

# Revisiting the advection-diffusion model for estimating evaporative discharge through soil profiles

Costelloe, J.F.<sup>1</sup>, E.C. Irvine<sup>1</sup> and A.W. Western<sup>1</sup>

<sup>1</sup> *Department of Civil and Environmental Engineering, The University of Melbourne, Victoria*  
Email: [jcost@unimelb.edu.au](mailto:jcost@unimelb.edu.au)

The application of the general advection-diffusion equation to model evaporatively-driven, groundwater flux rates from solute concentration soil profiles was developed in the 1980's and has been applied to a variety of arid zone locations, including salt lakes, valley floors and discharge zones of regional groundwater. In this paper we revisit and extend the model by accounting for the effects of variable water content and sediment type on the impedance factor, and in turn, effective diffusion coefficient. We also explore the sensitivity of the extended model to its major assumptions and parameter values. Early studies typically used a Penman tortuosity value of 0.66 to account for the impedance factor. In this study, we apply the constant slope impedance factor (CSIF) method to calculate the impedance factor relating the effective diffusion coefficient to the self-diffusion coefficient of the tracer and water content, from soil textural properties. The threshold water content is the water content at which flow paths become discontinuous and varies with soil type (e.g. gravel<0.04, sand<0.13, silt<0.21, clay<0.32 v/v). Relative to the Penman tortuosity value previously used, the CSIF method resulted in reductions in the mean effective diffusion rates of between 70-96% in field soil chloride profiles. The mean diffusion coefficient of the soil profile data used in the advection-diffusion model is dependant on the boundary conditions that set the length of the profile, particularly on the position of the evaporation front. In field soil profiles, there can be some uncertainty in the position of the evaporation front based upon the use of different solutes (e.g. chloride and  $\delta^{18}\text{O}$ ) that result in considerable variation in the mean diffusion coefficient for the profile. The CSIF method for calculating the mean diffusion coefficient is very sensitive to the volumetric water content of the profile, particularly at the top of the profile close to the evaporation front. The effective depth function results in samples substantially drier than lower samples having a large influence on the mean effective diffusion coefficient of the profile and hence on the modelled evaporation rates. The uncertainty in the position of the groundwater reservoir and its concentration has little effect where the lower part of the profile shows an asymptotic trend towards a representative value of groundwater concentration but can vary substantially with different values of groundwater depth and concentration if this is not the case.

**Keywords:** *arid zone, evaporative discharge, isotopes, tortuosity*

## 1. INTRODUCTION

Groundwater discharge via evaporation in the arid zone can form a critical component of the water balance of groundwater systems. Commonly the flux rates are low and difficult to measure with instruments and evapotranspiration algorithms and long-term monitoring is problematic in remote locations. The application of the advection-diffusion model to determine evaporatively-driven, groundwater flux rates from solute concentration soil profiles provides an attractive method for estimating long-term evaporative flux rates. This method was developed by Zimmermann *et al.* (1967) and later extended by Barnes and Allison (1983). The model has been applied to a variety of arid zone locations, including “dry” salt lakes (Allison and Barnes, 1985), valley floors (Fontes *et al.*, 1986) and discharge zones of regional groundwater (Woods, 1990). The model has been developed and experimentally tested on homogenous soil profiles under steady-state and unsteady evaporation conditions and under isothermal and non-isothermal conditions. However, its assumptions have not been formally tested under conditions of heterogeneous soil profiles although it has been applied in the field under these conditions (e.g. Fontes *et al.*, 1986; Woods, 1990). Barnes and Allison (1983) stated though that the main effect of non-uniformity of soil type would be on the tortuosity (or impedance) value used in the model. This paper does not aim to formally test the assumptions of the model but rather to explore the uncertainty bounds from applying the model to heterogeneous natural soil profiles. We also account for the effects of varying water content and sediment type on solute diffusion, specifically the impedance factor which is a major determinant of effective solute diffusion in soils.

## 2. THE ADVECTION-DIFFUSION MODEL FOR EVAPORATIVE DISCHARGE

The advection-diffusion model accounts for the concentration of a solute (ions or isotopes) through natural soil profiles resulting from steady-state evaporative flux (see example profile in Figure 1). The governing equation can be expressed differently depending on the assumption of the boundary condition defined by either a deep reservoir or a shallow reservoir supplying the evaporative flux. The model developed by Barnes and Allison (1983) used the following formulation:

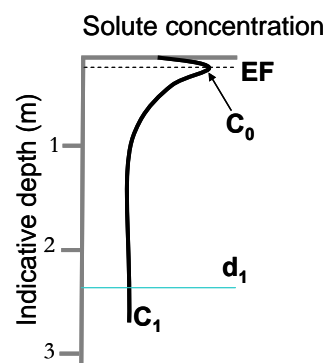
$$C(z) = (C_0 - C_1) \exp\left[-\frac{E}{D}z\right] + C_1 \quad \text{Equation 1}$$

Where  $C(z)$  is the concentration at some point with modified depth  $z$  in the profile,  $C_0$  is the concentration of the solute at the evaporation front,  $C_1$  is the concentration of the solute at the reservoir at depth,  $E$  is the steady-state evaporation rate and  $D$  is the mean diffusion coefficient. At steady-state, the plot of  $\ln[(C(z)-C_1)/(C_0-C_1)]$  versus  $f(z)$  should be linear with slope of  $E/D$  (see explanation of  $f(z)$  in the next section and Equation 4). Woods (1990) showed that this formulation assumes that the depth of the evaporation front is set at zero and that the bottom boundary ( $d_1$  - depth of the reservoir,) is set at infinity. This latter condition is considered by Woods (1990) to represent that the reservoir depth is deep enough not to affect the shape of the concentration profile in the unsaturated zone (i.e. where  $C(z)$  no longer changes with depth).

In the case of a shallow bottom boundary and still setting the evaporation front depth as zero, Woods (1990) derived the following ‘shallow reservoir’ formulation of the model:

$$C(z) = (C_0 - C_1) \frac{|\exp[-\frac{E}{D}z] - \exp[-\frac{E}{D}d_1]|}{1 - \exp[-\frac{E}{D}d_1]} + C_1 \quad \text{Equation 2}$$

Within these equations, the only unknown after collection of the soil profile data is  $E$ . The parameters  $C_0$ ,  $C_1$  and  $d_1$  form boundary conditions for the model. The diffusion coefficient  $D$  is a function of the water content and soil type through the profile.



**Figure 1.** Example of a solute concentration profile with depth typical of evaporative flux from the water table (at depth  $d_1$ , concentration  $C_1$ ) with an evaporation front located at EF with soil water concentration  $C_0$ . Note that the top of the profile is at the ground surface.

When well defined, the boundary condition parameters are independent of the diffusion coefficient of the profile. However, in field soil profiles, there can be some uncertainty in the position of the evaporation front and depth to the reservoir that results in considerable variation in the average value of  $D$  for the profile. Uncertainty in the position of the evaporation front and depth to the reservoir also introduces some uncertainty in the values used for  $C_0, C_1$ .

An alternative equation for evaporative flux from groundwater is a power approximation based upon the one dimensional solution to the steady state unsaturated flow equation (Gardner 1958; Gowing *et al.* 2006). This equation (3) relates the maximum upwards, evaporation-driven flux from the water table ( $q$ ) to the depth of the water table ( $z_w$ ) and depth of the evaporation front ( $z_{ef}$ ) using parameters ( $A, p$ ) related to soil profile properties:

$$q = \frac{A}{(z_w - z_{ef})^p} \quad \text{Equation 3}$$

### 3. FIELD DATA

The effects of different parameters and boundary condition on the results of the advection-diffusion model are illustrated using field data collected from groundwater discharge zones around the southern margins of the Great Artesian Basin in South Australia. In total, soil profile samples were obtained from 28 shallow boreholes in a variety of locations. Selected samples from each profile were analysed for chloride and isotope ( $\delta^{18}\text{O}$ ) concentration and volumetric soil water content ( $\theta$ ). Data from one borehole (FINN01) are used to illustrate the effects of differing parameter values and boundary conditions on the advection-diffusion model. The FINN01 data show that chloride concentration exceeded the halite solubility threshold ( $[\text{Cl}]=190 \text{ gL}^{-1}$ ) between 0.2-0.3 m depth and that the peak  $^{18}\text{O}$  value occurs in this interval (Figure 2). In addition, there is a large increase in the soil water content below this interval. These values indicate the evaporation front occurs between 0.2-0.3 m depth. This also coincides with a lithological boundary at 0.3 m between overlying unconsolidated sands and gravels (from surface to 0.3 m) and the Bulldog Shale, a consolidated mudstone of marine origin that forms the main aquitard to the GAB artesian aquifers (from 0.3 m to end of hole at 2.1 m). Unconfined groundwater was not intersected in this borehole (final depth of 2.1 m) but as the borehole was located within a few hundred metres of artesian springs, the groundwater table is expected to be shallow (*i.e.* <5 m deep). In the discharge zones the unconfined water table is often developed in the fractured upper section of the Bulldog Shale.

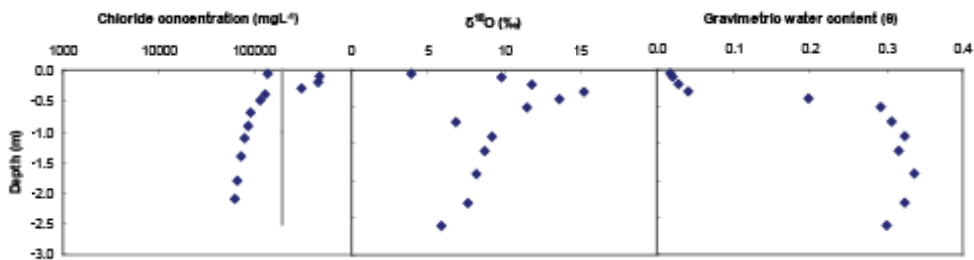


Figure 2. Chloride and oxygen isotope concentrations and gravimetric water content for borehole FINN01

### 4. PARAMETERS AND BOUNDARY CONDITIONS

#### 4.1. Diffusion coefficient

Barnes and Allison (1983) introduced a modified depth function ( $f(z)$  – see Equation 4) to account for the effects of variably saturated soils on the mean diffusion coefficient ( $D_s$ ) of the profile. This function calculates a modified length of each sample interval ( $z'$ ), based on the measured sample interval ( $z$ ) and its water content ( $\theta$ ), so that the whole profile, integrated over the interval between the evaporation front ( $z_{ef}$ ) and bottom boundary ( $z_b$ ), may be represented by a single representative water content ( $\bar{\theta}$ ) determined so that overall length of the modified depth profile remains the same as the measured depth profile.

$$f(z) = \bar{\theta} \int_{z_{ef}}^{z_r} dz' / \theta \quad \text{Equation 4}$$

$$D_s = \theta \omega D_0 \quad \text{Equation 5}$$

The effective diffusion coefficient,  $D_s$ , for a sample interval is given in (5), where  $D_0$  is the self-diffusion coefficient of the tracer (i.e. diffusion coefficient of water in the absence of a chemical potential gradient),  $\theta$  is the water content of that interval and  $\omega$  is the impedance factor. When the advection-diffusion model was developed, only limited assessments of  $D_s$  values for various soil types and moisture contents were available and a constant impedance factor was used throughout the profile. For instance, Allison and Barnes (1985) used a tortuosity value of 0.66 for the impedance factor, as defined by Penman (1940), which accounts for the diffusion of gases through soil and is only appropriate for isotope profiles. However, the impedance factor is more correctly used in the effective diffusion coefficient relationship through soil water as it incorporates geometric effects on diffusion (i.e. tortuosity) but also other effects related to the connectivity of pores and surface phenomena (e.g. electrostatic and viscous effects). Woods (1990) extensively reviewed the literature of impedance factors and found that a range of values have been used to represent  $\omega$  and that it also varied with porosity or water content. Woods (1990) used a value of 0.5, with an uncertainty of  $\pm 0.2$ , to represent profiles with clay dominant soils. Subsequent reports of solute diffusion in variably saturated media (e.g., Conca and Wright (1990, 1992); Olesen et al. (2001)) has meant bulk diffusion coefficients for each sample interval can be calculated. Here, the constant slope impedance factor (CSIF) method is used (Olesen et al., 2001) as shown in (6). The CSIF method allows the determination of the impedance factor ( $\omega$ ) that relates  $D_s$  to the self-diffusion coefficient of the tracer ( $D_0$ ) and water content ( $\theta$ ) for each sample interval, from soil textural properties. The threshold water content  $\theta_{th}$  is the water content at which flow paths become discontinuous and diffusion effectively ceases. The values adopted for each soil type encountered in this study, based on field descriptions, are presented in Table 1.

$$\omega = \frac{D_s / D_0}{\theta} = 1.1(\theta - \theta_{th}) \quad \text{Equation 6}$$

The modified depth function is further extended here (7) to include variation in the tracer diffusion coefficient resulting from changes in water content and soil textural properties, rather than just water content. In (7),  $D_s$  is the effective diffusion coefficient for each sample interval and  $\bar{D}_s$  is the weighted average bulk diffusion coefficient calculated so  $f(z)$  at  $z_r$  approximates the actual depth of  $z_r$ .

$$f(z) = \bar{D}_s \int_{z_{ef}}^{z_r} \frac{dz'}{D_s} \quad \text{Equation 7}$$

The diffusion coefficient and evaporation estimate are linearly related (see (1)). The revised method of calculating the diffusion coefficient results in significant decreases in these values compared to the original formulation of Barnes and Allison (1983). Relative to the Penman tortuosity value previously used, the CSIF method resulted in reductions in the mean effective diffusion rates of between 70-96% in field soil chloride profiles.

Table 1. Threshold water contents adopted for soils based on field descriptions.

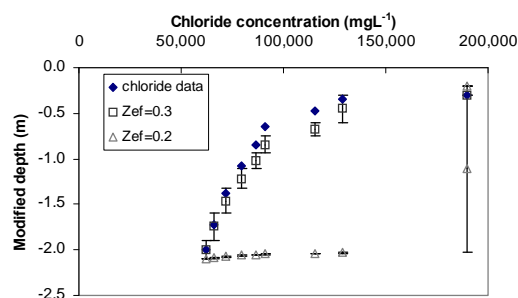
Soil Type	$\theta_{th} \pm \text{std. dev.}$	Data set	Reference
Clay	$0.17 \pm 0.05$	Clays and silty clays (n=5)	Olesen et al. (2001)
Loam	$0.11 \pm 0.03$	Sandy, silty and clayey loams (n=12)	Olesen et al. (2001)
Sand	$0.07 \pm 0.02$	Loamy sands and sands (n=5)	Olesen et al. (2001)
Gravel	0.02	Maximum values for river gravels (n=2)	Conca and Wright (1990) <sup>1</sup>

<sup>1</sup>determined following Olesen et al. (2001)

### 4.2. Evaporation Front

In this study, the evaporation front is considered to occur in the depth interval with chloride concentrations in excess of halite solubility ( $190 \text{ gL}^{-1} [\text{Cl}]$ ), and which is underlain by chloride concentrations below that threshold. It may otherwise be defined as occurring in the depth interval with the maximum isotope value. In general, the position of the evaporation front is well-defined for a given solute but broad peaks, or variation between peak positions defined by different solutes (discussed below) can introduce some uncertainty to this boundary condition. Defining the position of the evaporation front can have a large influence on the calculation of the mean diffusion coefficient and hence on the modelled evaporation rate. In the study area, the evaporation front condition was found to occur at depths from the surface (0.00-0.05 m) to a maximum depth of 0.75 m (0.65-0.75 m) in profiles showing probable steady state conditions. Out of 21 boreholes showing both chloride and  $\delta^{18}\text{O}$  evaporative discharge profiles, the evaporation front threshold concentration occurred in the same interval for six profiles, while the peak  $\delta^{18}\text{O}$  interval immediately underlay the chloride threshold in five profiles. For five profiles the oxygen isotope ( $\delta^{18}\text{O}$ ) peak interval overlay the chloride peak concentration by at least one 0.1 m interval. In only one profile was the  $\delta^{18}\text{O}$  peak interval clearly deeper than the chloride threshold by more than one interval. Gowing *et al.* (2006) reported that in experimental soil columns the zone of salt accumulation occurred up to 0.06 m below the evaporation front (defined as the change from liquid + vapour transport to vapour only transport) and occurred in the transition zone of vapour + liquid transport. Given the sampling interval across the continuously sampled upper 0.5 m of the field soil profiles was generally 0.1 m, it is reasonable to take the evaporation front as the upper margin of the sample interval that fulfils the evaporation front criteria, and the uncertainty in the position is only likely to be  $\pm 0.1$  m (i.e. one sampling interval either side).

The effects of the uncertainty of the evaporation front are illustrated using the FINN01 data. The evaporation front is quite well constrained in this borehole (Figure 2) and occurs between 0.2-0.3 m depth but setting the evaporation front at either 0.2 m or 0.3 m has a large effect on the modelled evaporative flux because of the low soil water content in the 0.2-0.3 m interval. Using the CSIF method for the chloride data with the evaporation front at 0.3 m resulted in a mean diffusion coefficient of  $6.42 \times 10^{-3} \text{ m}^2 \text{ y}^{-1}$  while setting the evaporation front at 0.2 m resulted in a mean diffusion coefficient of  $2.84 \times 10^{-4} \text{ m}^2 \text{ y}^{-1}$ . The plot of the chloride concentration data against the modified depth function using the two evaporation front conditions ( $z_{\text{ef}}=0.2$  and  $0.3$ ) shows the very large effect the uppermost sample interval (0.2-0.3 m) has on calculating the mean diffusion coefficient (Figure 3).



**Figure 3.** Chloride concentration data from FINN01 against modified depth function (Eq. 4) using two evaporation front boundary conditions ( $z_{\text{ef}}=0.2$  and  $z_{\text{ef}}=0.3$ ).

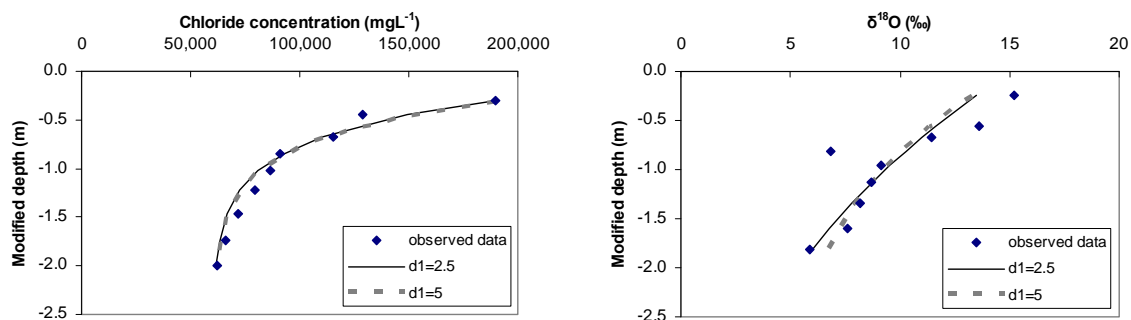
**Table 2.** Modelled results for FINN01 profile with different evaporation front and groundwater reservoir conditions. Groundwater concentrations were estimated based on being less than the lowermost soil profile values and were consistent with unconfined water table values observed in similar GAB discharge areas.

Solute	Evaporation front depth (m)	Reservoir depth (m)	Reservoir concentration (Cl- $\text{mgL}^{-1}$ ; $^{18}\text{O}$ -‰)	Evaporation rate ( $\text{mmy}^{-1}$ )	RMSE (Cl- $\text{mgL}^{-1}$ ; $^{18}\text{O}$ -‰)
Chloride	0.3	2.5	60,000	16.2	23,583
Chloride	0.2	2.5	60,000	19.0	100,179
Chloride	0.3	5.0	60,000	16.3	23,450
Chloride	0.3	5.0	50,000	10.4	38,523
$^{18}\text{O}$	0.2	2.5	4.0	6.6	1.28
$^{18}\text{O}$	0.3	2.5	4.0	25.4	1.44
$^{18}\text{O}$	0.2	5.0	4.0	12.1	1.31
$^{18}\text{O}$	0.2	5.0	0	6.7	1.28

The much lower soil water content of the 0.2-0.3 m interval results in a calculated diffusion coefficient that is nearly two orders of magnitude lower than for the lower part of the profile and so the uppermost interval has a disproportionately large effect on the modified depth profile than if the interval is excluded (i.e. by setting the evaporation front at 0.3 m). In the case of the chloride concentration, the model run with the evaporation front at 0.2 m has a modelled evaporation similar to that using an evaporation front at 0.3 m but with an extremely poor fit between the modelled and observed solute data (see difference in root mean squared error (RMSE) terms in Table 2). For the isotope data, model runs using the different evaporation fronts resulted in significant changes in the modelled evaporation rates with only modest changes in model performance (Table 2). Defining the position of the evaporation front would be improved by finer sampling intervals but this increases analytical costs and isotope extraction can be difficult for relatively dry soils and small sampling volumes.

### 4.3. Groundwater Reservoir

Depth to groundwater is one of the major controlling variables in the steady state discharge equation (3), with increasing depth to groundwater leading to lower evaporative discharges. In contrast, the deep reservoir formulation (1) of the advection-diffusion model implies that beyond some depth, where the concentration gradient no longer changes with depth, the discharge rate is independent of depth to the reservoir. We examine the sensitivity of the shallow reservoir formulation (2) using the FINN01 profile data. As the water table was not intersected in this borehole (final depth of 2.1 m), the discharge rate was calculated using water table depths of 2.5 and 5 m. For both cases, the mean diffusion coefficient was calculated for the length of the sampled profile rather than to the water table, however, this should make little difference to the diffusion coefficient due to the relatively high and uniform water content in the lower profile (Figure 1). The chloride model runs specified the evaporation front at 0.3 m and the isotope model runs at 0.2 m. All other parameters were kept the same for both water table scenarios and the results are shown in Table 2 and Figure 4.



**Figure 4.** Observed and modelled solute data (Cl – left panel;  $\delta^{18}\text{O}$  – right panel) for FINN01 against modified depth function (Eq. 4) using two shallow reservoir boundary conditions ( $d1=2.5$  and  $d1=5$ ).

The chloride model runs indicate that solving the shallow reservoir formulation of the soil profile model by curve-fitting is quite insensitive to the depth of the groundwater reservoir if the soil profile has a long asymptotic section in the sampled part of the unsaturated zone. In contrast, the isotope model runs demonstrate that the modelled discharge is sensitive to the bottom boundary condition when the sampled profile has not approached an asymptotic value with depth. The increase in the modelled discharge rate with the deeper groundwater depth, particularly for the isotope data, is a surprising result given that Equation 3 indicates that the discharge rate should decrease with increasing groundwater depth. It may be that the isotope profile has not reached steady state yet but typically the stable isotopes reach steady state more quickly than the chloride solute because of their faster diffusion rate.

The sensitivity to the concentration of the groundwater reservoir is also dependant on whether the concentration profile is showing asymptotic behaviour with depth. The chloride model run shows that a modest decrease in reservoir concentration results in a significant change in the modelled discharge but at the cost of a decrease in the model accuracy, as shown by the RMSE term in Table 2. The model accuracy continued to decrease as the groundwater concentration was lowered (results not shown). In contrast, model response to the relatively large change in the groundwater isotope concentration was dependant on both groundwater reservoir depth and concentration. At a groundwater depth of 2.5 m, the use of a groundwater isotope value of 0 ‰ resulted in an invalid model fit while at a groundwater depth of 5 m the same concentration resulted in a valid model fit with a discharge rate and RMSE value very close to first isotope

model run ( $d_1=2.5$  m,  $C_1=4$  ‰). The variation in the isotope results is facilitated by the absence of asymptotic behaviour with depth over the sampled interval.

## 5. DISCUSSION AND CONCLUSIONS

The mean diffusion coefficient of the soil profile data used in the advection-diffusion model is dependant on the boundary conditions that set the length of the profile, particularly on the position of the evaporation front. In field soil profiles, there can be some uncertainty in the position of the evaporation front based upon the use of different solutes (e.g. chloride and  $\delta^{18}\text{O}$ ) that result in considerable variation in the mean diffusion coefficient for the profile. The CSIF method for calculating the mean diffusion coefficient is very sensitive to the volumetric water content of the profile, particularly at the top of the profile close to the evaporation front. The effective depth function results in samples substantially drier than lower samples having a large influence on the mean effective diffusion coefficient of the profile and hence on the modelled evaporation rates. The uncertainty in the position of the groundwater reservoir and its concentration has little effect where the lower part of the profile shows an asymptotic trend towards a representative value of groundwater concentration but can vary substantially with different values of groundwater depth and concentration if this is not the case.

These results indicate significant uncertainty in the results from natural, heterogeneous soil profiles and suggest that further work is required in determining the suitability of the advection-diffusion model for these conditions.

## ACKNOWLEDGMENTS

Funding for this research was provided by the Australian Research Council Linkage grant LP0774814 and Discovery grant DP0450334, in conjunction with industry partners BHP-Billiton, Great Artesian Basin Coordinating Committee, Santos Limited and the South Australian Arid Lands Natural Resource Management Board. The second author was supported by a Land and Water Australia Postgraduate Scholarship.

## REFERENCES

- Allison, G. and C.J. Barnes, (1985), Estimation of evaporation from the normally “dry” Lake Frome in South Australia. *Journal of Hydrology*, 78, 229–242.
- Barnes, C.J., and G. Allison, (1983), The distribution of deuterium and  $^{18}\text{O}$  in dry soils, 1. Theory. *Journal of Hydrology*, 60, 141–156.
- Conca, J.L., and J. Wright, (1990), Diffusion coefficients in gravel under unsaturated conditions. *Water Resources Research*, 26 (5), 1055–1066.
- Conca, J.L. and J. Wright (1992). Diffusion and flow in gravel, soil and whole rock. *Applied Hydrology*, 1 (1), 5–24.
- Fontes, J., M. Yousfi, and G. Allison, (1986), Estimation of long-term, diffuse groundwater discharge in the northern Sahara using stable isotope profiles in soil water. *Journal of Hydrology*, 86, 315–327.
- Gardner, W.R. (1958), Some steady-state solutions of the unsaturated moisture flow equation with applications to evaporation from a watertable. *Soil Science*, 85, 228–332.
- Gowing, J.W., F. Konukcu, and D.A. Rose, (2006), Evaporative flux from a shallow watertable: The influence of a vapour-liquid phase transition. *Journal of Hydrology*, 321, 77–89.
- Olesen, T., P. Moldrup, T. Yamaguchi, and D. Rolston, (2001), Constant slope impedance factor model for predicting the solute diffusion coefficient in unsaturated soil. *Soil Science*, 166 (2), 89–92.
- Penman, H.L. (1940), Gas and vapour movements in the soil. I. The diffusion of vapours through porous solids. *Journal of Agricultural Science*, 30, 437–462.
- Woods, P. (1990), *Evaporative discharge of groundwater from the margin of the Great Artesian Basin near Lake Eyre, South Australia*. Ph. D. thesis, Flinders University, South Australia.
- Zimmermann, U., D. Ehhalt, and K.O. Munnich, (1967), Soil-water movement and evapotranspiration: changes in the isotopic composition of the water. In *Proc. Symp. Isotopes in Hydrology*, Vienna, pp. 567–584. IAEA.