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Scientific Notebook No. 813: Validation of Hydrus (07/26/2006 through 09/03/2007)

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Gary R Walter On 7/26/06

Investigator - Gary R. Walter

Project 20.06002.01.262

This notebook contains information and calculations used in the validation of the program ~~HYRRU~~ HYDRUS

On 7/26/06

When the milestone was originally formulated, it was anticipated that ~~HYRRU~~ Hydrus-2D would be validated.

On 7/26/06

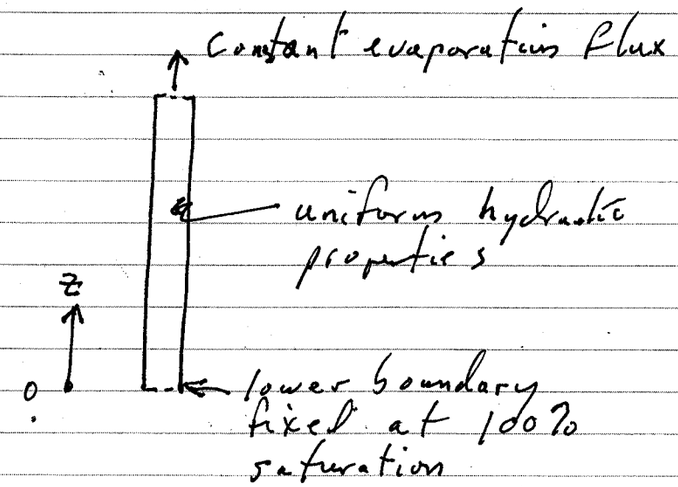
Hydrus-2D is no longer available and the validation was performed on Hydrus 2D/3D version Beta.03 obtained from PC-Progress s.r.o, Anglická 28, Prague, Czech Republic

The program is installed on Mage

8/2/06 Gary Walters

Validation Test Case 1

This test case is a comparison of Hydrus results with an approximate solution for steady flow through a vertical soil column subject to constant evaporation at its surface, as illustrated below



The approximate distribution of tension head is taken from

G. D. Salvucci. 1993. An approximate solution for steady vertical flux of moisture through an unsaturated homogeneous soil. Water Resources Research V. 29, No 11 pp 3749-3753

8/2/06 Gary

Based on Salvucci, the tension head distribution is given by

$$\frac{z}{\psi_1} = \frac{1}{1+q'}\left[\frac{q'}{1+q'} + \left(\frac{\psi}{\psi_1}\right)^{-n}\right]^{-1/n} \qquad (1)$$

where z is the vertical coordinate (cm)

ψ_1 is the bubbling head (cm)

$q' = q/K_s$

q is the specified flux (cm/s) and positive for evaporation

K_s is the saturated hydraulic conductivity (cm/s)

ψ is the tension head a z (cm)

n is an empirical coefficient used to describe the variation of hydraulic conductivity with tension head

$$K(\psi) = \frac{K_1}{1 + [\psi/\psi_1]^n} \qquad (2)$$

8/2/06 Cr

Eq'n (2) can also be written as

$$\frac{K(\psi)}{K_1} = \frac{\psi_1^n}{\psi_1^n + \psi^n} \qquad (3)$$

When $\psi_1 << \psi$ (note that ψ_1 and ψ are > zero in Saluucci's formulation)

Eq'n (3) can be approximated by

$$\frac{K(\psi)}{K_1} = \left(\frac{\psi_1}{\psi}\right)^n \qquad (4)$$

which is analogous to the Brooks-Corey equation used in Hydrus

$$\left(\frac{\psi_1}{\psi}\right)^n = \left(\frac{\psi_0}{\psi}\right)^{2+3m} \qquad (5)$$

where ψ_0 is the "air entry value" assumed to equal the bubbling pressure

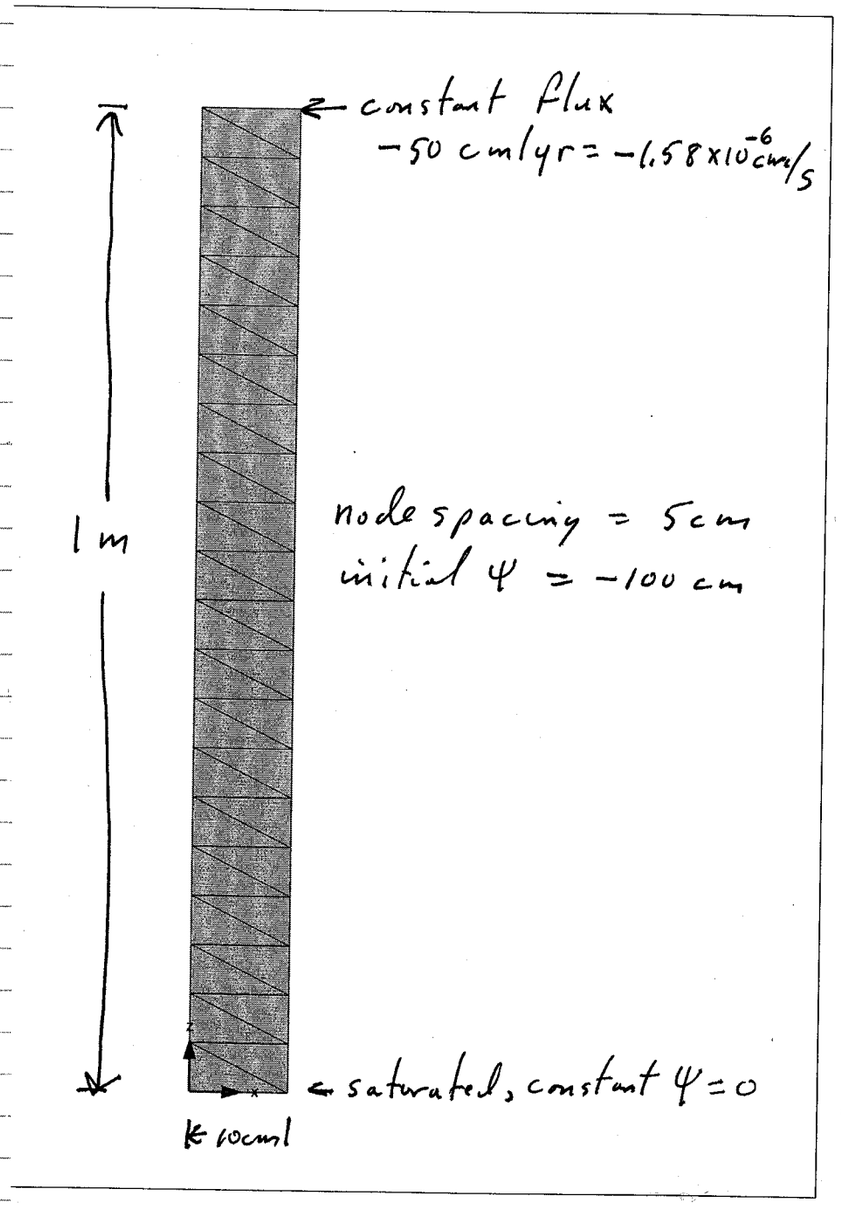
8/2/06 Cr

Thus from (5)

$$m = \frac{n-2}{3}$$

Eq'n (1) is implemented in the spreadsheet saluucci.xls. in directory hydrus\validation. Hydrus simulations were run using 1-d grid (actually 2 nodes wide because Hydrus requires at least a 2-d grid) with geometry illustrated on page 6.

On 8/2/06



8/2/06 On

Two Hydrus simulations were run, one using standard properties for a clay-loam and one for sandy loam that are provided with Hydrus. These properties are listed below

	$K_1 = K_{sat}$ (cm/s)	$\psi_1 = \psi_0$ (cm)	Salvucci n	Brooks-Corey m
clay loam	6.39×10^{-5}	25.9	2.582	0.194
sandy loam	7.19×10^{-4}	14.7	2.966	0.322

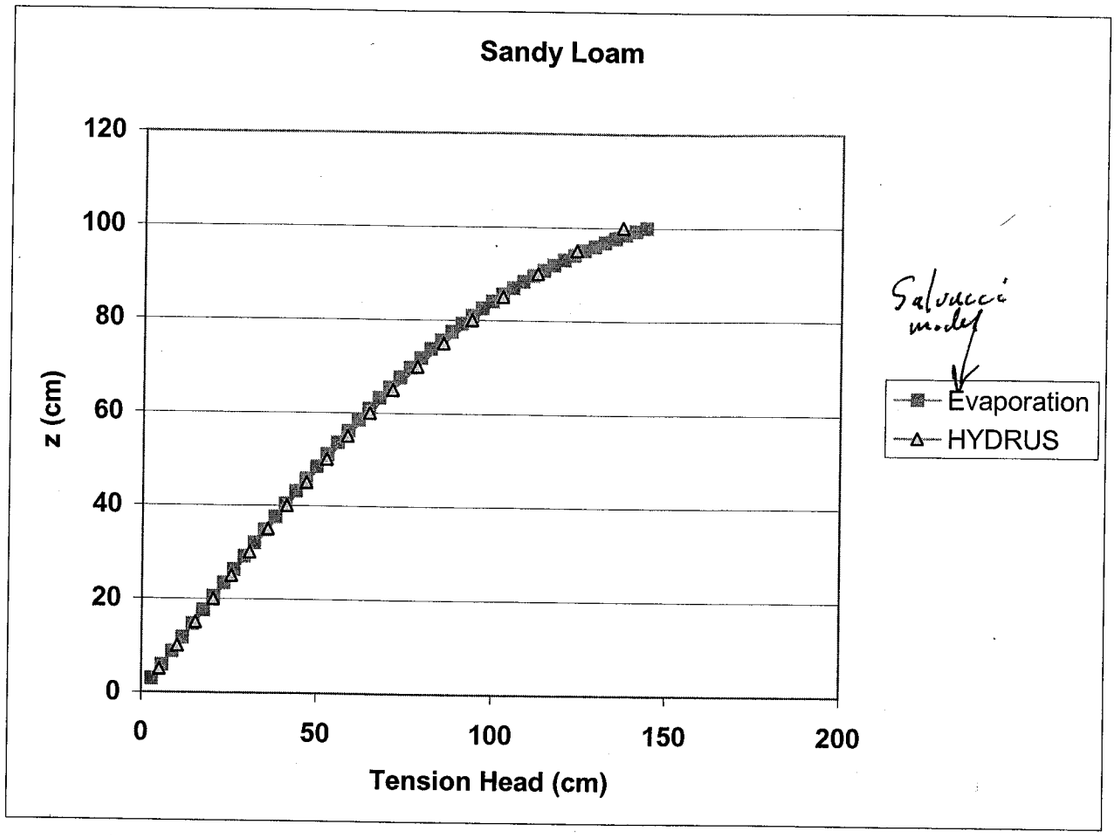
In both cases, the evaporative flux at the upper boundary of the Hydrus grid was held steady at −50 cm/yr ≡ -1.58×10^{-6} cm/s. The simulations were run for 8.64×10^5 seconds to establish steady conditions. The Hydrus input/output files are in directories

H3D_1-d salvucci clay loam

H3D_1-d salvucci sandy loam

8/2/06 CR

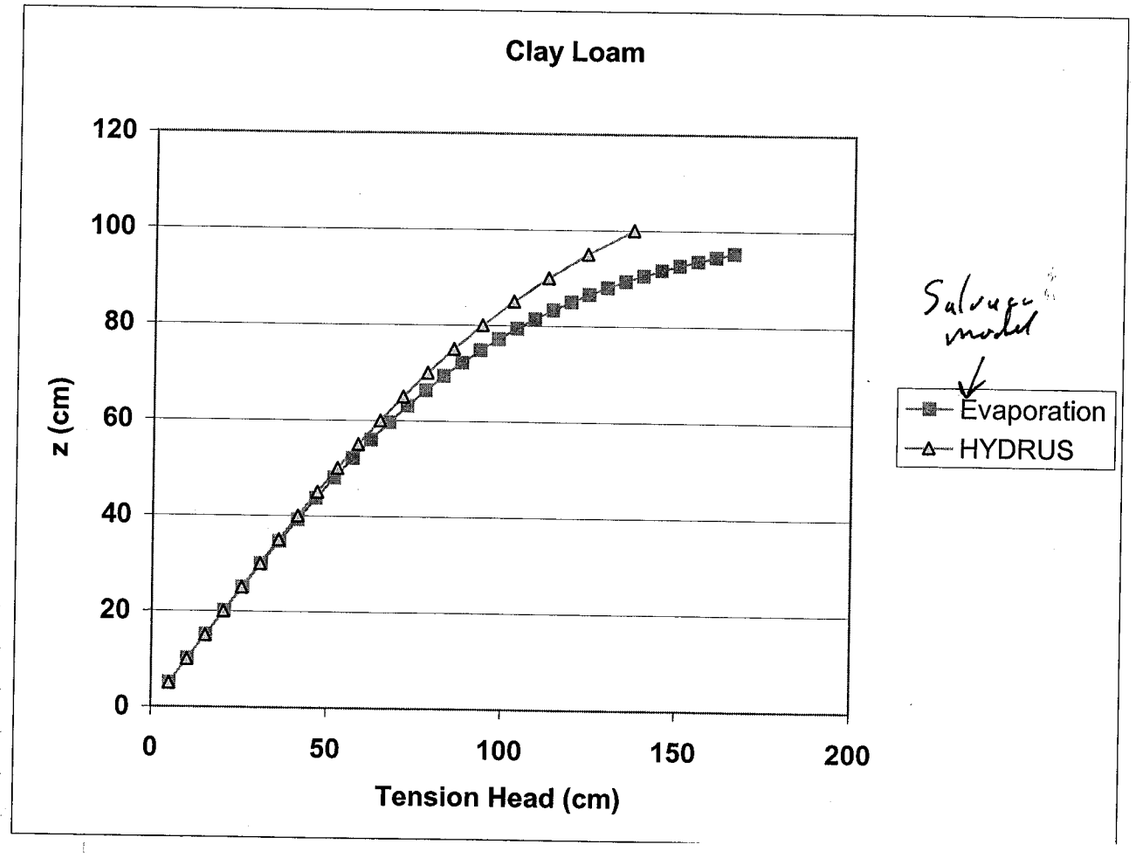
The results of the sandy loam simulation are shown below. The Hydrus results agree quite well with the analytical



model calculations.

8/2/06 CR

The results of the clay loam simulations are shown below. Hydrus agrees well with the Salvucci solution at low tensions



but deviates at higher tensions. This is consistent with Salvucci's finding and is consistent with the approximations in his

8/2/06 OR

analytical model. Thus, Hydrus passes Test 1

8/03/06 OR

Test 2 Simulation of transient flow around a landmine

This test is based on results reported by J. B. Rhebergen, H. A. Lensen, P. B. W. Schwering, G. R. Morin and J. M. H. Hendrickx,

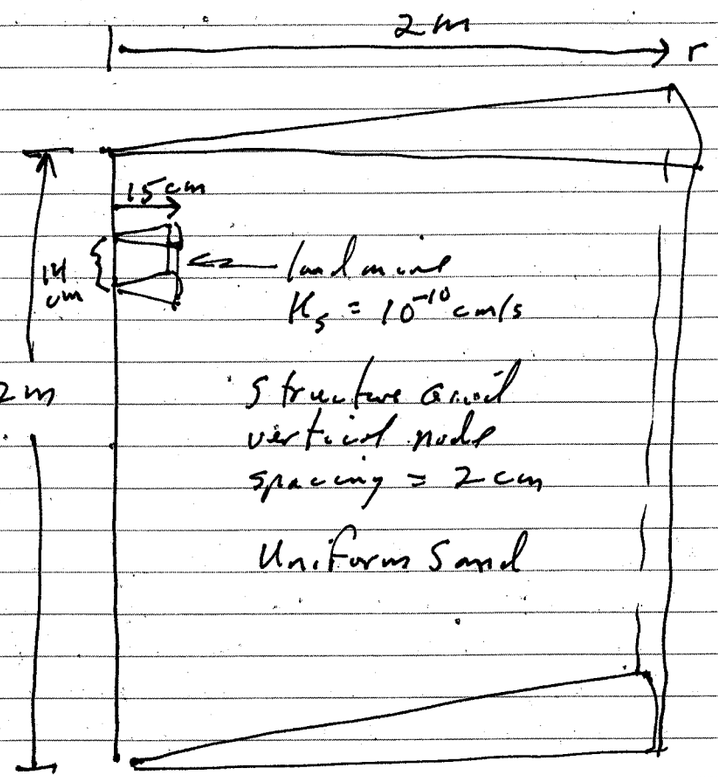
"Soil moisture distributions around landmines and the effect on relative permittivity."
Third Demining Technologies Information Forum, Ispra, Italy
September 24-25, 2002
maica.jmu.edu/dtif/Conferences/Ispra2/papers/~~rot~~ rhebergen2.pdf
OR 8/3/06

Rhebergen et al. used Hydrus 2D to simulate flow and water content near a buried landmine. Because all aspects of their simulations are not fully specific, the ~~HYR~~ OR 8/3/06

the HYDRUS results performed here will only be qualitatively compared with those of Rhebergen et al.

8/3/06 GW

The Hydrus simulation was performed using a radially symmetric 2-D grid as illustrated below



The landmine was represented as a zone of very low saturated hydraulic conductivity sand $K_s = 10^{-10}$ cm/s

The rest of the domain was ~~repren~~ GW 8/3/06 represented as sand using the van Genuchten model

8/3/06 GW

Default hydraulic properties from Hydrus were assigned to the sand

residual ~~saturation~~ GW 8/3/06 water content = 0.045

saturated water content = 0.43

$\alpha = 0.145$

van Genuchten exponent = 2.68

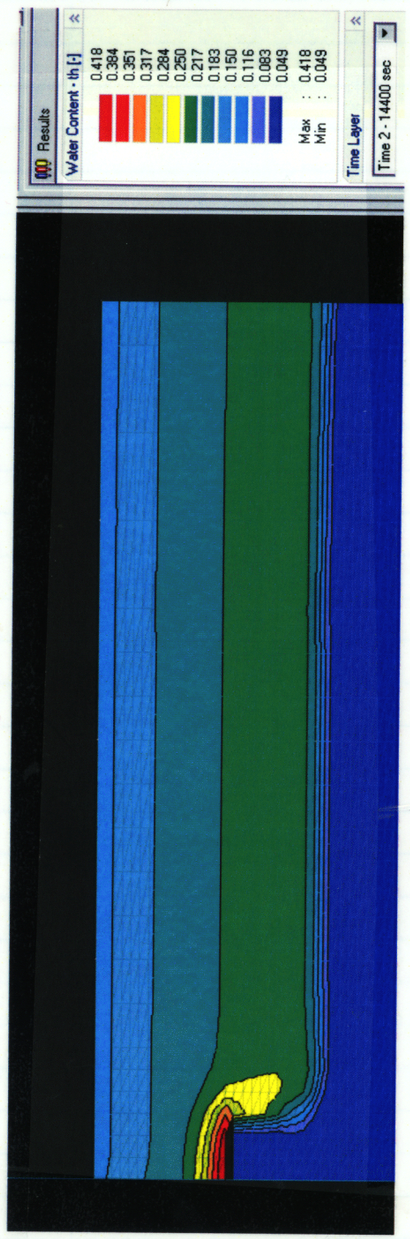
$K_s = 8.25 \times 10^{-3}$ cm/s

The simulation was started with an initial tension head of −100 cm through the model.

80 mm of water was applied to the upper model boundary for 1 hour ~~sta~~ GW 8/3/06 starting the 2nd hour of the simulation and ending at the start of the 3rd hour.

Water content was monitored at nodes on the left model boundary at depths of 10 cm, 28 cm, and 46 cm

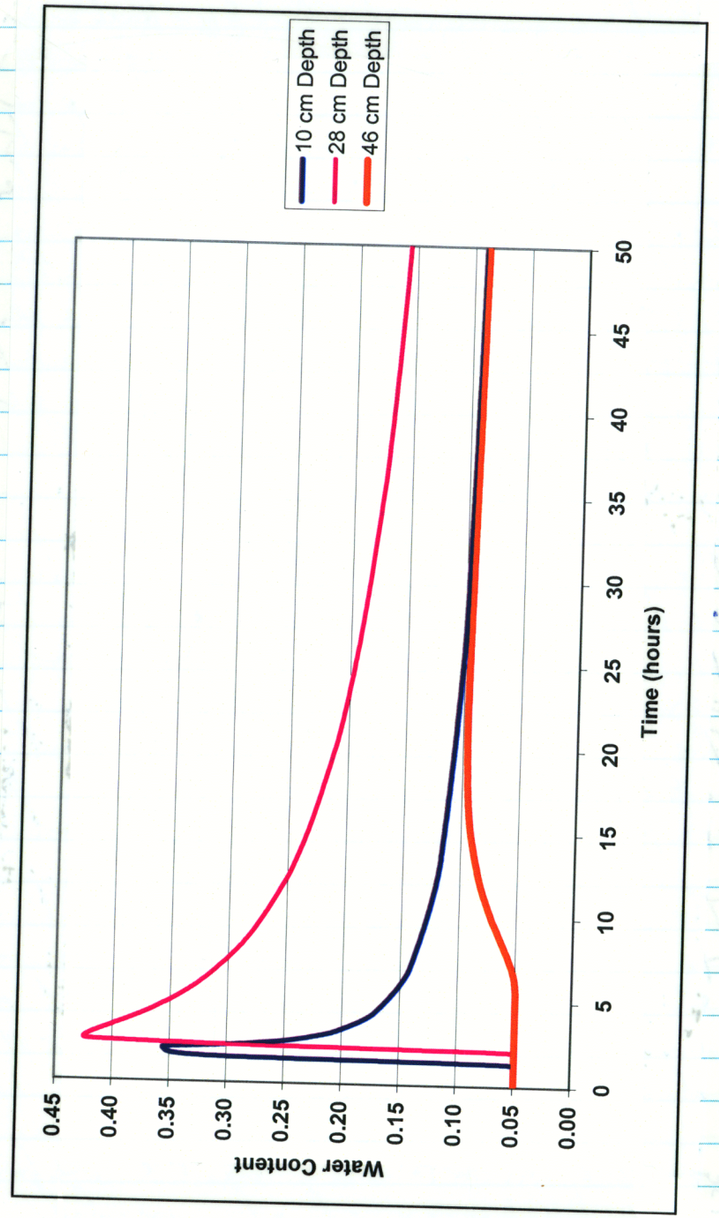
8/3/06 a



The illustration to the left shows the water content distribution after 4 hrs. The distribution is reasonable and shows the "shadowing" effect of the mains

Time histories of water content at the observation nodes are shown in the graph on p.15

8/6/06 a



8/3/06 a

The Hydrus results are consistent with but slightly different from those reported by Rhebergen et al

For the 10 cm observation point, the peak in the water content curve occurs immediately after the onset of water application and has a value of about 0.35, consistent with Rhebergen et al. After 48 hours, however, the water content approaches 0.09 as opposed to 0.15 as reported by Rhebergen et al. 8/3/06 a

The peak of the 28 cm water content occurs slightly later than the 10 cm curve, reasonable and consistent with Rhebergen et al. The 28 cm curve peaks at about 0.43 as opposed to 0.35 reported by Rhebergen et al

The 46 cm curve doesn't start to rise until about 6 hrs into the simulation. Rhebergen et al indicated their 45 cm curve didn't increase until about 11 hrs.

Given the uncertainties in the details of the Rhebergen et. al. model, the results of my simulation indicate that HYDRUS is producing reasonable results.

8/5/06 a

All input and output from the Test 2 simulations are contained in the directory "H3D-landmine"

The water content time histories are tabulated in the spreadsheet "landmine-observation-Nodes-Water-Content.xls"

8/14/06 [illegible]

Validation of HYDRUS against 1-D transport solution. The analytic solution used to check the Hydrus solution is that given by Javandel, I., Doughty C. and C-F Tsang ~~Hon~~ Groundwater Transport: Handbook of Mathematical Models. American Geophysical Union Water Resources Monograph 10

Ca 8/14/06

The specific solution used is Javandel et al. eqn (41) pp 16-17 for flow through a semi-infinite column with constant input concentration

The solution is given on p. 19 of this notebook with the retardation factor assumed to be 1

8/14/06 Ca

$$\frac{C(x,t)}{C_0} = \frac{v}{v+\beta}\exp\left\{\frac{x(v-\beta)}{2\delta v}\right\} erfc\left[\frac{xv-\beta t}{2(\delta v t)^{1/2}}\right] + \frac{v}{v-\beta}\exp\left\{\frac{x(v+\beta)}{2\delta v}\right\} erfc\left[\frac{xv+\beta t}{2(\delta v t)^{1/2}}\right]$$
$$+ \frac{v^2}{2\delta\lambda}\exp\left\{\frac{x}{\delta} - \lambda t\right\} erfc\left[\frac{xv+\beta t}{2(\delta v t)^{1/2}}\right]$$

~~(7) is above~~ Ca 8/14/06

where $C(x,t)$ is the concentration at distance x from the upstream boundary and time t,

C_0 the upstream concentation,

v is the fluid pore velocity [cm/s],

θ is the water-filled porosity,

δ is the hydrodynamic dispersivity [cm],

λ is the decay rate [1/s].

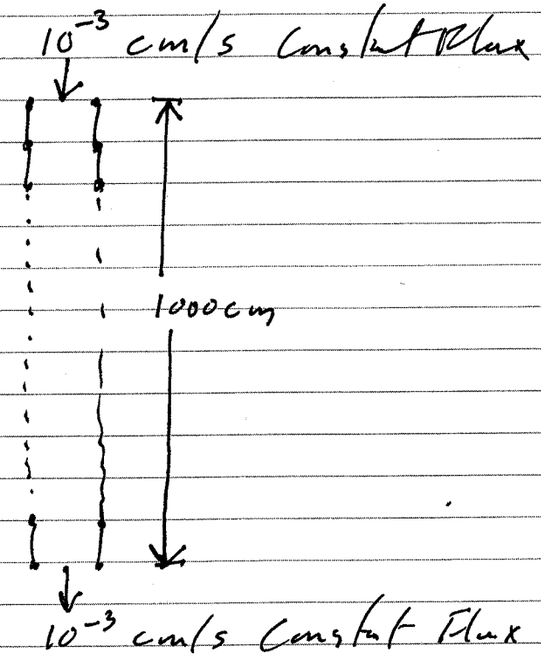
and

$$\beta = (v^2 + 4\delta v\lambda)^{1/2} \quad (8)$$

The Javandel solution is implemented in the spreadsheet javandel.xls. The Hydrus simulation was performed using a quasi-1D vertical grid with uniform properties. The input files are in directory H3D_1-d transport

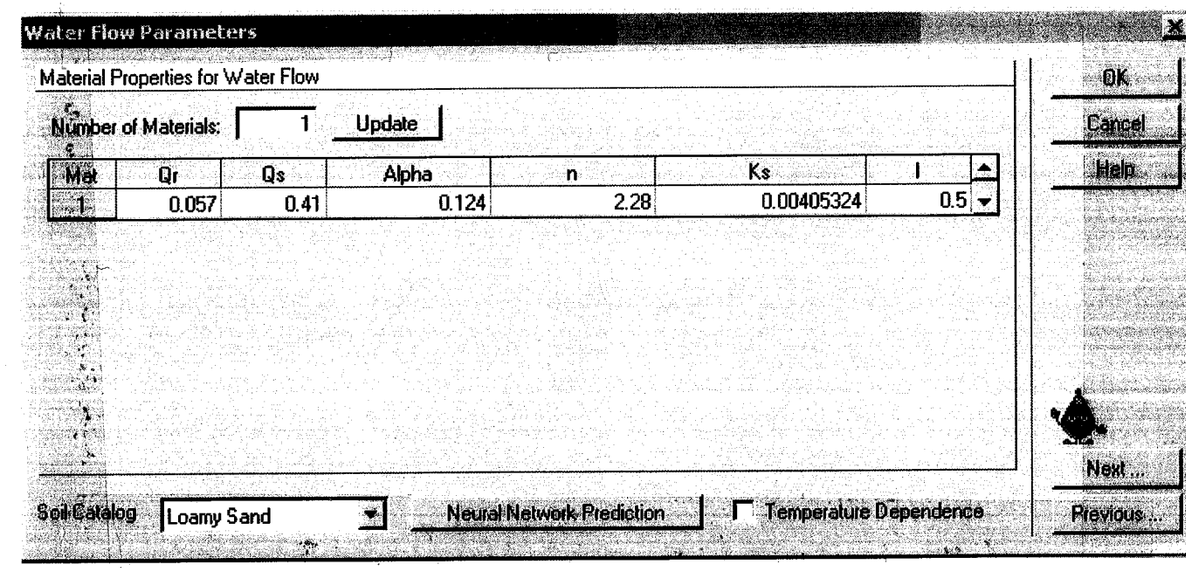
7/14/06 CW

The Hydrus grid was 2 nodes wide and 100 nodes long as illustrated below



The hydraulic properties assigned to the model were the default properties for a sandy loam using the van Genuchten model from Hydrus (see print out p. 21)

7/14/06 CW



Mat	Qr	Qs	Alpha	n	Ks	l
1	0.057	0.41	0.124	2.28	0.00405324	0.5

q_R is the irreducible water content

q_s is the saturated water content

Alpha is the Van Genuchten α or bubbling pressure [1/cm]

K_s is the saturated hydraulic conductivity [cm/s]

and n is the empirical exponent

8/14/06 Cw

The Hydrus simulation was first run to establish a steady water content consistent with the specified boundary fluxes. This water content was 0.352. This value was then assigned as the initial value to all nodes in the model and the simulation was restarted with a constant concentration of 1.0 assigned to the upper boundary using the "Third Type" boundary condition which is the Cauchy boundary condition. Simulations were run with a dispersivity of 1 cm and no decay using each of the three solution methods provided in Hydrus. These are:

8/14/06 Cw

1. Conventional Galerkin Finite Element
2. An upstream weight finite element formulation
3. A Galerkin finite element formulation with artificial dispersion.

These methods are described in the Hydrus technical manual.

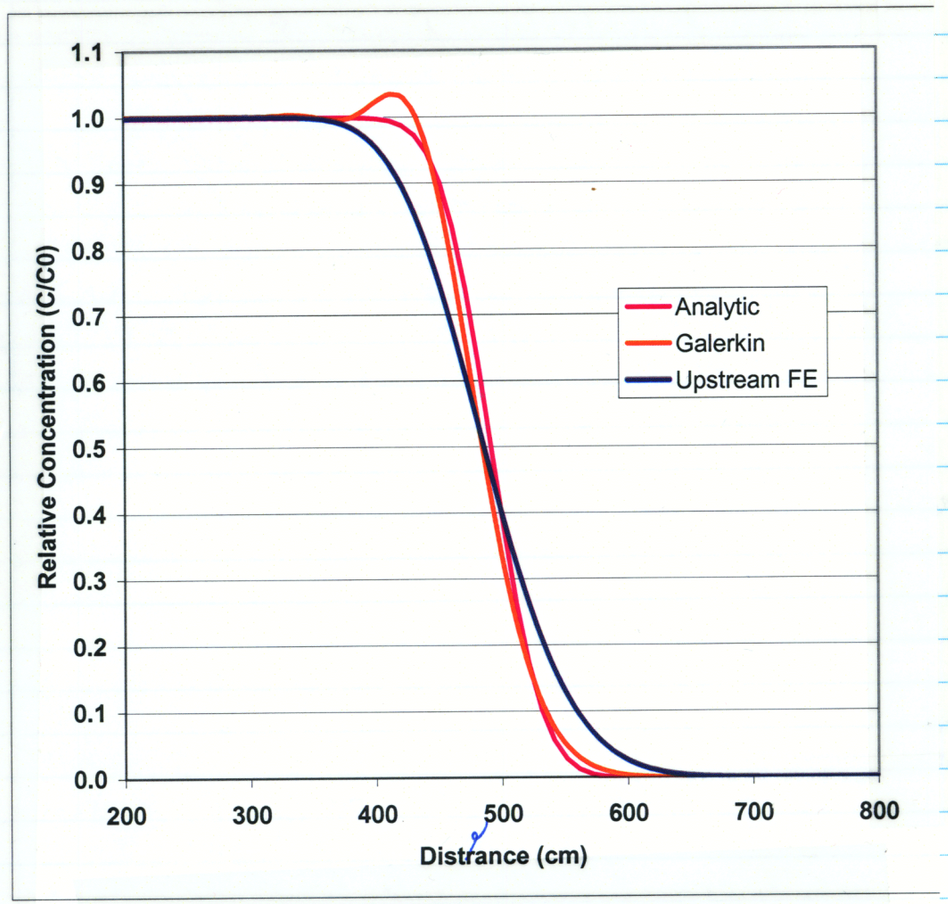
The Hydrus results were extracted using the cross-section tool into the following files at time = 172800 seconds

1-dtransport_Concentration_galerkin_-_172800_sec.txt
1-dtransport_Concentration_UpStrmFE_-_172800_sec.txt
1-dtransport_Concentration_GFEartdisp_-_172800_sec.txt

The results of the method 3 simulations were practically identical to those for method 2. The results are compared to the analytic solution in the graph on page 24

8/14/06 AW

Comparison of Hydrus results to analytic solutions



The results are consistent with expectations with the Galerkin method ~~match~~ matching the

AW 8/14/06

8/14/06 AW

the analytic solution reasonably well between relative concentrations of 0.9 and 0.1 but displaying an oscillation ($C/C_0 > 1$) at $C/C_0 > 0.9$. Methods 2 and 3 display numerical dispersion but not oscillations, as would be expected.

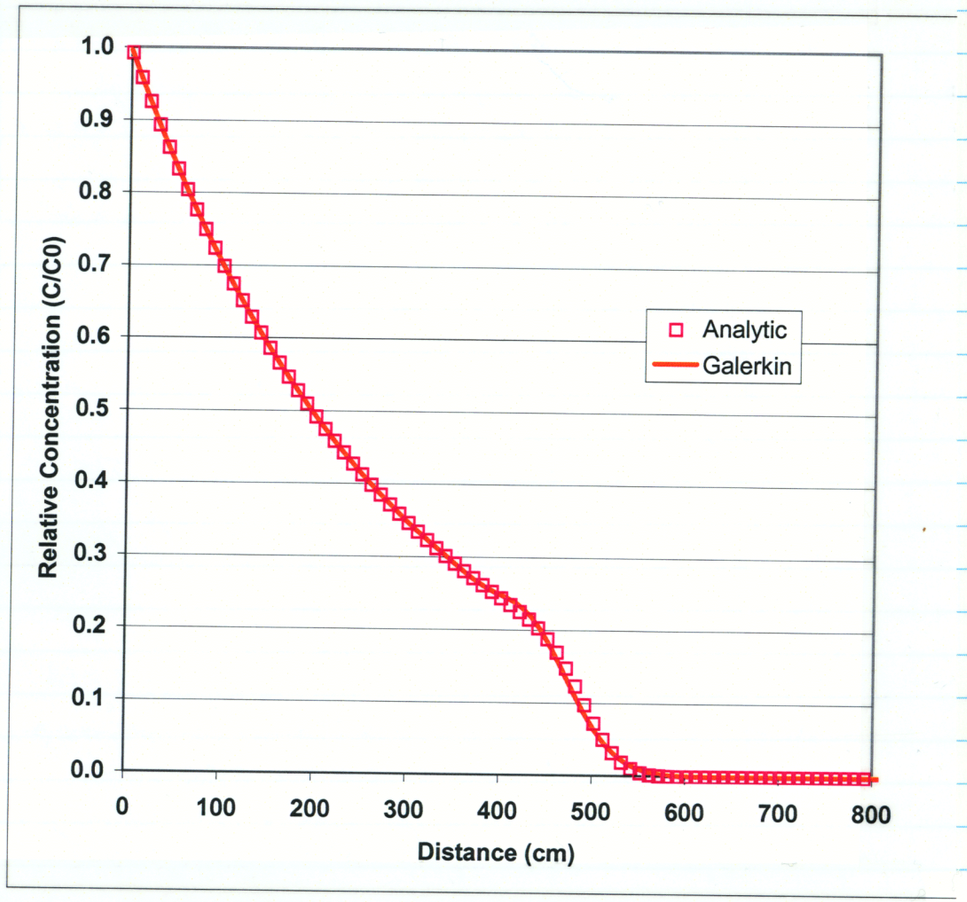
A simulation was then run with the 1st order decay rate set to 1×10^{-5} 1/s using the Galerkin method. The results are in

1-d transport_concentration_decay_178200sec.txt

The Hydrus results are compared to the analytic solution on p. 26 and p. 27 and agree very well.

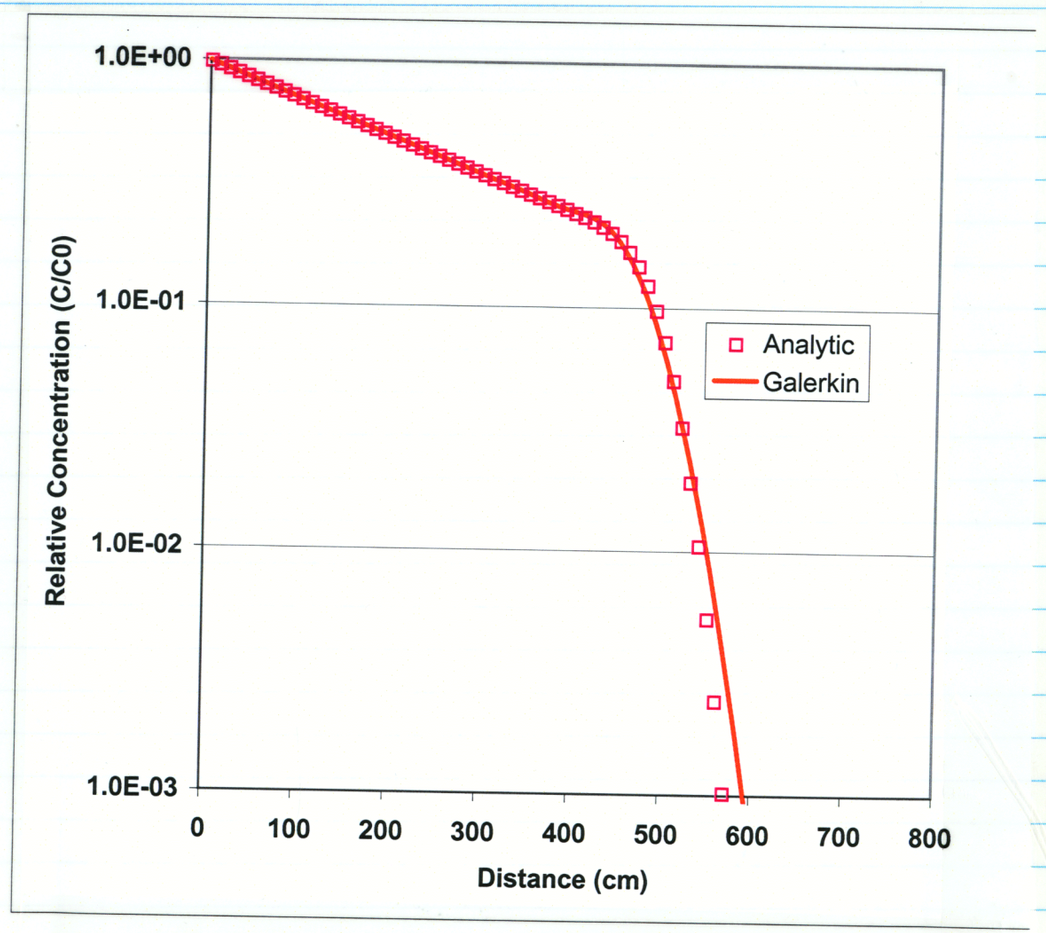
8/14/06 Cw

Comparison of Hydrus solution to 1-d analytical solution, decay ~~rate~~ constant = 1×10^{-5} 1/s



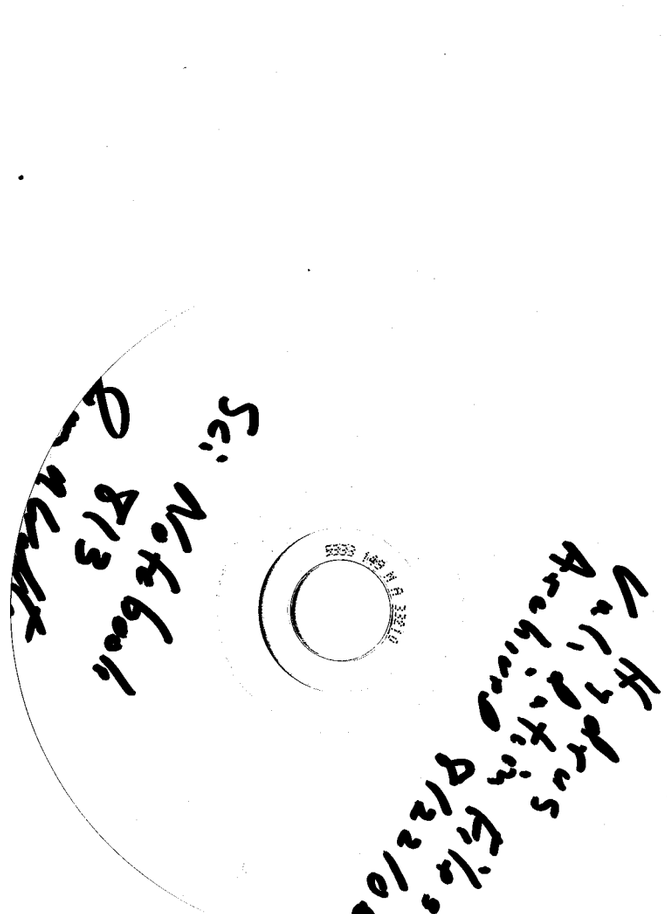
8/14/06 Cw

Comparison of Hydrus to analytical solution, decay constant = 1×10^{-5} 1/s



8/22/06 [signature]

The attached CD contains input/output files for Hydrus Validation as of this date



9/3/07 [signature]

I am submitting this note book for closure

ADDITIONAL INFORMATION FOR SCIENTIFIC NOTEBOOK NO. 813

Document Date:	08/22/2006
Availability:	Southwest Research Institute® Center for Nuclear Waste Regulatory Analyses 6220 Culebra Road San Antonio, Texas 78228
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File Types: (.exe, .bat, .zip, etc.)	xls, jpg, gif
Remarks: (computer runs, etc.)	Media contains: Input/output files for Hydrus

GEOSCIENCES AND ENGINEERING DIVISION

SCIENTIFIC NOTEBOOK REVIEW CHECKLIST RECORD

Scientific Notebook No. ___ 813 ____Project Numbers: ____20.06002.01.262._____

Accomplished

✓ RL	1. Initial entries per QAP-001
✓ RL	2. Dating of entries
✓ RL	3. Corrections (crossed out, one line through w/initials/date)
✓ RL	4. No White out used
✓ RL	5. Page number visible on copy or original notebook
✓ RL	6. In process entries per QAP-001
✓ RL	7. Figure information present
✓ RL	8. Text readable
none	9. Copyrighted material is identified
✓ RL	10. Permanent ink or type only
✓ RL	11. Signing of entries (not required on each page)
✓ RL	12. Electronic media in the scientific notebook properly labeled
✓ RL	13. NRC Supplementary Scientific Notebook Questions are addressed.
✓	14. The independent, two person verification required by AP-019, Section 5.2.1.2(b) is complete

Any discrepancies must be resolved before notebook closeout.

==========

I have reviewed this scientific notebook and find it in agreement with QAP-001.

Manager's Signature _____ Date 11/16/07

Attach this completed form to the last page of the notebook.

Form QAP-01 (03/2007)