of duration, $t_r$, and intensity $P$, one needs to first determine the time at which surface ponding occurs (Eqs. B4 & B5). If $t_r < t_p$ or $P < K_S$ then the amount of infiltration, $F = Pt_r$ and the infiltration rate, $f = P$. If $t_d > t_p$, then Eq. B4 is used to find, *by trial and error*, the value $F_p$ that gives $t = t_p$.

The Green & Ampt equation describes the infiltration capacity as an implicit function of time. In other words, the infiltration capacity cannot be determined for a given time by a formal algebraic method of substitution.

Unfortunately, equation B4 cannot be inverted to give F(t) as an explicit function of t. Thus, application of Equation B4 requires arbitrarily choosing values of F(t) and solving for t. If the chosen value of F(t) gives t< Tp or t >Tr, it is invalid. The corresponding infiltration rate f(t) is then found by substituting valid values of F(t) into equation B3a.

Figure C2 identifies the parts of an infiltration-rain intensity analysis with respect to Green & Ampt. The curved dash line is what equation B4 describes, and for times < Tp, it deviates from the actual infiltration line (solid line). Hence, the mathematical results for **F vs t** Eq. B4) and **f vs t** (Eq. B3) are incorrect for times < Tp. For times > Tp the **F vs t** and **f vs t** are correct.

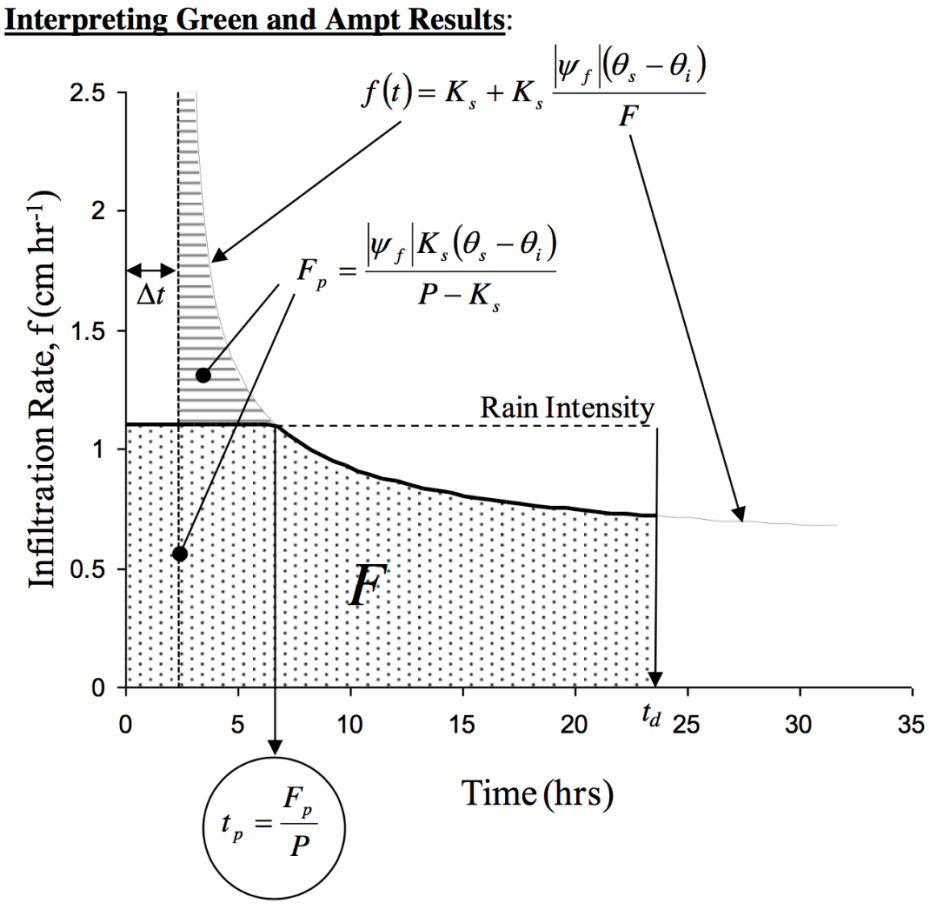



*Figure C2. Schematic of actual infiltration behaviour under steady rainfall compared with that predicted by Green & Ampt theory as quantified by Equation B4 (from Cornell University 2011)*

The use of trial-and-error solutions method make direct use of the Green & Ampt model inconvenient for incorporation into hydrology models. Consequently, Salvucci and Entehkhabi (1994) developed a close approximation of the Green & Ampt equation that gives f(t) and F(t) as explicit functions of t. Their approach requires the computation of three time parameters; (1) *characteristic time* which depends on soil type and initial water content, (2) *compression time* which is the equivalent time to infiltrate Fp under ponded conditions, and (3) an *effective time* which is a function of Tp and compression time. More detail on this approach may be found in Chapter 8 of Dingman (2015).

Further complexity occurs when the intensity varies throughout the rainfall event. Chu (1978) has adapted the Mein and Larson equations to accommodate non-steady rain, and his approach is used in 3 of the 18 hydrology models summarised by Ladson (2021). Green & Ampt has also been extended to soils where Ks decreases continuously with depth (Beven 1984) or decreases in discrete layers (Rawls et al. 1992).

The preceding methodology is a complex calculation to perform for each storm in say a 20- to 30-year water balance model run, but nonetheless Green & Ampt is used in the CREAMS, SWAT and WEPP models. Hence, I suggest a further project could assess the computational time in using Green & Ampt in MEDLI type run lengths (decades), as well as comparing the predicted runoff for selected storms (of different ARIs) for different soil water deficits, for a range of soils typically considered in MEDLI application. Runoff predictions from CN have been well validated for dryland cropping systems (e.g. Ghahramani et al. 2019), but less so for irrigated soils. Indeed, the higher antecedent soil moisture of irrigated soils may reduce the importance of Smax in predicting runoff using CN.

Taken overall the Green & Ampt model captures the essential aspects of the infiltration process - in particular the complete infiltration of rain up to the time of ponding, and the quasi-exponential decline of the infiltration rate thereafter. The minimum infiltrability of a soil is its saturated hydraulic conductivity. A valuable feature of the model is that its parameters are measurable bulk physical properties of the soil that affect infiltration in intuitively logical ways (Dingman 2015).

## References

Beven, K, (1984). Infiltration into a class of vertically non-uniform soils. *Hydrological Sciences Journal* **29** 425-434

Chu, SH, (1978). Infiltration during unsteady rainfall *Water Resources Research* **14,** 461-466

Dingman, SL, (2015). Physical Hydrology. Chapter 8 *Infiltration & Water movement in soils.* Third Edition. - https://b-ok.org/book/2613918/8a39dc

Ghahramani, A, Freebairn, DM, Sena, D, Cutajar, JL, and Silburn, DM, (2019). A pragmatic parameterisation and calibration approach to model hydrology and water quality of agricultural landscapes and catchments. *Environmental Modelling & Software* (*accepted for publication).*

Ladson, AR (2021). MEDLI science review: Hydrology – model and process. Report to the Queensland Water Modelling Network, Department of Environment and Science by Moroka Pty Ltd.

Rawls, WJ, Ahuja, LR, Brakenseik, DL, and Shirmohammadi, A, (1992). *Chapter 5. Soil Water Movement and Infiltration* in Maidment, D.R. (Editor). Handbook of Hydrology. McGraw- Hill.

Salvucci, GD, and Entehkhabi, D, (1994). Explicit expressions for Green-Ampt infiltration rate and cumulative storage *Water Resources Research* **30,** 2661-2663.

Salvucci, GD. and Entekhabi, D, (1994). "Equivalent steady moisture profile and the time compression approximation in water balance modelling." Water Resources Research **30** 2737-2749.

Silburn, DM, and Freebairn, DM, (1992). Evaluation of the CREAMS model. 3 simulation of the hydrology of Vertisols *Aust J Soil Research* **30,** 547-564.

# Appendix D: Solute Leaching equations

Nitrate leaching is one of the major criteria to assess the environmental sustainability of any effluent irrigation scheme. Its occurrence depends on the concentration of $NO_3$ in the crop root zone that coincides with deep drainage events. Hence the importance of predicting deep drainage, as discussed previously. In MEDLI, the $NO_3$ leaching from any layer is calculated as the soil solution concentration of that layer (mg N/L) multiplied by the deep drainage (mm) moving through that layer. When this $NO_3$ enters the contiguous lower layer, it is assumed to fully mix with the $NO_3$ of that layer which then is transported with the deep drainage exiting this lower layer. At the bottom of the plant zone, $NO_3$ leaching is considered a loss to the plant system as it can no longer take part in root water uptake processes. Hence the NO3 exiting the root zone depth is considered an irreversible leaching loss (kg N/ha).

Th MEDLI algorithm has a pragmatic utility, but ignores the solute transport processes that have been studied in great detail over the last 4 decades; viz that solutes move due to convective flow (the assumption used in MEDLI) as well as hydrodynamic and solute gradient dispersion, and that not all the water in a soil layer takes part in the leaching process - the fractional *immobile water content* (Dyson and White 1987, Addiscott and Cox 1976, Clothier et al. 1995). One of the more rigorous approached used to describe non-reactive solute movement in uniform soil is the convective dispersion equation which was derived by combining Richards equation with Ficks law of diffusion. It has the form:

$$\frac{\partial(\theta c)}{\partial t}+\frac{\partial(\rho s)}{\partial t}=\frac{\partial}{\partial x}\left(\theta D\frac{\partial c}{\partial x}\right)-\frac{\partial(qc)}{\partial x}+\varphi$$

Where *c* and *s* are solute concentrations (ppm) in solution or adsorbed to the soil surface, *D* is the combined dispersion and diffusion coefficient ($cm^2\ h^{-1}$), *q* is the water flux ($cm\ h^{-1}$), ρ is the soil bulk density ($g\ cm^{-3}$), and φ is the source/sink term for solute ($ppm\ h^{-1}$) ( Huth et al. 2012).

This equation is used in the SWIM module of APSIM to describe the movement of non-reactive solute including $NO_3$ leaching. Apart from the numerical difficulty of solving this strongly non-linear equation, the input variable required are the Diffusion coefficient, the soil hydraulic properties (**K-** $\boldsymbol{\theta}$, $\boldsymbol{\psi}-\boldsymbol{\theta}$) and the assumption of no preferential convective flow paths from macropores (Magesan et al. 1999). Although well tested in laboratory soil columns, its success in describing real world behaviour is more questionable (Addiscott and Wagenet 1985). None the less, Huth et al. (2012) argue that its use in SWIM (within APSIM) makes it a viable method for describing water and solute fluxes in cropping systems where more detail on infiltration, deep drainage and solute leaching is required.

At the other end of the spectrum is the Burns leaching equation (Burns 1974, 1975) which assumes that when rainfall/infiltration enters a soil it causes a temporary increase in its water content. The incoming water and solutes are assumed to mix with the water and solutes already in the layer. If the new water content of the layer exceeds the Field Capacity, the surplus water and (mixed) solutes are transferred to the next layer where the procedure is repeated. This continues down the profile until a layer is encountered which is either bottom layer (of interest), or in which the incoming water does not cause the water content to exceed Field Capacity (Addiscott and Wagenet 1985). It can be seen that this description is very similar to the assumptions used in the MEDLI model, but Burns developed his own equation which has the form:

$$X=\left(\frac{I}{I+\theta\Delta z}\right)^{z/\Delta z}$$

where X is the fraction of solute leached below depth z in a soil with volumetric soil water content at Field capacity, $\theta$, by drainage **I**. The quantity $\Delta$ z is the thickness of the notional thin soil layers that Burns considered when deriving his equation, and for which he suggested 10 mm as a suitable thickness.

The equation may be written more simply as:

$$X = \exp(-z\theta \,/\, I),$$

which is the independent of the layer thickness (Towner 1983). Burns (1975, 1976) and Burns and Greenwood (1982) went on to show that his simple equation could explain quite well the leaching of chloride and nitrate behaviour in a number of irrigated and dryland experiments reported in the literature. The soil science literature largely ignored the Burns equation for almost 20 years, when interest was reignited by the work of Scotter et al. (1993) and Magesan et al. (1999) who placed the equation in the context of stochastic convective behaviour that could be quantified by a transfer function (Jury and Roth 1990) of a resident solute. Scotter et al. (1993) went onto argue that the Burns equation was consistent with a soil showing some preferential flow (ignored by the CDE) and operating as a system of independent flow tubes in which the water and solutes travel at varying speeds. This is the complete opposite of a well-mixed system assumed by Burns (1975) in which "*the soil solution within each layer is in equilibrium with its drainage water at all times*". A consequence of this stream tube explanation is that the solute concentration measured in the soil solution (e.g. via ceramic samplers) is very different from the concentration in the soil solution actually transporting the solutes. When this latter parameter is multiplied by the deep drainage flux, the product is the actual solute leaching flux - the output of interest to MEDLI. **Hence it would appear that the algorithm used in MEDLI to calculate $NO_3$ leaching may be in error.**

This phenomenon is explored further in Figures D1a and D1b where the dimensionless concentration of a solute is expressed either as a *resident concentration* **Cr** (the volume average concentration in the soil in kg/m3 soil) or a *flux averaged solute concentration* **Cf** (kg/m3 solution) for the same conditions of deep drainage ( $I$) and a $\theta$ of 0.3. In both cases **M** (kg/m2) is amount of solute (soluble fertilizer) introduced to the soil surface. Figure D1a shows a shape that would be expected if much of the invading water by passed the less mobile soil solution, whereas Figure D1b shows the bell shape more expected from the CDE. The shape of D1a & D1b are very different, and it is Figure D1b that provides the more accurate estimate of leaching.

Other analytical solution for different initial conditions including a solute spread uniformly throughout the whole soil profile, or just to a certain soil depth, are also reported by Scotter et al. These better approximate an effluent irrigated soil, and the Scotter approach should be investigated in more detail by a solute transport expert (i.e. an expert soil physicist) for its adaption to MEDLI (see Cook 2021).

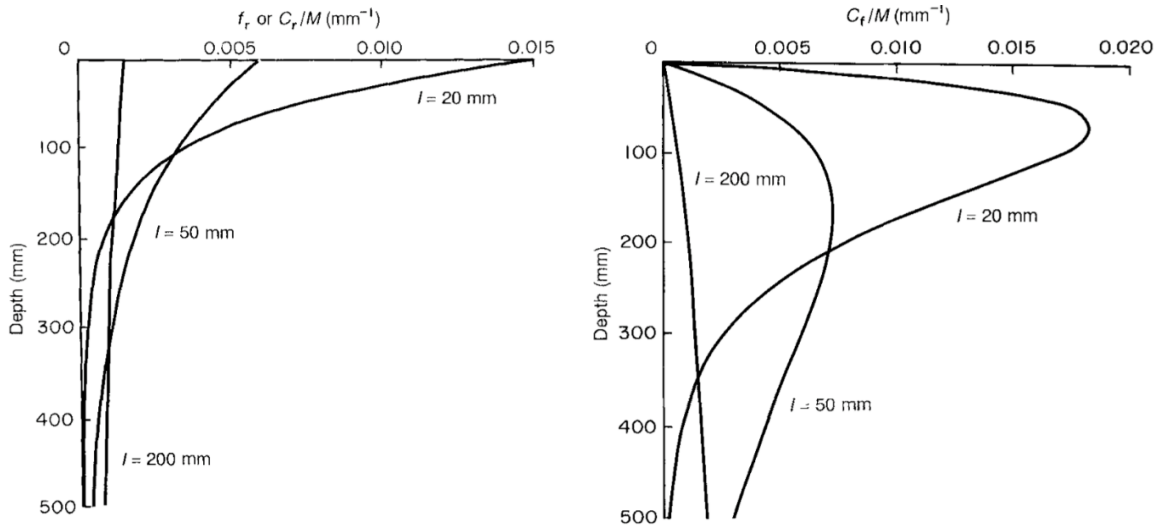



*Figure D1. Normalized resident solute concentration profiles (a) and flux averaged solute concentration profiles (b) for different amounts of deep drainage $I$ and a solute transport volume $\theta$ of 0.3. The profiles were calculated based on the Burns equation modified by a specific analytical transfer function described in Jury and Roth (1990). The graphics come from Scotter et al. (1993).*

Scotter et al. argue the main justification for the continued use of the Burns equation is its ability to simulate the leaching of non-reactive conservative solutes in a range of soils (except swelling and cracking soils) using easily obtained inputs. However, because of the phenomena of mobile/immobile water, the value of $\theta$ in the above equations may be very different from Field Capacity. Rather $\theta$ should be treated as a *fractional solute transport volume* which depends in a complex way on pore geometry and leaching condition (Jury et al. 1986). Experimental studies (White et al. 1986) have shown that measured and predicted fractions of leached fertilizer in structured soils were in better agreement when $\theta$ < FC was used. In some cases, the best fit was the water storage between FC and a $\psi$ of -200cm (Addiscott and Cox 1976). However other field studies that predicted solute loss from mole drained paddocks using the modified Burns equation showed the results were not very sensitive to the chosen value of $\theta$, with fair to good predictions occurring using $\theta$ from 0.25 to 0.45 cm3/cm3 (Heng and White 1996, White 1998).

Referring back to the Burns equation, one can see that z $\theta$ /I is the inverse of the number of pore volumes which have leached through a soil layer of depth z, noting that z $\theta$ is the equivalent depth of water in one Pore Volume, assuming that leaching must pass through a soil volume with volumetric water content $\theta$. Cichota et al. (2012) used this approach to develop a simple dimensionless relationship between the fraction of N leached from a soil profile (subjected to urine input) and the number of pore volumes of deep drainage.

The cumulative drainage (*P)* was normalised by the effective soil water storage depth (*D*), which makes the model applicable to a wide range of soils. The value of *D* was defined as the equivalent depth of soil water stored between wilting point and the drained upper limit (or field capacity) from the soil surface to a depth of 750 mm. A typical response is shown in Figure D2 where no $NO_3$ leaching occurs until about one pore volume has passed through the soil profile, and complete $NO_3$ leaching has occurred after about 2.5 pore volumes. The actual shape of the breakthrough curve depends partially on soil type and was developed using APSIM simulations to predict N losses for a wide range of NZ soils. The P1 and P2 were estimated using empirical regression functions (based mainly on rainfall and D) and then used in the monthly time step OVERSEER model (Wheeler et al. 2006, Watkins and Selbie 2015) to estimate the fraction of N lost in any given month, provided the soil N storage (calculated in OVERSEER) and monthly deep drainage (calculated in OVERSEER) were known. Deep Drainage was converted into pore volume units.

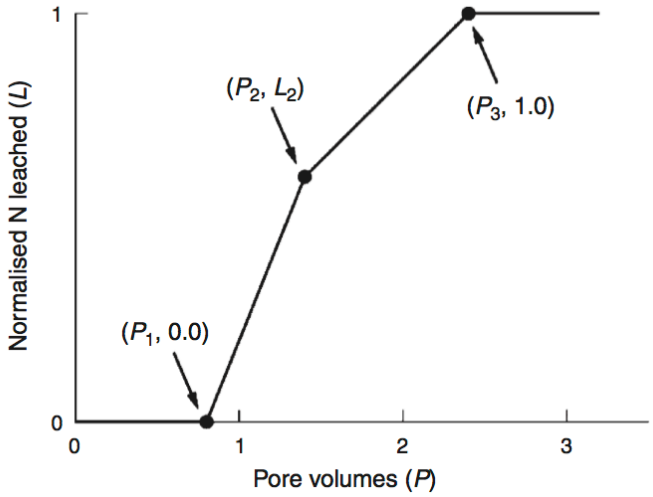



*Figure D2. Schematic of a simplified breakthrough curve to characterise N leaching losses from urine patches. The actual N losses were "measured" using APSIM simulations and expressed as a fraction of the NO3-N store in the soil depth considered (750mm). (From Cichota et al. 2012).*

The predictions from this Transfer Function model approach were checked against experimental (lysimeter) data for a range of NZ soils, which varied from a loamy sand to a clay with Ks's varying from 10 to 100mm/hr. The results are shown in Figure D3 and apart from the very high N leaching losses under urine patches (c 600 kg/ha/yr) the agreement between the predicted and measured values is generally quite good.

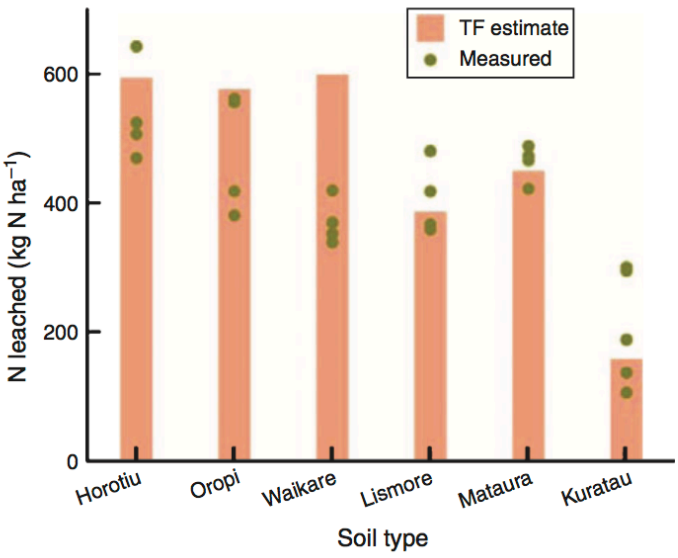



*Figure D3. Measured and estimated (from the Transfer Function of Fig D2) leaching losses of nitrogen from replicated lysimeter experiments for different soil types in NZ (from Cichota et al 2012).*

For application to MEDLI, it seems that APSIM simulations could be done for a range of soils often used for effluent irrigation in Australia (e.g., Dermosols, Chromosols and Rudosols) to develop the general shapes of the breakthrough curves of Figure D2.

**Transfer Function Model**

Because of the high micro scale variability in the physical transport of a non-conservative solute through a soil matrix, application of the CDE using single values of pore water velocity and dispersion coefficients is often of limited predictive value (Biggar and Nielsen 1976) . Jury et al. (1986) argued that the advection and dispersion mechanisms governing solute transport can be ignored, and the mass rate of solute transport through a defined layer of soil at any time can be treated as a stochastic function of the input at an earlier time. The approach has similarities with a continuous *flow- through* reactor volume, where the elution of the solute is described by an exponential decay function, which in turn can be incorporated into a Transfer Function model. Heng & White (1996) developed a Transfer Function model to describe the movement of a conservative non-reactive solute through soil, for a solute inputted at the soil surface to the output surface at any depth Z, viz:

$$C_{ex}(z,I) = \int_0^I C_{ent}(z, I - I')f(z,I')dI'$$

Where $C_{ex}$ and $C_{ent}$ are the solute output and input concentrations (mass per unit volume), **I** is the cumulative drainage depth (mm), *f(z,I) is the probability density function for the solute travel times through the soil* (units of depth$^{-1}$)and I' is a dummy variable of integration.

For the leaching of a solute such as $NO_3$ that is initially distributed uniformly throughout the soil to depth Z, the transfer function equation becomes:

$$C_{ex}(z,\ I) = C_0\left(1\ -\ \int_0^I f(z,\ I')\ \mathrm{d}I'\right)$$

Where **Co** is the average initial value of the NO3 concentration in the soil solution (mass per unit water volume).

For a log normal distribution of the travel time function, the solution for f(z,I) becomes:

$$f(z,I) = \frac{1}{(2\pi)^{\frac{1}{2}}\sigma I}\exp\left(-\frac{(\ln I - \mu)^2}{2\sigma^2}\right)$$

Where μ and σ are the Mean and Standard Deviation of the distribution of the **I** values respectively.

After manipulating the above equations, Heng and White (1996) showed that the Transfer Function model for $NO_3$ leaching based on a log normal pdf is:

$$C_{ex}(z,I) = \frac{M}{(2\pi)^{\frac{1}{2}}\sigma I}\exp\left(-\frac{(\ln I - \mu)^2}{2\sigma^2}\right) + \frac{1}{2}(C_0 + C_b)\left[1 - \mathrm{erf}\left\{(\ln I - \mu)/2^{\frac{1}{2}}\sigma\right\}\right]$$

Where M is the mass of solute per unit surface area applied to the soil surface and $\mathbf{C_b}$ is the net nitrification, adjusted for plant uptake.

Assuming M and $C_b$ are zero, the first term goes to zero and the second term retains just (the known) $C_o$ as the multiplier. When the Burns equation assumptions are introduced (fractional solute leaching vs the inverse of the pore volumes of drainage), the pdf can be converted into a simpler analytical form, and the *flux concentration* in the drainage **I** at any depth Z is given by:

$$C_{ex}(z,I) = C_0[1 - \{(z\theta/I) + 1\}exp(-z\theta/I)]$$

Where $\theta$ is the volumetric water content of the mobile water that is effective in transporting the solute through a range of stream tubes.

The first approximation of the mobile water content is Field Capacity, or perhaps the water content corresponding to a $\psi$ of -0.2 bar suction (Addiscott 1977). It would appear the *above equation* could be used to predict $NO_3$ leaching in the MEDLI model provided the daily $C_o$ values are known (effectively already done by existing mass balance calculations in MEDLI), and the fractional soil volume effective in solute transport (the mobile water content - Clothier et al. 1995) is known.

In cases where the above analytical expression does not apply, the values of $\mu$ and $\sigma$ must be estimated using knowledge of the measured leaching behaviour of a prior solute such as chloride as a surrogate for $NO_3$ (e.g. see White et al. 1998). This requirement, combined with the dense mathematical arguments, has meant that the Transfer Function model has not been used widely in agriculture except by the developers (White, White and colleagues, Scotter et al.). However just as the empirical Burns equation was revisited two decades after its development and shown (by David Scotter) to be a special case of a stochastic convective process that could be adapted to a log normal pdf form, it is possible that a similar expert may show how other forms of the Transfer Function model could be applied to MEDLI.

## References

Addiscott, M, and Wagenet, RJ, (1985). Concepts of solute leaching in soils: a review of modelling approaches. *Journal of soil Science* **36**, 411-424

Addiscott, TM, and Cox, D, (1976). Winter leaching of nitrate from autumn applied calcium nitrate, urea and sulphur coated urea in bare soil. *J Agric. Science* **87,** 381-389

Addiscott, TM, (1977). A simple computer model for leaching in structured soils. *J. Soil Sci*. **28,** 554–563.

Biggar, JW, and Nielsen, DR, (1976). Spatial variability of the leaching characteristics of a field soil. *Water Resour. Res*., **12**, 78-84, 1976.

Burns IG, (1975). An equation to predict the leaching of surface-applied nitrate. *Journal of Agricultural Science* **85**, 443--454.

Burns, IG, (1974). Model for predicting the redistribution of salts applied to fallow soils after excess rainfall or evaporation *Journal Soil Science* **25,** 165-178.

Burns, IG, (1976). Equations to predict the leaching of nitrate uniformly incorporated to a known depth or uniformly distributed throughout a soil profile. *The Journal of Agricultural* Science **86,** 305-313.

Burns, IG, and Greenwood, J, (1982). Estimation of the year-to-year variations in nitrate leaching in different soils and regions of England and Wales. *Agriculture and Environment* ***7,*** 35-45.

Cichota, R, Snow, VO, Vogeler, I, Wheeler, DM and Shepherd, MA, (2012). Describing N leaching from urine patches deposited at different times of the year with a transfer function. *Soil Research* **50.** 694-707.

Clothier, BE, Heng, LK, Magesan, GN, and Vogeler, I, (1995). The measured mobile-water content of an unsaturated soil as a function of hydraulic regime. *Australian Journal of Soil Research* **33** 397-414.

Dyson, JS and White, RE, (1987). A comparison of the convection dispersion equation and transfer function model for predicting chloride leaching through an undisturbed structured clay soil. *J Soil Science.* 38, 157-172

Heng, LK, and White, RE, (1996). A simple analytical transfer function approach to modelling the leaching of reactive solutes through field soils *European J Soil Science.* **47,** 33-42.

Huth, NI, Bristow, KL, and Verburg, K, (2012). SWIM 3: Model use, calibration, and validation. *Transactions of the ASABE*. **55,** 1303–1313.

Jury, WA, (1982). Simulation of solute transport using a transfer function model. *Water Resources Research* **18,** 363-368.

Jury, WA, and Roth, K, (1990). *Transfer Functions and Solute Movement through Soil: Theory and Applications*. (Birkhauser Verlag; Basel.)

Jury, WA, Sposito, G, and White, RE, (1986). A transfer function model of solute transport through soil. 1. Fundamental concepts. *Water Resources Research*, **22**, 243-247.

Jury, WA., Stolzy, LH, and Shouse, P, (1982). A field test of the transfer function model for predicting solute transport. *Water Resources Research* **18,** 369-375.

Magesan, GN, Scotter, DR and White, RE, (1999). The utility of Burns equation to describe solute movement through soil under various boundary and initial conditions. *European Journal of Soil Science.* **50,** 649-656.

Nielsen, R, & Biggar, JW, (1962). Miscible displacement. **3.** Theoretical considerations. *Soil Science Society of America Proceedings* **26**, 216-221.

Scotter, DR, White, RE, and Dyson, JS, (1993). The Burns leaching equation. *Journal of Soil Science,* **44**, 25-33.

Towner, D, (1983). A theoretical examination of Burns' (1975) equation for predicting the leaching of nitrate fertilizer applied to a soil surface. *Journal of Agricultural Science* **100,** 293-298.

Watkins, N, and Selbie, D, (2015). Technical description of OVERSEER for Regional Councils: Report prepared for Bay of Plenty Regional Council, AgResearch NZ, RE 500/2015/084.

Wheeler DM, Ledgard SF, Monaghan RM, McDowell R and deKlein CAM, (2006). OVERSEER Development– What it is, what it does. In: Implementing sustainable nutrient management strategies in agriculture. (Eds. L.D. Currie and J.A. Hanly). Occasional Report No. 19. Fertilizer and Lime Research Centre, Massey University, Palmerston North, New Zealand.

White, RE, Heng, LK, and Magesan, GN, (1998). Nitrate leaching from a drained sheep grazed pasture 2. Modelling nitrate leaching losses *Aust J Soil Research* **36,** 963-977.

White, RE, (1986). Leaching. In *Advances in nitrogen cycling in agricultural ecosystems* CAB International, pp 193 -211.