

VOLUME XI – SOFTWARE VALIDATION

Scientific Notebook 432

Notebook started February 21, 2005

RF 2/21/2005

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06/10/2008 RF

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(page numbers added at notebook submittal date)

Collaborators: Roger Smith (Sci Ntbk # 473)
David Woolhiser (Sci Ntbk # 444)

Role of This Scientific Notebook in KINEROS2 Testing

Roger implemented the software test plan with David's and my help. The entries in this scientific notebook began after the first draft of the software validation report when I had noted some inconsistencies in version numbers and began to re-run the simulations. In addition, problems with the equation for the first test case were identified and fixed. Thus, this notebook volume is a supplement to the earlier work contained in Roger Smith's notebook.

KINEROS2 VERSION 1.13 was added to Software Validation exercise, as was Version 1.9. Version 1.13 contained fixes for problems we identified in Version 1.12. Version 1.9 was specially modified to output intermediate results along a plane specifically for the third test case. All three versions are being run through the software validation exercises.

Entries in May 2008 are interspersed with the 2005 entries, thus topics are kept together (at the expense of chronologic order of entries). Also, figure numbers. When numbered, are not necessarily sequential. Gaps in numbering occur, but all figures are traceable from the text to the correct figure. Also, spreadsheets from 2005 were updated and corrected in 2008 (thus, 2008 files are more reliable).

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02/21/2005 RF

Computer and Software

As of February 2002, the personal computer in my office (called bubo) was:

Primary computer running WindowsNT 4.00.1381 is called bubo

(Acer, x86 Family 6 Model 4 Stepping 2; AT compatible with 512 MBytes RAM).

Adobe Acrobat & Distiller version 5.0, Adobe Illustrator 8.0

Excel 97 SR-2, WORD 97 SR-2

KINEROS2 Version 1.9 and 1.12

In general the results and files are stored in

bubo: E:\SoftwareValidation\KINEROS2\

bubo: E:\KINEROS\Fortran_WebVersion_Feb2005\

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03/25/2005 RF

Window PC was upgraded March 21, 2005 to Windows2000 operating system

Adobe Acrobat & Distiller version 5.0
Adobe Illustrator 10.0.3
ArcView 3.2a
Excel 2002 (10.4302.4219) SP-2 (Office XP)
Lahey/Fujitsu Fortran 95 version 7.1
Mathematica 4.2
Sigma Plot2000 version 6.00
Word 2002 (10.4302.4219) SP-2 (Office XP)
Word Perfect version 10

End 03/25/2005 RF

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Start 05/19/2008 RF

M70 Precision Laptop running Windows XP

Excel 2003 SP3
Lahey/Fujitsu Fortran 95 version 7.1
Word 2003 SP3

Files stored on

C:\RFedors\Kineros\Version1.9\
 .\Version1.12\
 .\Version1.13\
 .\Feb2005* [files from 2005 entries in this sci ntbk]
 .\RogerSmithFiles* [files obtained from Roger at start of 2005]
 .\Downloaded_WalnutGulchData* [data obtained May 2008]
 .\Fortran-SourceCode* [source code 2003 vintage, downloaded]

For each of the Version directories, there are subdirectories for each of the 6 tests. These subdirectories are labeled Test1, Test3a, Test3b, Test3c, Test 4, and Test5. Spreadsheets with analysis of output are stored in many of the test subdirectories, and typically include the test name and KINEROS2 version as part of the filename. For the 2008 analysis, output file from KINEROS are retained in the subdirectories of each KINEROS2 version to keep things organized. Where multiple output files have been saved, a description and filename are included in this scientific notebook.

Earlier work (2005) was copied to C:\RFedors\Kineros just to organize, then to revise analysis in May 2008. This other work is listed in this scientific notebook with the old directory path, but the last part of the path names remains the same so that everything is traceable.

For the version numbers, which are labeled as some number with a "ws" (i.e, 1.12ws), I have dropped the "ws" part in this notebook and the software validation report.

Comments on Version Numbers – Historical Usage

Based on the output files (version stamp in the output) provided by Roger Smith:

Test 1 – Roger used Version 1.9

Test 2 – No simulations needed, we used calculation published in a journal article

Test 3a – Roger used Version 1.9

Test 3b – Roger used Version 1.8

Test 3c – Roger used Version 1.9

Test 4 – Roger used Version 1.12

Test 5 – I believe Woolhiser provided results to Roger for Test 5 simulations;
Woolhiser was using Version 1.12 at that time (but I do not have output files to confirm the version number, but other simulations Dave was performing at that time were with Version 1.12; Woolhiser's notebook should have this)

Email from Stothoff on Woolhiser's notebook on versions:

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From: Stuart Stothoff [mailto:ssstothoff@cnwra.swri.edu]

Sent: Thursday, May 15, 2008 4:35 PM

To: Randall Fedors

Subject: RE: percolation rates

Randy

I now have physical possession of notebook 444.

Page 202 (dated 5/6/05) states that Upper Split Wash runs from page 173 (dated 9/30/03) were run with version 1.12ws.

Pages 202 through 209 present a comparison of versions 1.12ws and 1.13ws for three control files. The comparison indicates that total runoff volumes agreed to within 1 percent for each of the three control files and there were no differences in channel infiltration (to 2 significant digits). The plane elements with the largest differences are for elements disturbed by roads.

Are the relevant KINEROS2 files from 9/03? The updates to TPA 5.0.1 document does not specify a version number for KINEROS2. I can dig in deeper to verify version numbers if the abstraction work was done with earlier files.

stu

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Additional Notes on Version Numbers

The draft Upper Split Wash report (dated Dec 2003) mentioned using KINEROS2 Version 03_2; this draft report included the abstraction for updating TPA for runoff. The confusion in version numbers arose because we previously used a different version naming scheme. After starting the software validation plan, I had figured out Woolhiser and Roger Smith were using different versions of KINEROS2 Version 03_2 for the validation work. To avoid future confusion, back in 2005, I switched the validation documentation to the 1.9 and 1.12 versions naming scheme. Note that 1.9 can be thought of as 1.09, for consistency with 1.12 and 1.13. So, we started using the other U.S. Department of Agriculture - ARS version number scheme. Specifically,

I checked through my electronic files for information relating to the comparison test of KINEROS2 versions 1.12 and 1.13. From my statement for May, 2005, I see that the comparisons were made in the period 5-06-05 - 5-12-05 and may be referenced in Scientific Notebook #444 pp. 202 - 209. In my progress report for May, 2005 (attached), I state that the comparison has been done and was reported to you and Roger Smith. However, I don't find a specific report in the folder and Roger hasn't a record of a report. I think that I summarized the comparisons with the attached Figures (see files Program versions.wpd and CDF KINEROS VERSIONS.wpd) and submitted them as an e-mail attachment. My

conclusion was that the minor differences between the results are insignificant insofar as conclusions that were reached in the report of our previous tests (SVTP_both-11-30.wpd) , given the degree of uncertainty of the modeling activity.

I assume that these figures are shown in the notebook, but can't check the information because I haven't received a copy of the notebook I returned to you.

Let me know if you need this to be summarized in a form other than in the notebook.

I have not received my new contract as yet, so couldn't do extensive work until it arrives..

>>>>>>>>>>> [email sender was apparently Woolhiser, Stu just tacked it on to his email]

End 05/9/2008 *RF*

02/21/2005 RF

KINEROS2 Version 1.12 Software Validation

Objectives

Develop and implement software validation test cases for KINEROS2 Version 1.12 so that KINEROS2 can be used for calculations that may be part of the safety evaluation report for Yucca Mountain or any other location for NRC licensing.

Collaborators

Roger Smith and David Woolhiser

Running KINEROS2

The graphical user interface is now standard with software releases. However, I can not get the user interface to read the input control correctly. Instead I have to manually set the input files (START -> click "No run file ..." option, then go to Options to specify parameter file and precipitation file and output file) and the simulation control parameters, if the information was not picked up from the control input file.

Also, difficulties with long path names meant that I usually ran the program in a .tmp directory with short subdirectory path names, then transferred all the files back to an archival directory.

To get diagnostics output file with more intermediate results, use the PR=4 setting in the parameter input file. PR=4 is not documented, only PR=1, PR=2, and PR=3 are documented in the user guide.

Test Results

Roger Smith implemented most of the test case simulations; David Woolhiser and Randy Fedors helped as needed. Roger Smith's input and output files for the five test cases are included with his scientific notebook

bubo: E:\SoftwareValidation\KINEROS2\Dec2003\RogerSmithFiles\

When the draft test plan and test result reports were reviewed, a number of changes were needed. The changes noted below were done by R. Fedors, including running all test cases with the newly-obtained Version 1.13. Hence, Roger Smith's scientific notebook should be consulted for all of the original calculations and information.

Change in Equation (10) of Test Report

The software test plan went through the technical and programmatic process with only one change. Gary Walter (technical reviewer) noted that he had derived an expression for the discharge Q as a function w in the rill:

$$Q(w) = \frac{1}{n} S^{1/2} [(w - BW) \{b + (w - BW)z / 4\}]^{5/3} \left[\frac{2b}{z} + z(w - BW) \sqrt{1 + \frac{1}{z^2}} \right]^{-2/3} \quad \text{Eqn (XI-2a)}$$

where S is the slope, n the Mannings coefficient, and the remainder of the terms are shown in Figure XI-6 below. The expression Gary derived was in similar form and exponents, but the terms inside the brackets were different. At first glance, the equation did seem to be in error. However, using the expression for b derived from the geometry shown in the figure on page XI-2, and substituting $b = z \cdot BW / 2$ into the equation above and rearranging, the following expression in Eqn (XI-2b) was derived, which was identical to that derived by Gary Walter. All the steps showing the relationship between Eqn (XI-2a) and Eqn (XI-2b) were handwritten on the comment sheet of the technical review for the test plan.

$$Q(w) = \frac{1}{n} S^{1/2} [(w - BW)(w + BW)z / 4]^{5/3} [BW + (w - BW) \sqrt{1 + z^2}]^{-2/3} \quad \text{Eqn (XI-2b)}$$

Because Roger Smith used Eqn (XI-2a) for the calculations in his notebook, both equations were left in the report on the test plan description.

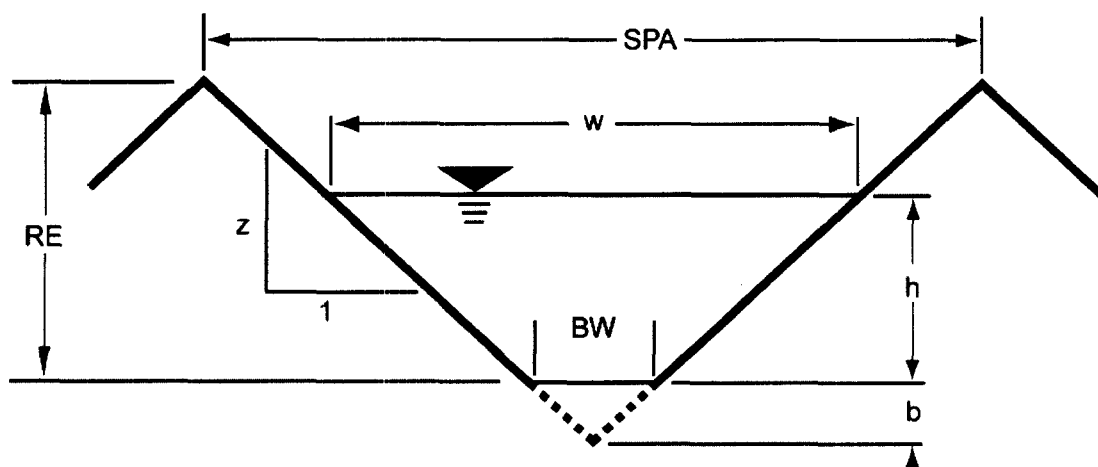


Figure XI-6. Schematic for Rill Geometry

Problem with Test Case 1, Infiltrability Estimates

During technical review of the test results, a problem was noted in the Test Case 1 where the equation was not providing the points displayed on the figure with KINEROS2 results.

The test case was re-simulated using both KINEROS2 Version 1.9 and Version 1.12. There were nuances to this problem that were not clearly discussed in the test description, and more importantly, the equation was not the one implemented in KINEROS2.

First the issue of the equation. The equation put into the report was not the one implemented in KINEROS2 source code obtained from the USDA website for KINEROS2 (do a google search for KINEROS2 to find the KINEROS2 homepage, and then go to downloads). Roger and I had this same discussion 1-1/2 years ago, and we still got the wrong equation into the draft report.

Discussions in 2003 with Roger, in regards to the equation for infiltrability in the software validation plan, $f_c = K_s * [\exp(I/G') - 1] / \exp(I/G')$ was used; but the KINEROS2 website documentation uses a slightly different equation and fixes the γ term, and uses $f_c = K_s * [1 + (\gamma / \{ \exp(\gamma I / G') \} - 1)]$; whereas Smith et al (1995, page 700) has $f_c = K_s * \exp(I/G') / [\exp(I/G') - 1]$ and Smith (2002, page 105) has a more general discussion with $f_c = K_s + [\gamma (K_s - K_i) / \{ \exp(\gamma I / G') - 1 \}]$ where G' is the combination of the capillary drive term and the soil water deficit. The file 2LAYINF.DOC, provided with the KINEROS2 documentation, describes the infiltration model in KINEROS2 and shows that the equation is the same as that provided on the website documentation of KINEROS2 (i.e., Eqn (XI-3a, below). To further verify which equation is in KINEROS2, the source code was downloaded from the KINEROS2 website and the code was searched. The relevant algorithm is found at lines 2038 to 2064 in the "fgex" function routine of the file infiltr.for. The source code confirms that Eqn (XI-3a) is the correct equation to use. The source code was stored in

bubo: E:\KINEROS\Fortran_WebVersion_Feb2005*

The revised equation put into the draft report was

$$f_c = K_s \left[1 + \frac{\gamma}{\exp\left(\frac{\gamma I}{G'}\right) - 1} \right] \quad \text{Eqn (XI-3a)}$$

where f_c is the infiltrability, K_s is the hydraulic conductivity, I is the cumulative infiltration, G' is the capillary drive term {where the prime denotes the modified term, $G' = (G + h_w) \cdot (\theta_s - \theta_i)$ }, and γ a coefficient dependent on soil type ($\gamma = 0.8$ for most soils; e.g., loams).

Smith, R.E., 2002. Infiltration Theory for Hydrologic Applications. Water Resources Monograph 15, American Geophysical Union, Washington, D.C.

Smith, R.E., D.C. Goodrich, D.A. Woolhiser, and C.L. Unkrich. 1995. KINEROS – A Kinematic Runoff and Erosion Model. Chapter 20 in Computer Models of Watershed Hydrology, V. P. Singh, editor. Water Resources Publications, Highlands Ranch, Colorado.

The input files to run Test Case 1 (infiltrability) and output files are located in

bubo:\SoftwareValidation\Kineros2\Feb2005\Test1_Redone*

Because the input files for parameters and precipitation are short, they are included below. The options to use in the "Files and Options" menu window of the graphical user interface for KINEROS2 are (i) select appropriate parameter, precipitation, and output files, (ii) enter a title

for the simulation, (iii) set duration of run to 45 minutes and leave time step at 1.0 minutes, and (iv) select "Write Summary Table" if so desired.

The parameter input file, "infilval.par," contains:

BEGIN GLOBAL test plane for validation infiltration test

!

CLEN = 50., UNITS = METRIC, NELE = 1 !

END GLOBAL

!-----

BEGIN PLANE

ID = 2, LEN = 100., WID = 10.0, SL = .09, MANNING = .02

SAT = .25, CV = 0.0, PR = 4

RELIEF = 0., SPACING = 1.

KS	G	DIST	POR	ROCK
5.0	50.	0.25	.40	0

END PLANE

!-----

This parameter file specifies that the plane is 100 m long and 10 m wide with a slope of 0.09. The Mannings n is 0.02, the initial saturation is 0.25, the coefficient of variation for heterogeneity of hydraulic conductivity is 0.0, and the diagnostic output file is requested (PR=4). The saturated hydraulic conductivity is 5.0 mm/h, the capillary drive term is 50 mm, the pore size distribution term (DIST) is 0.25, the porosity is 0.40, and no rock fragments are in the soil. With these inputs, the initial saturation is 0.1295 and the saturated water content is 0.38 because of automatic adjustments by the KINEROS2 code. Thus, $G' = (G + h_w)(\theta_s - \theta_i) = 12.525$ mm, neglecting the contribution of the surface water height (h_w) for now.

The precipitation input file, "R40mmh.PRE," is self explanatory.

BEGIN STORM simple r=

N = 3

TIME	DEPTH
------	-------

! (min)	(mm)
---------	------

0.	0.
----	----

60.	40.
-----	-----

100.	40.
------	-----

END

Relevant results of the simulations are output into a file called "diagno.out," which I renamed to included values of parameters of interest

diagno.out.lambda.25

diagno_Lambda.25_Version1.12.out

diagno_lambda75_Version1.12.out

diagno_lambda25_Ver1.12_step.25.out

results using KINEROS2 Version 1.9

results using KINEROS2 Version1.12

results using DIST=0.75

results using a time step = 0.25 minutes

Visual inspection of these output files:

- showed that the choice of the DIST coefficient (pore size distribution term) value did not affect results significantly;
- showed that the time step size did not affect results significantly, thus implying that using the average value of the cumulative infiltration for a time step led to insignificant error;

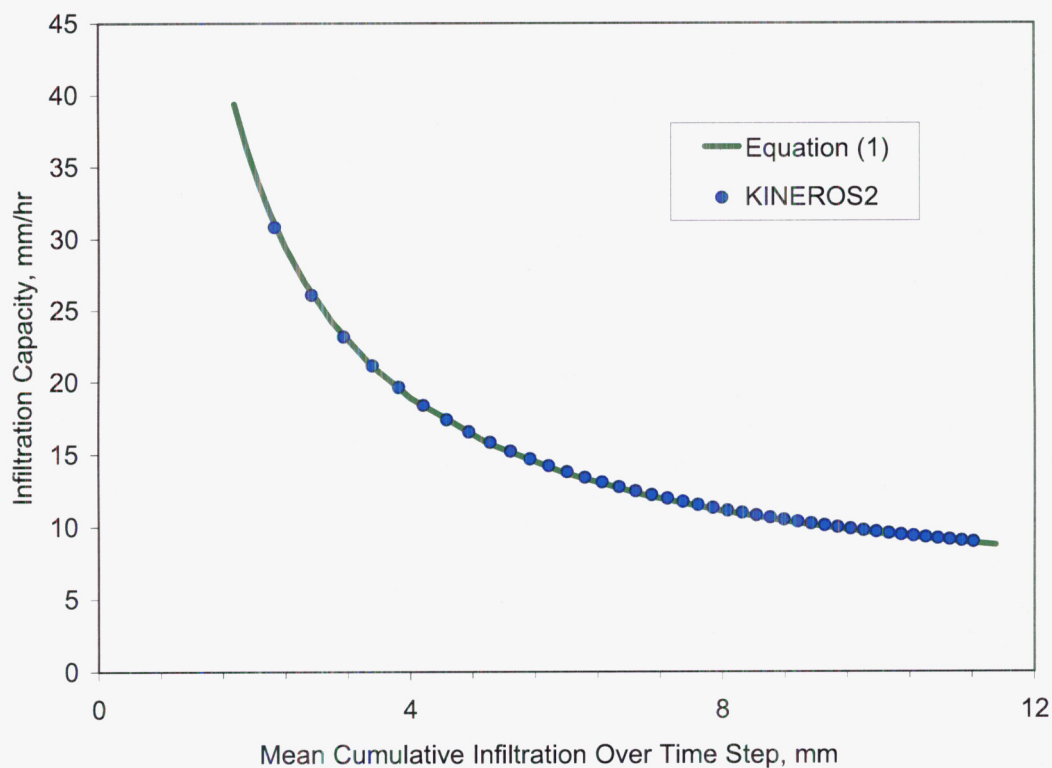
The diagnostic output file data of interest were manually tabulated in a spreadsheet. Confirmed by checking the code output statements for the diagnostic file, the values of interest are labeled as "net inf:" and "f"

bubo: E:\SoftwareValidation\KINEROS2\Feb2005\Test1_Redone\Test1.xls

The figure below comes from the file Test1.xls. The "Equation (1)" curve was derived using a range of cumulative infiltration values between 1.74 and 11.5 mm. The "KINEROS2" curve is a plot of the mean cumulative infiltration for the time period versus the infiltration rate for the time period (note that the infiltration rate from KINEROS2 is equal to the infiltration capacity after the infiltration capacity drops below the rainfall rate).

Note that the KINEROS2 infiltrability data should be plotted against the mean cumulative infiltration for the time step in order for the comparison with the results from the equation.

The curves are visually close, but do differ by small amounts. The error varies over time. Thus a closer inspection of the algorithm was warranted.



Four possible errors were identified. The surface water pond height was identified as the most important.

- The term G' is not only a function of the capillary drive parameter and water initial water deficit, but also the surface water height. A slope of 0.09 reduces the surface water height, but its effect is still present. Note that the surface water height varies along the plane and with time.
- Whereas a cumulative infiltration value is recorded at the end of time steps in KINEROS2, a representative value of cumulative infiltration for the time step is needed for comparison with Eqn (XI-3a). Any nonlinearity over a time step would introduce some error when using mean values of cumulative infiltration.
- Variations in the pore size distribution term lead to small changes in infiltration; but this is not integrated into the equation for G' .
- Use of large initial water contents would amplify errors in Eqn (XI-3a) for representing infiltration because the initial effective conductivity is assumed to be small. These errors are minimized by using a small initial water content in this test case.

A quick calculation of approximate initial effective conductivity indicates that $K_i = 1.2 \times 10^{-6}$ mm/h, thus we can safely assume that $(K_s - K_i)$ can be approximated as K_s in the general 3-parameter formula for infiltrability in Smith (2002); $f_c = K_s + [\gamma (K_s - K_i) / \{ \exp(\gamma / G') - 1 \}]$. Because K_i is small, the Smith (2002) equation reduces to that in Eqn (XI-3a). The calculation for K_i is not straightforward. First, noting that

$$G = G(O) = \int_{-\infty}^0 \frac{K(h)}{K_s} dh$$

where h is the capillary tension head. Using the Brooks-Corey characteristic relation

$$\frac{K(\psi)}{K_s} = \left(\frac{\psi_b}{\psi} \right)^{2+3\lambda} \quad \text{Eqn (XI-6a)}$$

we can see that

$$G = \psi_b \frac{2+3\lambda}{1+3\lambda}$$

which can be rearranged to solve for the bubbling tension head. Then using the Brooks-Corey relation for saturation as a function of tension, which can be rearranged to

$$\psi = \frac{\psi_b}{S^{1/\lambda}}$$

Once the tension head ψ is calculated, the initial effective hydraulic conductivity can be calculated using Eqn XI-6a.

The dominant reason for expected differences in infiltrability is the neglect of the surface water height in the hand calculations using Eqn (XI-3a), specifically in estimating G' . Surface water heights are estimated to range from approximately 0 to 2.5 mm over time and distance along the plane; note that KINEROS2 has grid points along a plane, the number of these internal grid points are automatically determined. Before infiltrability becomes less than the precipitation rate, the surface water height is 0. At early times when infiltrability is less than rainfall rate, the surface water height is smaller than at later times. When a representative surface water height for early times is used to estimate G' , the errors are ≤ 1.1 percent for all times. When a representative surface water height for later times is used to estimate G' , the errors in infiltrability estimates are less than 0.5 percent, except at the earliest times.

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Start 5May2008 *RF*Additional comments on Test Case 1:

Results for Kineros2 Version 1.9 stored and plotted in

.\Version1.9\Test1\Test-1_1.9.xls

Using data from diagnostic file=.\Version1.9\Test1\diagno.out

Results for Kineros2 Version 1.12 stored and plotted in

.\Version1.12\Test1\Test-1_112.xls

Using data from diagnostic file=.\Version1.13\Test1\diagno.out

Results for Kineros2 Version 1.13 stored and plotted in

.\Version1.13\Test1\Test-1_113.xls

Using data from diagnostic file=.\Version1.13\Test1\diagno.out

Of the 4 reasons on page XI-10, the comment on pore-size distribution should not be relevant because pore-size distribution does not show up in equation XI-3a.

As before (in 2005),

1. infiltration, I (mm), is taken from "net inf" in the diagnostic file; note that another decimal place can be obtained by using the "Infil" value multiplied by the 10-m width of the plane;
2. infiltration capacity f_c (mm/hr) taken from "f" in the diagnostic file;
3. estimate of pond height h_w (m) taken from "h2" node 5; i.e., the 5th node for the plane is taken as representative of the pond height for the entire plane.

G' is calculated from $G'=(G+h_w)(\theta_s-\theta_i)$, and thus is variable along the time profile. $G=50\text{mm}$ is an input to the simulation. Per Roger Smith (and confirmed in the output file – check input value for porosity, then check output), note that KINEROS2 uses $\theta_s=\phi-0.02$; thus, full porosity is not used for saturated water content.

For the estimate of the ponding height, h_w , I stayed with the original choice of the 5th node on the plane. Originally, this node was chosen by visual estimate as being representative of the ponding height for the entire plane for all times. This approach for estimating the representative ponding height is simple, but certainly may lead to some unknown level of error. It is not clear how much error is created in approximating h_w . Also, note that the nonlinearity error for estimating infiltration created when using the interpolation of the KINEROS2 output is more important early, and less important later in time.

End 5May2008 *RF*

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RF Start 19May2008

Confirmed the two following points by checking the code or by checking output files, knowing the inputs:

- Confirmed that KINEROS2 output had saturated water content $\theta_s=0.38$ when porosity $\phi=0.4$ in input and $\theta_i=0.1295$ when saturation $S_i=0.25$ as input

- Confirmed $\gamma=0.8$ hardcoded in version 3.2 from fortran code of web site (noted in 2005)

Version 1.13 results differ from the analytical results for infiltrability by $<0.45\%$ for all times, and $<0.01\%$ for all times beyond 13 minutes (of the 45 minute-event) in the simulation. Also, in the absolute difference in infiltrability between KINEROS2 and the hand calculation is generally 0.01 (the original validation criteria), except for early times when the maximum difference ranges up to 0.1 mm/hr.

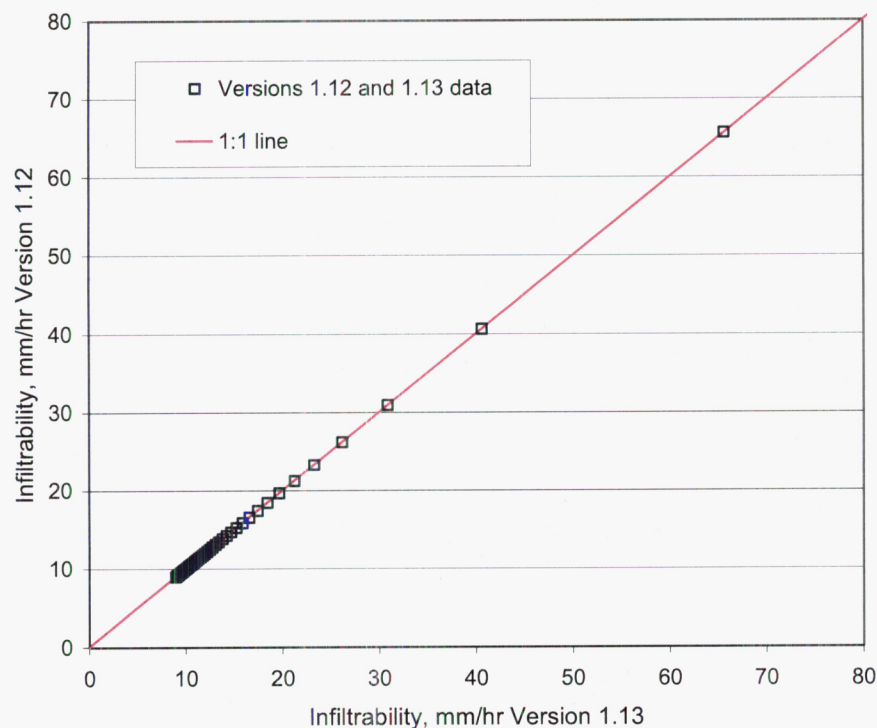
- Files in .\Version1.13\Test1*
- Inputs: infilvalid.fil, infilvalid.par, R40mmh.PRE
- Outputs: infilvalt.out and diagno.out; calculations in Test1_113.xls

Version 1.12 results differ from the analytical results for infiltrability by $<0.45\%$ for all times.

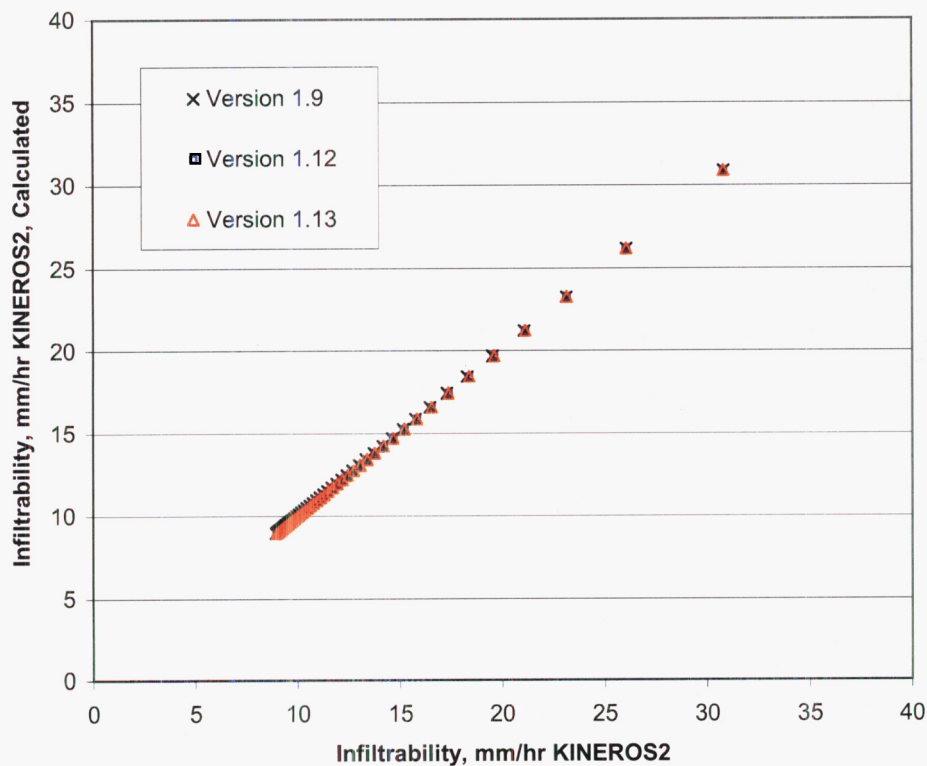
- Started with the old Test1.xls which had a representative ponding height after early times.
- Files in .\Version1.12\Test1*
- Inputs: infilvalid.fil, infilvalid.par, R40mmh.PRE
- Outputs: infilval_lambda25_Version1.12.out and diagno_Lambda.25_Version1.12.out; calculations in Test1_112.xls

Version 1.9 results differ from the analytical results for infiltrability by $<0.7\%$ for all times, and $<0.5\%$ for the later half of time in the simulation.

- Files in .\Version1.9\Test1*
- Inputs: infilvalid.fil, infilvalid.par, R40mmh.PRE
- Outputs: infilvalt.out and diagno.out; calculations in Test1_19.xls



Results from Versions 1.12 and 1.13 do not differ, as shown by the figure to the left (on this page).



Quantitatively, Versions 1.12 and 1.13 are identical, and differ slightly from Version 1.9. (see above figure on this page). There were minor differences between version 1.9 and versions 1.12/1.13. The maximum percent difference (normalized to KINEROS2 f_c) is 0.03% (very small). Calculations are in Test1_113.xls.

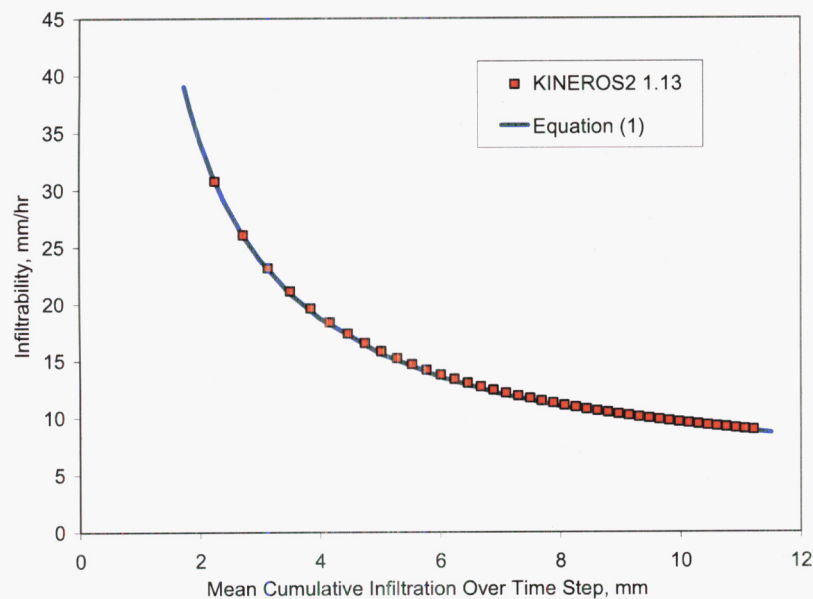


Figure used in the report is the figure to the left, as copied from test1_113.xls, worksheet "Plot".

End 19May2008 RF

RF 8 April 2005

Test Case 3a

Test Case 3a was re-simulated using KINEROS2 Version 1.12, and results plotted. The results did not vary much from those produced by Roger Smith, who used version 1.9.

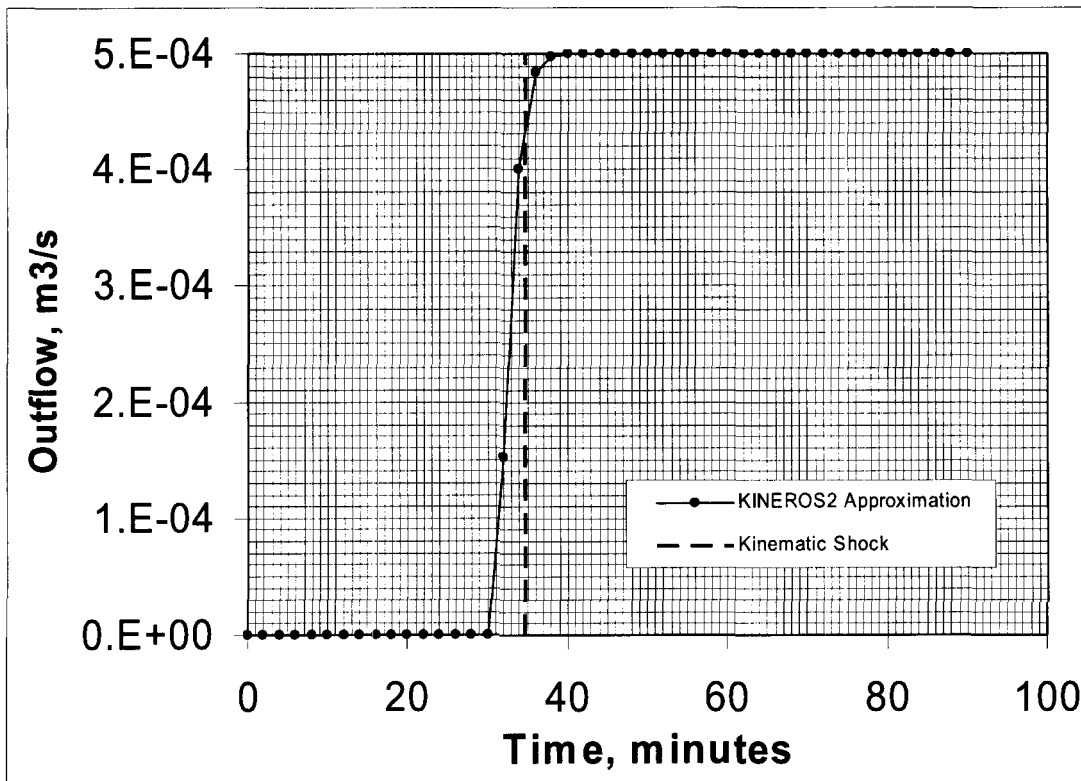
Again, simulations are run in the D:\tmp\KIN\ directory to avoid the KINEROS2 problem with long directory names. Results were then transferred to the following directory for storage:

bubo: E:\E_Drive\SoftwareValidation\KINEROS2\Feb2005\Test3a\

Input files are norain.pre, ronvalid0n.par, inject2.dat (rate=0.0005 m³/s/m); a total of 90 minutes were simulated using a time step of 2 minutes.

My output files are check112.out, which was imported into Excel and the outflow m³/s column of data was plotted for Figure 3 of the software validation report.

File: check112.out.xls



For the shock front, velocity will equal the input flux (m³/s/m) Q_o divided by the flow depth H_o ; and the position of the front will be equal to the velocity multiplied by time. The normal flow depth can be estimated using a simplified and rearranged form of the Manning's equation:

$$H_o = \{Q_o / \alpha\}^{1/m} = [(0.0005 \text{ m}^3/\text{s} / 10 \text{ m}) / \sqrt{0.05} / 0.151]^{1/(5/3)} = 0.002075 \text{ m}$$

Where the roughness coefficient $\alpha = \sqrt{(\text{slope})/m}$, noting that m is 5/3 and using a slope of 5 percent for a 50-m long plane element that is 10 m wide. Output file diagno.out shows that this value of flow depth is estimated by KINEROS2 Version 1.12.

Thus $V = Q_o/H_o = 0.0005 \text{ m}^3/\text{s}/0.002075 \text{ m} = 0.024093 \text{ m/s}$
 And, time = advance distance / velocity = $50 \text{ m} / 0.024093 \text{ m/s} = 2075 \text{ s} = 34.588 \text{ min}$

The 50% breakthrough occurs at about 32.7 minutes (visually extracted from figure on previous page); at 34.588 minutes, 86% breakthrough occurs. Error in shock front breakthrough time (when 50% is used as "front") is $(34.588-32.7)/34.588 = 4.88\%$

How good is the estimate of flow depth using $H_o = \{Q_o/\alpha\}^{1/m}$?

This approximation neglects the perimeter [set perimeter equal to 1 in the equation for estimating the hydraulic radius ($R = \text{area} / \text{perimeter}$)]. Then the Manning equation can readily be rearranged to solve directly for flow depth. The Manning equation, in metric form (multiply by 1.49 to use feet instead of meters)

$$Q = \frac{1}{n} A R^{2/3} S^{1/2}$$

Where the area is $H_o \times \text{width}$, and the hydraulic radius is $(H_o \times \text{width}) / (2H_o + \text{width})$
 Just use regular Manning equation and solve iterative (trial and error). This was done in the .\Test3a\check112.out.xls spreadsheet and the results are copied below. The conclusion is that the simplified approach leads to a pretty good estimate. Below is the excerpt from the calculations in check112.out.xls.

Shock Front calculations - Flow Depth & Flux Check

0.0240931	Velocity(m/s) = injection / flow depth
2075.2822	time (s) = distance / velocity = shock front arrival at bottom of plane element
34.588037	time (minutes)
50	length of plane element
10	width of plane element
0.00005	calculated injection (m ³ /s/m)
0.0005	injection Q (m ³ /s) from inject2.dat file
0.0020753	calculated normal depth of flow (m), $H_o = [(Q/w) / \text{roughness coef}]^{1/(5/3)}$
1.4808397	roughness coefficient = $\text{sqrt}(\text{slope}) / n$
0.05	Slope
0.151	Mannings n

Check on depth using full Manning Equation (instead of simplified approach with perimeter neglected)

$Q = A R^{2/3} S^{0.5} / n$ where n in Manning coef, S is slope, R is hydraulic radius = Area/perimeter

0.0020756	guess for depth, m
0.0005	injected Q, m ³ /s from above
0.0020748	R, hydraulic radius
0.0005	$A R^{2/3} S^{0.5} / n = \text{estimated Q}$
7.222E-10	difference between injected Q and estimated Q

Therefore, the simplified and rearranged Mannings Eqn for estimating flow depth is a pretty good approach

Test Case 3b

Test Case 3b was re-simulated using KINEROS2 Version 1.12, and results plotted. The results did not vary much from those produced by Roger Smith, who used version 1.8.

Again, simulations are run in the D:\tmp\KIN\ directory to avoid the KINEROS2 problem with long directory names.

Results were then transferred to the following directory for storage:

```
bubo: E:\E_Drive\SoftwareValidation\KINEROS2\Feb2005\Test3b\
      .\LargeFluxInjected\*      q > f * L scenario
      .\SmallFluxInjected\*      q < f * L scenario
```

Input files are norain.pre, ronvalid.par, injectry.dat; a total of 100 minutes were simulated using a time step of 0.5 minutes. The value in file "injectry.dat" was varied between the two scenarios, from 0.001 m³/s (SmallFluxInjected) to 0.0022 m³/s (LargeFluxInjected). Roger Smith had the value of 0.001 m³/s in his input file. I calculated that a value of 0.0022 m³/s would be needed to get discharge off the bottom of the plane element. The injection value of 0.001 m³/s would lead to a stable profile with the leading edge of the front stopping at about the 50 m downslope position.

Large Flux (Q_o=0.0022 m³/s)

A large injected flux will lead to runoff occurring from the bottom of the plane element. A flux of 0.002 m³/s leaves the front just barely reaching the bottom, thus the injected flux was increased a small arbitrary amount to 0.0022 m³/s. For the first part of Test Case 3b, the timing of the front arrival at the bottom of the plane element will be compared against an analytical result. The difference with Test Case 3a (no infiltration allowed) is that infiltration will delay the front. The input parameters are Mannings n = 0.09, slope = 0.05, soil Ksat = 7.2 mm/hr (which determines steady state infiltration rate), width of plane = 10 m, length of plane = 100 m, 100 min simulation time, 0.5 minute time steps.

The shock front without infiltration would reach the bottom at about 28 minutes (using equations from Test Case 3a, calculated H_o is 0.00307 m and velocity is then 0.0594 m/s; then 100/0.0594/60= 28.04 minutes). However, with infiltration, the front is delayed. Cunge and Woolhiser (1977) solution provided in the software validation test plan for KINEROS2 (eqn 3, and repeated below) is implemented in the spreadsheet

$$t' = m \left[1 - (1 - x')^{1/m} \right]$$

where t' and x' are normalized to account for injected flux, infiltration rate, plane length, and roughness coefficient. This solution is described more clearly in Roger Smith's scientific notebook (#473, page 51-52). The scalings are implemented in the spreadsheet (test3b_v1112.xls, worksheet 'Calcs Large Flux') and copied to the table below with the input parameters:

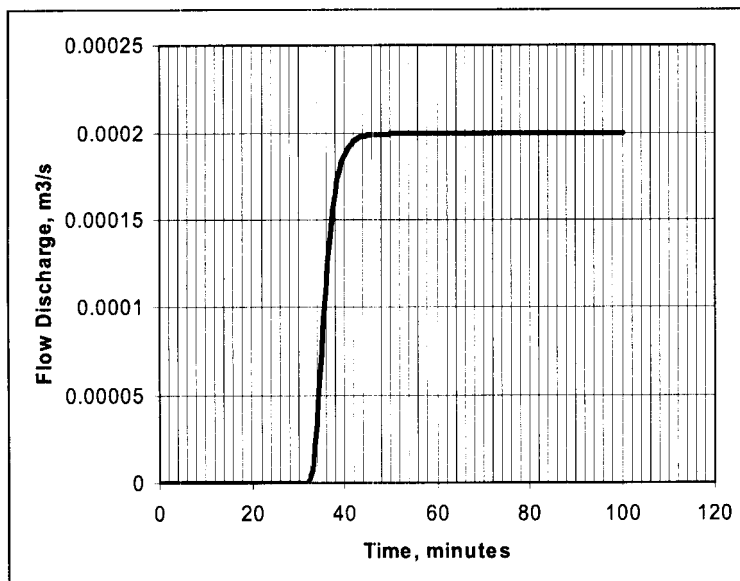
7.2	= steady infiltration, i = Ksat, mm/hr KINEROS2 input in parameter file
2.0E-06	= steady infiltration, i = Ksat, m/s
0.0022	= injection Q _o , m ³ /s from injectry.dat file
10	= width of plane, m
2.48452	= α, sqrt(slope)/mannings n
0.09	= mannings n
0.05	= slope
1.6666667	= m = 5/3, exponent of hydraulic radius in Manning equation

$3.071\text{E-}03$ = H_o , flow depth at top, from diagno.dat file (m)
 0.0037009 = H_o , m, calculated from $H_o = (Q/w/\alpha)^{1/m}$, Q in m^3/s injected
 $1.9\text{E+}03$ = T_o (s) = $H_o/\text{infiltr}$, infiltration in m/s
 $1.1\text{E+}02$ = X_o (m) = $Q/w/i$, where Q is m^3/s injected

 $9.1\text{E-}01$ = $x' = x/X_o$, where x is bottom position of plane
 1.2712881 = $t' = m (1 - [1 - x']^{1/m})$
 $2.4\text{E+}03$ = t (s) = $t' * T_o$, rearranged from scaled relation $t' = t/T_o$
 39.207653 = t , minutes

Cunge, J.A. and D.A. Woolhiser. "Irrigation Systems," Chapter 13 in Unsteady Flow in Open Channels, Volume 2, pp. 522-533. Water Resources Publications, Fort Collins, CO, 1975.

Hence, infiltration delays the shock front arrival at the bottom of the plane to 39 minutes, compared to the 28 minutes without infiltration. A plot of the data in the output file is included below; test3b_large_q.out was included in the spreadsheet.



Visually the front reaches the bottom of the plane between 32 and 44 minutes, depending on how the "front" is defined.

- at 39 minutes 89.3 percent of steady discharge rate has been attained;
- at 39.5 minutes 91.8 percent of steady discharge rate has been attained;
- Therefore, if the front is defined as 90% of the steady discharge, then the analytic result is matched;
- 50% breakthrough occurs as about 36 minutes.

Clearly, dispersion at the leading edge of the front brings some of the flow before the front.

Low Injected Flux ($Q_o = 0.001 \text{ m}^3/\text{s}$)

At a lower injected flux, the front will stall somewhere along the plane. For this case, the depth profile and front position can be compared between KINEROS2 and analytical results. In KINEROS2, at steady state, results of the flow depth were extracted from the diagno.out file for some time after steady flow was reached (just used last time step, and confirmed that the flow depths were not changing from previous time steps). The flow depths are in two records with

the labeling of “h2” at each time step in the diagno.out file. These values were plotted in the worksheet ‘Calcs Small Flux’ of the Excel spreadsheet

File: test3b_v112.xls

Analytical results were calculated using the equations in section 6.3.2; the calculations are included in the spreadsheet file in worksheet ‘Calcs Small Flux’ and are copied to the table below. Equation 5 in the third column refers to equation 5 of the software validation test plan and is reproduced below. Other calculations are explained the table.

$$h(x) = \left(\frac{Q_o - f \times w}{\alpha w} \right) \text{ where } h(x) \text{ is the depth at } x \text{ meters down the plane element, } Q_o \text{ is the}$$

injected flux, f is the infiltration, w is the width of the plane element and α is the roughness coefficient.

Inputs and calculation of intermediate parameter values:

7.14285714 = spacing (m); 15 points on 100-m long plane, thus spacing is 100/14

7.2 = steady infiltration = Ksat, mm/hr KINEROS2 input in parameter file

2.0E-06 = steady infiltration = Ksat, m/s

0.001 = injection Q_o , m³/s from injectry.dat file

10 = width of plane, m

2.48451997 = α , sqrt(slope)/mannings n

0.09 = mannings n

0.05 = slope

1.66666667 = $m = 5/3$

Calculation of normal flow depth and flow rate at each x location:

At time = 100 minutes

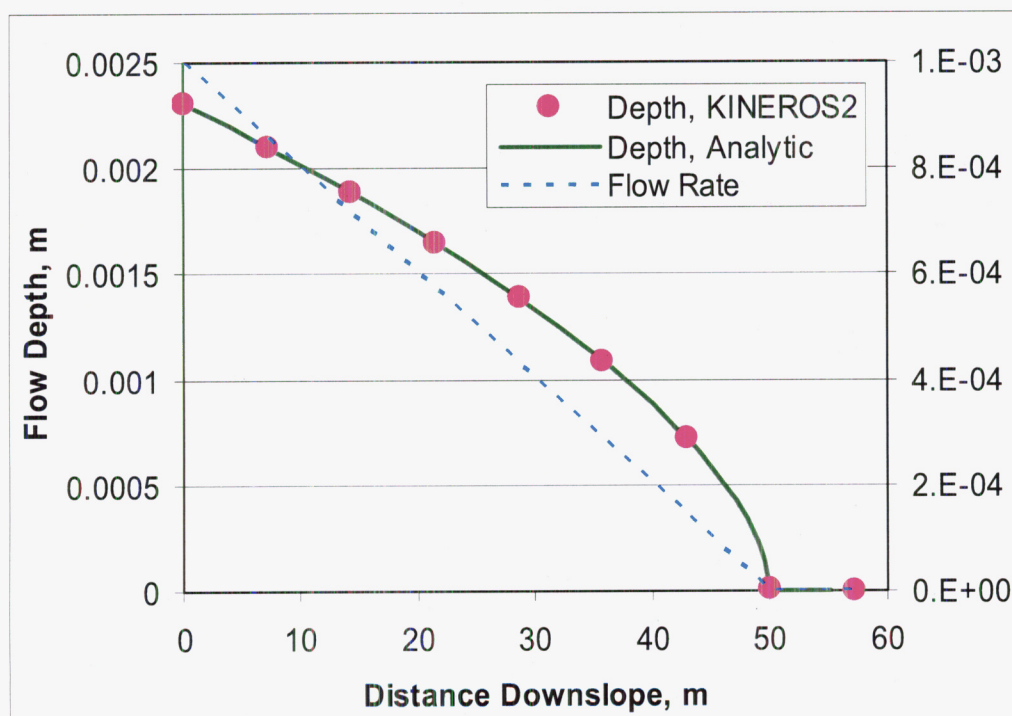
	KINEROS2	calc using	$q = \alpha h^m$	$Q = q w$
	diagno.out	eqn 5	calculated	calculated
calculated	diagno.out	eqn 5	flow at x_i	flow at x_i
distance, m	flow depth, m	Flow depth, m	m ³ /s/m	m ³ /s
0	2.306E-03	0.00230597	1.000E-04	1.000E-03
7.14285714	2.102E-03	0.00210226	8.570E-05	8.570E-04
14.2857143	1.884E-03	0.00188442	7.140E-05	7.140E-04
21.4285714	1.648E-03	0.00164828	5.713E-05	5.713E-04
28.5714286	1.387E-03	0.00138697	4.286E-05	4.286E-04
35.7142857	1.087E-03	0.00108746	2.855E-05	2.855E-04
42.8571429	7.175E-04	0.00071746	1.429E-05	1.429E-04
50	6.950E-06	0	6.289E-09	6.289E-08
57.1428571	0.000E+00	#NUM!	0.000E+00	0.000E+00

46.6

0.00045958 essentially zero depth, eqn 5

0.1992991 = $h(i)/h(0) \sim 0.2$

The analytic result for the front location is 46.6 m downslope when the front edge of the overland flow is defined as 20% of the flow at the top of the plane element. Note that there is not a sharp front analytically when there is infiltration occurring, unlike the situation with overland flow on an impervious surface where analytically there is literally a sharp front.



Plot of the data provided in the table above, plus the analytical results calculated in worksheet "Calc Small Flux" of test3b_v112.xls.

=====

Start June 9, 2008 *RF*

Test 3a

Just needed to clean up the spreadsheets and extract the criteria for the report. The simulations for all three KINEROS2 versions were completed in 2005.

.\Version1.9\Test3a\check19.out.xls and test3a_1.9.out output file

.\Version1.12\Test3a\check112.out.xls and test3a_1.12.out output file

.\Version1.13\Test3a\check113.out.xls and test3a_1.13.out output file

Previously calculated (this volume of Sci Ntbk 432 Volume XI) breakthrough time for a shock front is 34.588 minutes. Calculations are also in the spreadsheets for each version.

Estimated breakthrough for each version uses 50% of the simulated flux (front) for defining the front. Mass balance is from bottom of the output files (summary for event) based on volume in and out and change in storage.

Version	Estimate of Front Reaching End of Plane	Error for Time Reaching End of Plane	Mass Balance Error for KINEROS2 Simulation
Version 1.9	33.6 minutes	2.86%	2%
Version 1.12	32.7 minutes	5.49%	3%
Version 1.13	33.4 minutes	3.43%	2%

A visual comparison of the results, focusing in near the breakthrough time, shows that Version 1.9 had the most dispersion, but nearly the same 50% breakthrough time. Version 1.12 had the earliest 50% breakthrough time. The difference between the results for each version are not thought to be significant.

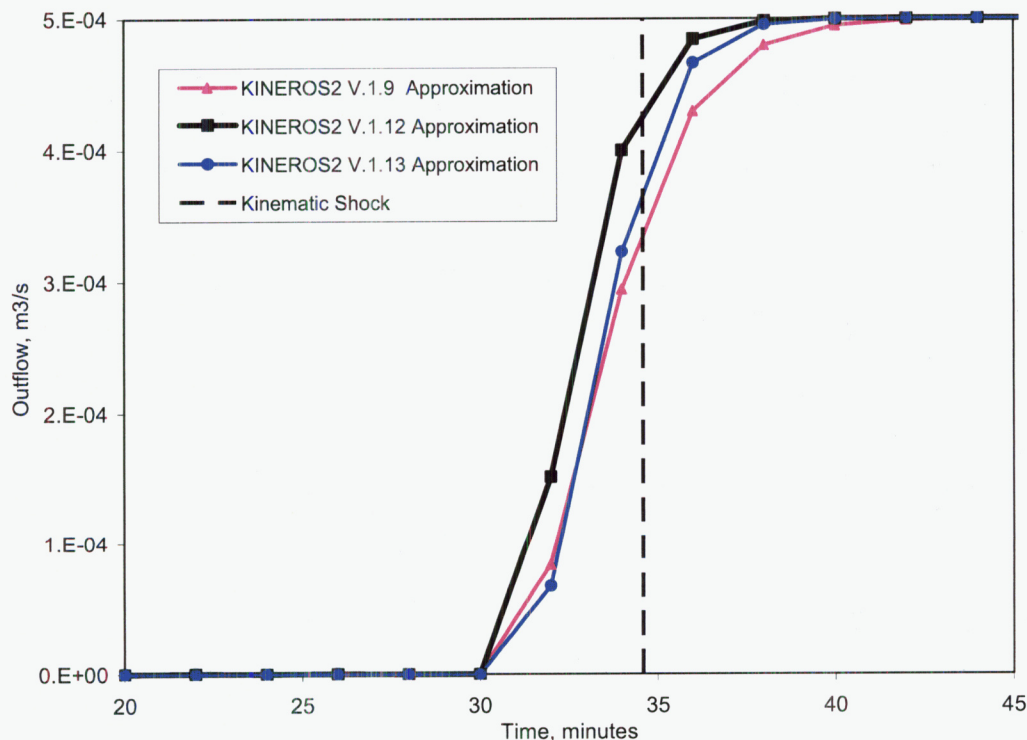


Figure - Comparison of version results for Test 3a (worksheet "Compare 1.9, 1.12, 1.13" in the spreadsheet check113.out.xls.

Test 3b

Much of the calculations were done in 2005 (see earlier entry in this volume of the scientific notebook).

Because versions 1.12 and 1.13 were not modified to spit out the extra intermediate results along the plane element, the approach for Version 1.9 (intermediate water heights and fluxes along the plane in diagno.out) differed from that for Versions 1.12 and 1.13 (water heights in diagno.out, but flux was calculated using equation (4) noted below). The calculations for all versions were done in:

.\Kineros\Version1.12\Test3b\Test3b_v112.xls

Input files, same directory: .ronflatval.fil, injectry.dat, ronvalid.par, norain.pre

Output files: .diagno.out and test3b_v112.out

Version 1.13 results are in (input filenames are the same):

.\Kineros\Version1.13\Test3b\test3b_v113.xls and diagno.out

For Version 1.9, the diagno.out file provides the water height and flux (the latter needs to be multiplied by the plane width).

.\Kineros\Version1.9\Test3b\diagno.out and test3b_v19.xls

For the analytical results, I used the following equations; these are eqn (4) and (5) from the software validation report.

Equation (4) $Q = \alpha h^m$

Equation (5)
$$h(x) = \left(\frac{Q_0 - f x w}{\alpha w} \right)^{\frac{1}{m}}$$

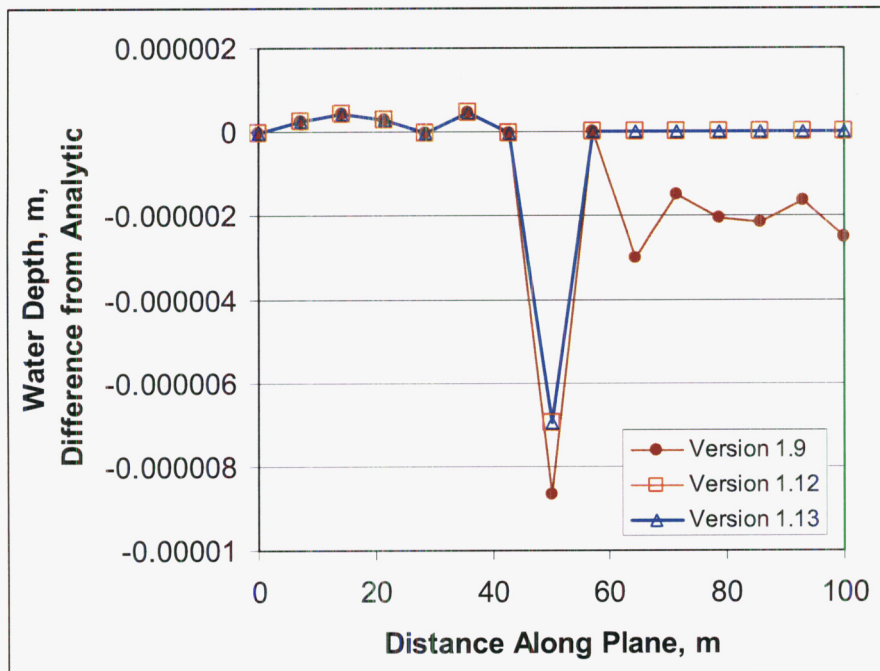
To create the analytical data set, choose values of x (distance along the plane) for equation 5; h is depth of water, $Q_0=0.001 \text{ m}^3/\text{s}$ is injected water at top of the plane, $f=7.2 \text{ mm/hr}$ is the infiltration rate, $w=10 \text{ m}$ is width of plane, $m=5/3$ is the exponent from the Manning equation, and $\alpha=2.4845$ is the roughness coefficient that is equal to the square root of the slope ($=0.05$) divided by the Mannings $n(=0.09)$.

The worksheet "Calcs Small Flux" in the spreadsheet test3b_112.xls contains the calculation

Comparison of water depths taken from the diagno.out files is done in

.\Kineros\Version1.12\Test3b\testb_v112.xls, worksheet "Compare 1.9, 1.12, 1.13"

The differences are minor. Results from Versions 1.12 and 1.13 are identical. Version 1.9 had slightly more dispersion at the toe of the front, and had numerical artifacts downstream of the front (nonzero, but extremely small water heights). The extremely small differences from 0 to 42 meters along the plane are likely just roundoff errors in the KINEROS2 output. The figure below illustrates the minor differences between the analytical water height and the results from Versions 1.9, 1.12, & 1.13:



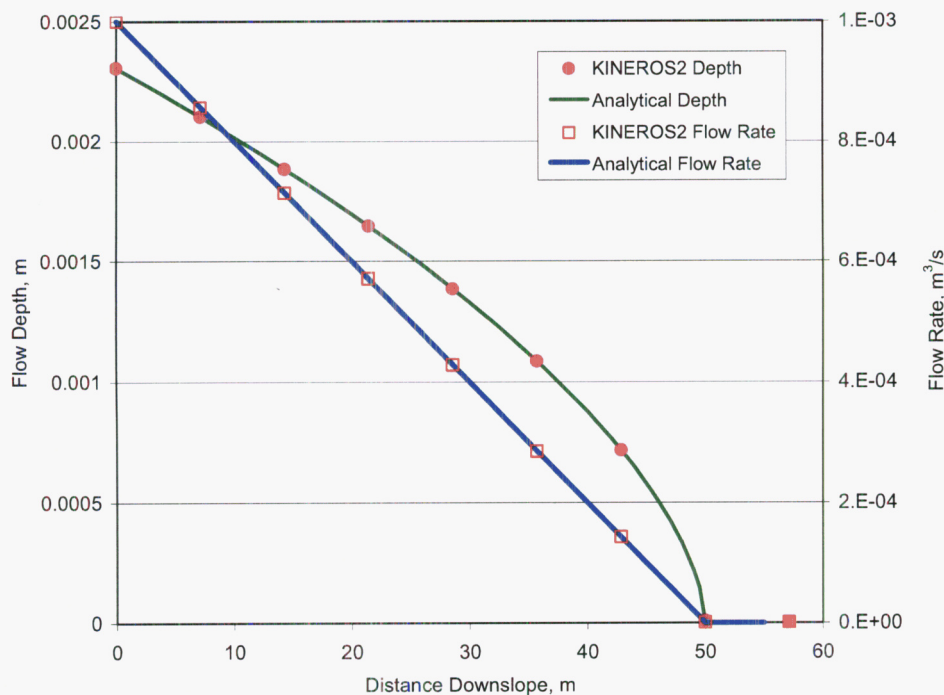
The figure for Version 1.9 results is used in the report (worksheet “Plot” in test3b_v19.xls), with a comment that the results for Versions 1.12 and 1.13 for water height along the plane do not differ from the analytical result.

Using equations (4) and (5) on the previous page, the front can be delineated assuming some fraction of the water height or discharge has been reached. At 49.5 meters down the plane, the flux is 1% of that at the top of the plane (i.e., the flux at 49.5 m is 1% of the injected flux at the top of the plane). At 49.98 meters, the water height is ~1% of the water height at $x=0$ m. See trial and substitutions in the “Calcs Small Flux” worksheet of the test3b_v112.xls spreadsheet.

For all three versions (1.9, 1.12, and 1.13), a simulation was run using the large flux, $q_0=0.0022$ m³/s, injected at the top of the plane. These were estimated graphically or by mental interpolation of the data out table in the test3b_large_q.out files in worksheets “Calc Large Flux” of each version’s test3b_V???.xls spreadsheet file.

KINEROSION Version	Time to 50% Breakthrough
1.9	36.5 minutes
1.12	36 minutes
1.13	36 minutes

The figure (below) I put into the software validation report is the one I created using KINEROS2 Version 1.9. It appears to reproduce Roger’s figure visually-speaking. I used Version 1.9 because that version spit out the water heights and fluxes along the plane. The other two versions only spit out the water heights in the diagno.out files. The same figures for versions 1.12 and 1.13 look the same as the one below for version 1.9. But the flux values for Versions 1.12 and 1.13 are calculated for KINEROS2 outside of the program, but using the water height values from KINEROS2 output.



Version 1.9 results for Test 3b, used for software validation report

Test 3c

Roger used a modified version of KINEROS2 Version 1.9 that also printed out intermediate flux values along the plane in the diagno.out file. Normally, only h_w and t_w (rill, water width) are printed out in the diagno.out file for version 1.13; when there are no rills, a flux is printed (like in Test 1). Hence, I will use Roger's Figures for Test 3c in the software validation report (he used Version 1.9). Then, I will show that the flow depths are the same for Versions 1.9 (Roger's) and 1.13 (mine). Version 1.12 has the known problem at the toe of the front as the front is moving down the plane. I'll just show the main part of the height profile at steady state is the same as it is for versions 1.9 and 1.13. Note that Woolhiser has shown that Versions 1.12 and 1.13 produce only slightly different results (~1%) for the Upper Split Wash watershed events he checked (see Woolhiser Sci Ntbk #444).

Also rerun his integration fortran code to get the analytical code. The latter is straightforward – results were saved in the test3c_v113.xls spreadsheet; 3 worksheets called:

- "TEST3.OUT Integration, Re=50"
- "TEST3.OUT Integration, Re=100"
- "TEST3.OUT Integration, Re=150"

The code results, code, and executable are saved in

.\Kineros\Version1.13\Test3c\Case3c_Integrate*

The input files are *.CON, the output files are *.OUT. For example, the input file for the integration is:

```
LENGTH (M)  SLOPE    n      RE (MM)      SPA (M)      Q0 (CMS)  KS (MM/H)  NINC
1000.        0.05    0.151    50          1.0          0.0001    22.5       50.
TEST3.OUT
```

The integration Roger solved with the interate.f95 fortran code refers to equations 10 and 11 in the software validation report: a Runge-Kutta integration is used on equation 11; but the width of the water in the rill as a function of flow $w(Q)$ is needed for equation 11, so a Newton-Raphson iteration is used with equation 10 to get $w(Q)$. For reference and clarity, the equations are included here (without symbol definitions):

$$Q(w) = \frac{1}{n} S^{1/2} [(w - BW)(w + BW)z/4]^{5/3} [BW + (w - BW)\sqrt{1 + z^2}]^{2/3} \quad (10)$$

$$\frac{dx}{dQ} = \frac{-1}{K_s w(Q)} \quad (11)$$

Roger provided his KINEROS2 version 1.9 output and diagno.out files. Extraction of results from the diagno.out files is needed to plot the discharge and to calculate the simulated flow depths. Start with 2nd to last time entry (or any earlier entry that where it appear that steady behavior has been reached) in the diagno_xxx.out file (the last entry appears to be affected by the sudden change in boundary conditions at the end to the simulation). While I could have just put Roger's figures into the revised report, I wouldn't be able to compare version 1.9 results with Versions 1.12 and 1.13 results. This also shows that the flow depths are taken from the same place in the output files. Because Versions 1.12 and 1.13 have not been revised to output the flux along the plane, as version 1.9 had been, I will just compare the flow depths along the plane to show that Versions 1.9, 1.12, and 1.13 all produce the same results for Test Case 3c.

Plot flux, q2 entry in diagno_xx.out file, along the plane; no manipulation of flux data is needed. For the flow depth, h2 in the diagno_xx.out file does not account for the rills. Hence, need to adjust the flow depths before plotting against the analytical results. Adjust the flow depths using the tw entry in the diagno_xx.out file. The tw entry is the width of the water in the rill. The equation to adjust the flow depth is: $h_w = 2 * h_2 / (0.1 + tw)$

The files used to produce the output and diagno.out file for KINEROS2 Versions 1.13 are:

- .\Kineros\Version1.13\Test3c*
 - .\ronmicv50.fil input control file
 - .\ronvalidm50.par parameter file with PR=4 to produce diagno.out
 - .\norain.pre no precipitation
 - .\inject4.dat referred to in the parameter file

Similar input files for rill widths of 100 and 150

The output files are

- .\diagno_50.out, diagno_100.out, and diagno_150.out
- .\ronmalm50.out, ronmalm100.out, and ronmalm150.out

Results are collected in the spreadsheet:

- .\test3c_v113.xls, worksheet "KINEROS2 Results"

Note that the Distances Along the Plane have to be calculated knowing the length of the plane (100m for Re=50mm, 120m for Re=100 and 150 mm), and knowing the number of calculation nodes in the plane (15 nodes). These calculations are done in the worksheet "KINEROS2 Results". The distances match up with the data in the diagno.out files.

Note that Roger used nonsequential numbering to name his files (Re=100 uses "3", Re=150 uses "2"):

- Re=50: ronvalidm1.par, rondiagm1.out, and ronvalm1.out
- Re=100: ronvalidm3.par, rondiagm3.out, and ronvalm3.out
- Re=150: ronvalidm2.par, rondiagm2.out, and ronvalm2.out

I re-ran version 1.9 with Rill=50mm depth to confirm that I got the same results as Roger.

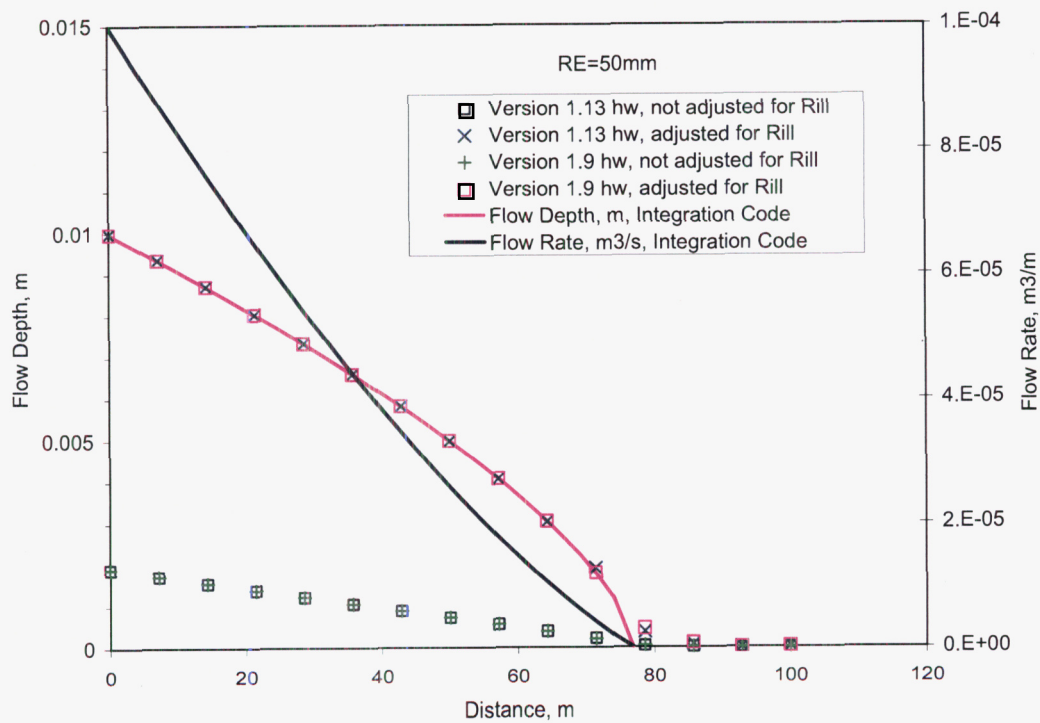
- .\Kineros\Version1.9\Test3c\diagno.out

This file had the same results as Rogers

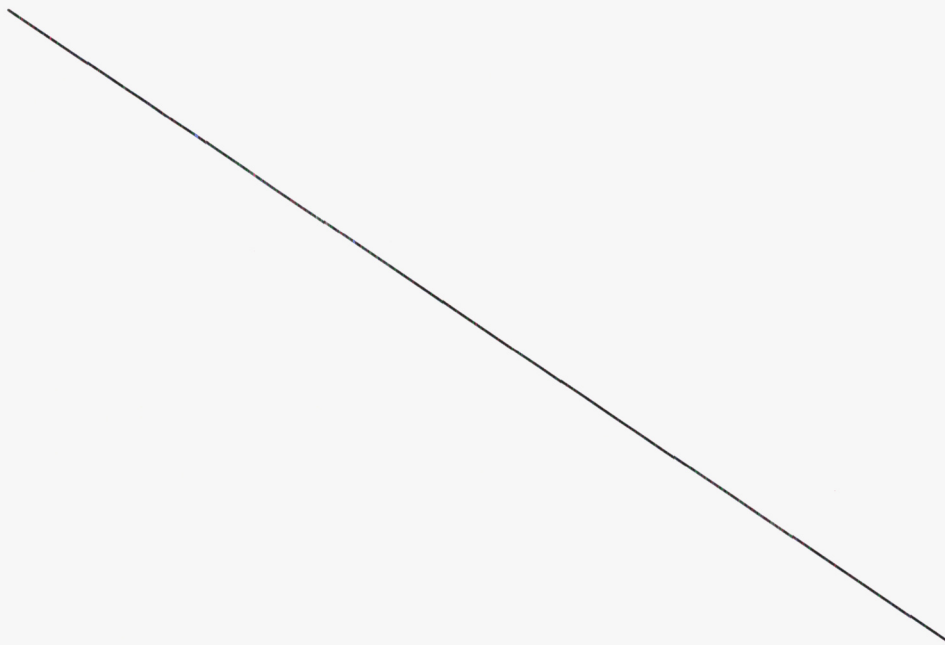
- .\Kineros\Version1.13\Test3c\Rogers\rondiagm1.out

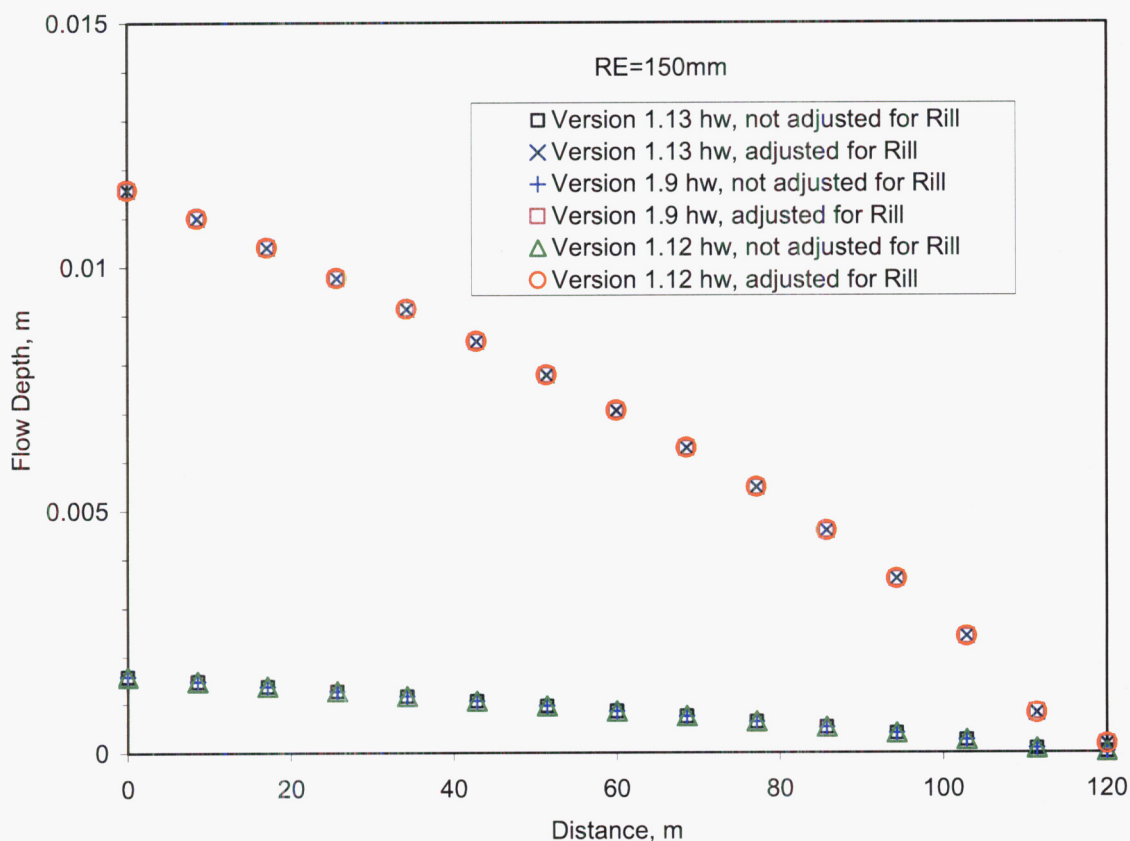
The figure on the next page (XI-25) shows that Versions 1.9 and 1.13 produce the same water height profiles, both "h2" from the diagno.out files and the water height adjusted for rill geometry. As noted, Version 1.13 does not spit out flux profiles along the plane in the diagno.out files, hence a comparison could not be made. The adjusted water height was calculated as noted a few paragraphs back.

The figure is from the "Plot" worksheet in the spreadsheet test3c_v113.xls.



The next figure (page XI-26) directly compares the "h2" output in diagno.out files for each version (1.9, 1.12, and 1.13) and the adjusted water depths (using "tw" from diagno.out files). The three versions of KINEROS2 clearly produce the same water profile along the plane element. The figure below is from the "Plot RE=150" worksheet in the test3c_v113.xls spreadsheet.





End June 9, 2008 RF

Start May 27, 2008 RF

Test Case 4, Versions 1.9, 1.12, and 1.13

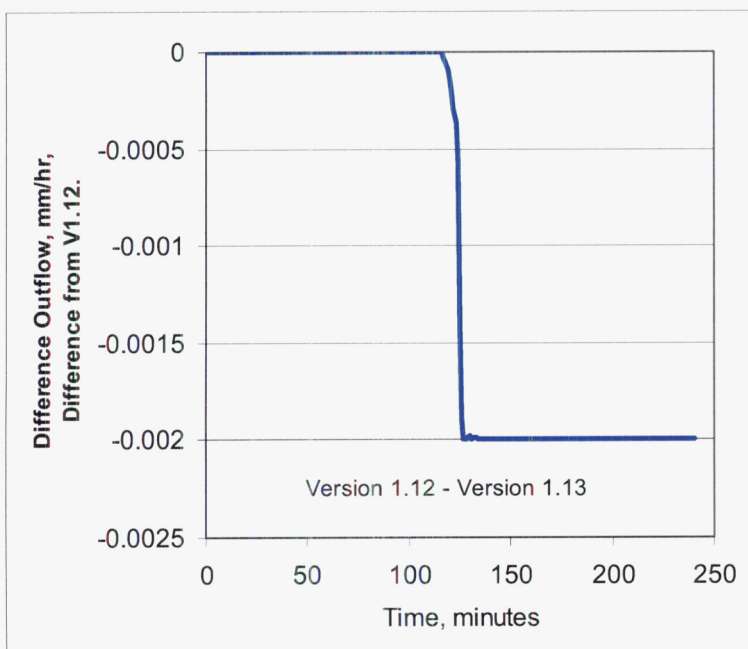
Version 1.9 simulation did not run to completion because of negative infiltration values. The problem appears to be with the parameter input value for G for the bedrock. When $G=0$ for bedrock, Versions 1.12 and 1.13 run fine; however Version 1.9 simulation aborts. Therefore, I used a value of $G=0.01$ mm for the bedrock in the Version 1.9 simulation. This should not change the results much as this value of G is very small compared to the other layer (soil layer above the bedrock has $G=50$ mm). I note that Roger used Version 1.12 for this test case, thus, he was not aware of this problem. (Roger used Version 1.9 for his Test 1, Test 3a, and Test 3c simulations; Version 1.8 for Test 3b, Version 1.12 for Test 4; Woolhiser appeared to have used Version 1.1.2 for Test 5).

In 2005, I replotted Roger's results from Version 1.12, dated Nov 2003. I re-ran the simulation using Versions 1.9 and 1.13 in May 2008 to compare the results of the two versions.

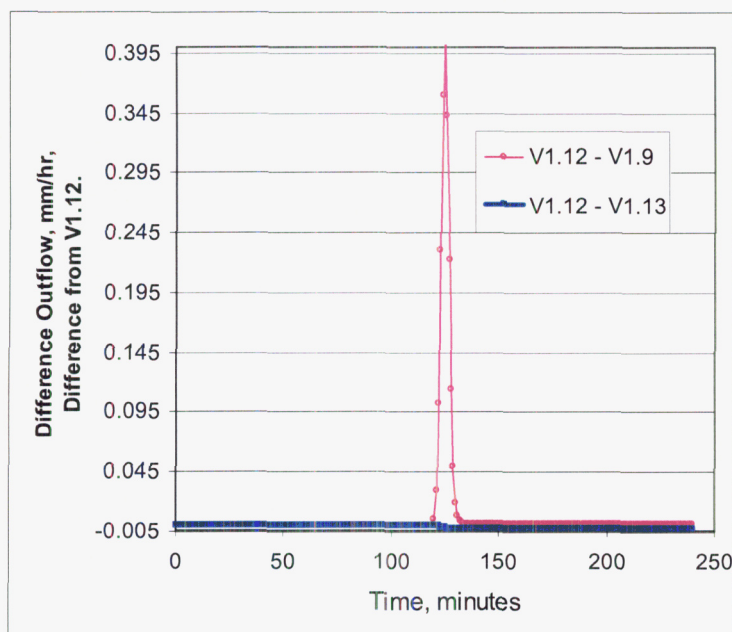
.\\Kineros\\Version1.9\\Test4* (no spreadsheet, results imported into test4_v1.13.xls
.\\Kineros\\Version1.12\\Test4_replotted.xls
.\\Kineros\\Version1.13\\Test4\\test4_V1.13.xls
(contains comparison of Versions 1.9, 1.12 & 1.13)

The input files for each version are: SAT_TEST1.PRE, SAT_TEST2L.PAR, SAT_TEST3.FIL.
Note that the parameter input file (SAT_TEST2L.PAR) for Version 1.9 uses a G value of 0.01 for the bedrock, instead of a value of 0.

There is a small difference between output of Versions 1.9, 1.12, and 1.13 (see next figure, after this paragraph; page XI-27). For the time period just after the soil capacity has filled and extending through the time when the asymptotic infiltration value is reached (time 117 to 129 minutes), the difference increases (in an absolute sense) from zero to -0.002 mm/hr. Version 1.13 results show a slightly faster increase in runoff, once runoff starts; the first non-zero value of runoff at 116 minutes for both versions is identical. Note the difference in the following figure is calculated as Version 1.12 outflow – Version 1.13 outflow. At the steady runoff period following the transition (129 minutes to the end of the precipitation at 240 minutes), Version 1.13 runoff results are a uniform 0.002 mm/hr larger. Note that Version 1.13 more closely matches the expected 19.5 mm/hr outflow (runoff), thus appears to be more precise. But for all practical purposes, the error in either version is small (0.01%, 0.01%, and 0.0001% for versions 1.9, 1.12, and 1.13, respectively) for the steady runoff rate. Versions 1.9 and 1.12 slightly underpredicted the runoff rate, whereas version 1.13 ever-so-slightly overpredicted the runoff.

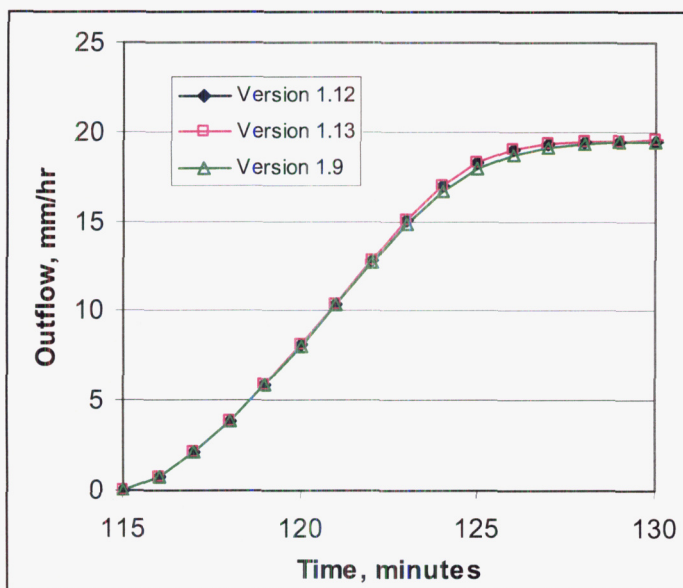


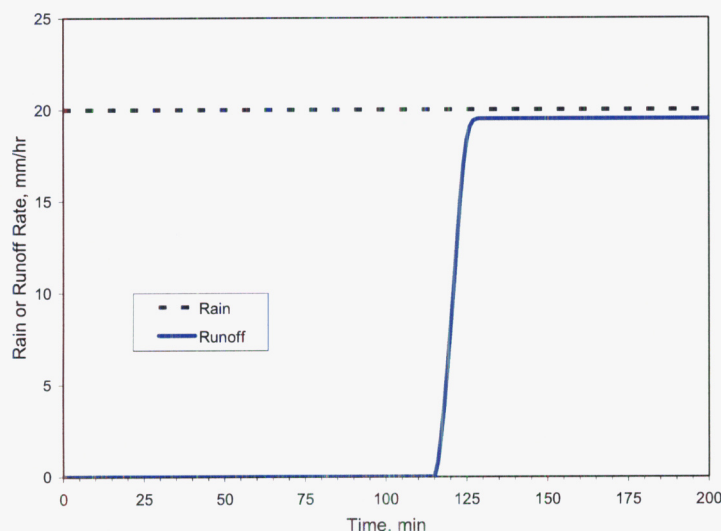
The steady value of runoff for
Version 1.9 is 19.49790
Version 1.13 is 19.49802
Version 1.13 is 19.50002



Version 1.9 had the same values of runoff for the first 5 or 6 steps when runoff started. However, from 120 minutes to 130, Version 1.9 was slower to reach the asymptotic value of approximately 19.5 mm/hr. The sharp peak in the figure above reflects this difference between Version 1.9 results, and those of Versions 1.12 and 1.13. This may be caused by the nonzero value of G for bedrock used for the Version 1.9 simulation. This minor difference does not change the conclusion of the software validation test (criteria are onset of runoff and asymptotic value of runoff).

The figure below illustrates the slightly slowly approach to asymptotic outflow (runoff) for Version 1.9 results. This difference is minor, calculated as max difference with Version 1.12 results divided by the outflow for Version 1.12 for that time step $\rightarrow 2.2\% = (0.4017/18.31)$ mm/hr





The results shown on the figure to the left, which is included in the software validation report, are from KINEROS2 Version 1.13. The figure is in the "Plot" worksheet of the test4_V113.xls spreadsheet. Both versions have runoff initiating between 115 and 116 minutes, as indicated by the first non-zero value of runoff. Closer estimation of runoff initiation is not warranted because of the nonlinearity.

Besides the predicted value is 115 minutes, and maximum difference between KINEROS2 and predicted onset is 1 minute, which is easily less than the 2% criteria for software validation.

Test Case 5, Versions 1.9, 1.12, and 1.13

Output collected in test5_v19.xls, test5_v112.xls, and test5_v113.xls spreadsheet files located in the respective version directories (i.e., test5_v19.xls is in .\Version1.9\Test5*).

Obtaining Measured Data from Walnut Gulch

Measured data from Walnut Gulch were not provided by Roger Smith or Dave Woolhiser for this test case. Thus, measurements of rain rates and runoff for the Lucky Hills watershed at Walnut Gulch were obtained on the web. Lucky Hills is referred to as watershed #106. The closest rain gage is #384, which appears to be near the edge of the watershed. A second rain gage is located to the northeast, and is called #83. Rain gage #83 is approximately 150 meters from the edge of the Lucky Hills watershed (#106). Rain for the 4 events registered first at rain gage #83. Roger Smith used data from both rain gages for the test case input file for precipitation. KINEROS2 combines the two rain gage data sets for use in the computations. When comparing simulation results with measured runoff values, the clock time inherently becomes important in terms of when a watershed sees the rain

The website for Walnut Gulch runoff data sets was obtained from http://www.tucson.ars.ag.gov/dap/runoff_event.asp##

The options on this data request page are

- Walnut Gulch (63)
- Select Flume 106
- Choose 4 dates of the 4 events listed in the software plan
 - July 19, 1974; Event 50
 - July 12, 1975; Event 62
 - July 17, 1975; Event 63
 - Sept 26, 1977; Event 75
- Choose options for hydrograph, excel, cfs

Similarly, for rain data, choose gages 384 and 83 from the web site:

<http://www.tucson.ars.ag.gov/dap/event.asp>

Options are to choose dates, breakpoint data, and excel

This data sets, with appropriate file names, were stored in
.\KINEROS\Downloaded_WalnutGulchData*

A map of the site can also be obtained from the web site to help locate the watershed and rain gages (not reproduced here because of potential copyright issues). Just click on the Walnut Gulch map button on either of the websites listed above, or,

http://www.tucson.ars.ag.gov/dap/images/WalnutGulch_map.jpg

Two journal articles were published in support of the data:

Goodrich, D.C., et al. Long-term precipitation database, Walnut Gulch Experimental Watershed, Arizona, United States. Water Resources Research 44, W05S04, doi:10.1029/2006WR005782, 2008.

Stone, J.J., et al. Long-term runoff database, Walnut Gulch Experimental Watershed, Arizona, United States. WATER RESOURCES RESEARCH, VOL. 44, W05S05, doi:10.1029/2006WR005733, 2008

It was confirmed that the downloaded rain data matched the KINEROS2 precipitation input file data provided by Roger Smith. Note that the plots of rain in the software validation report include KINEROS2 output of rain, not measured rain values from the 2 gages. My comparison of rain downloaded from the web and Roger's precipitation input files was done to gain confidence that the correct events and files were downloaded. Also, the precipitation and runoff measurement files contain clocktime needed for the comparison of measured versus simulated runoff. The focus of the test case was to compare actual measured runoff data against simulated runoff data. The downloaded runoff data was visually compared with the plots of Roger's for this test case, and found to be the same.

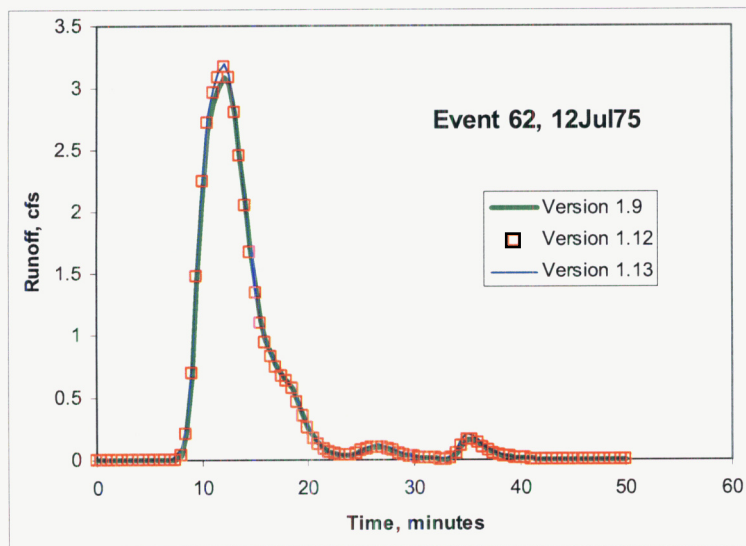
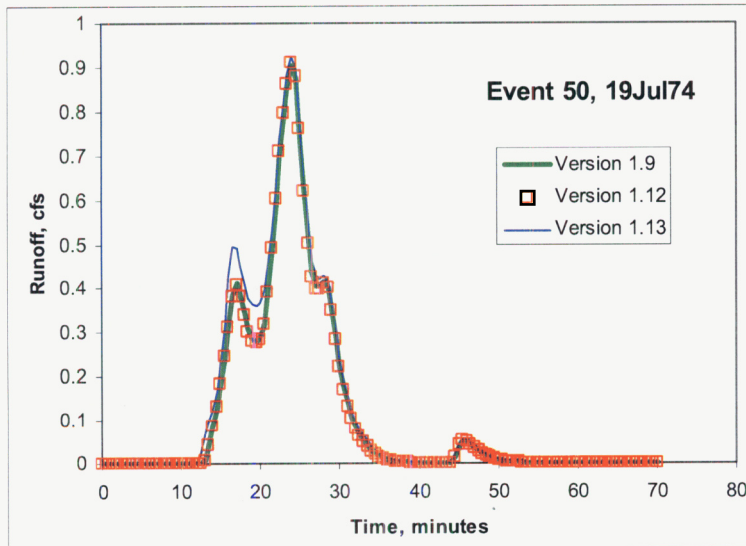
To resolve the difference in timing between the (i) rain gage times and flume flow rates, and (ii) KINEROS2 times (which start at zero), the measured runoff rates had to be adjusted by the difference between the precipitation event start time and the flume start time. This had to be done in order to plot the measured runoff data against the simulated runoff data. While an average difference could have been used (average of the two rain gages), it makes more sense to use the start times from the rain gage located right at the watershed boundary. Use of either approach likely leads to some error in terms of timing of the runoff peaks because gage or gages probably do not represent the timing of the rain across the Lucky Hills watershed exactly.

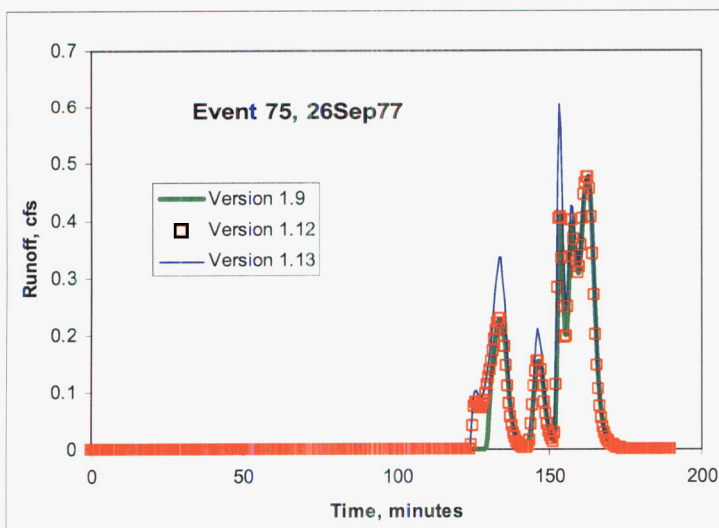
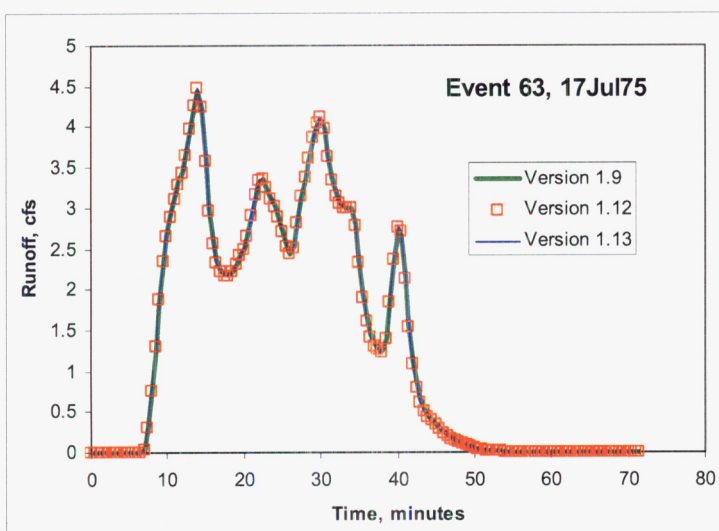
Problem with Rain Output for Version 1.12

Version 1.12 rain rate (mm/hr) output in the tabulation of time and rain is wrong. This was noted when comparing the rain output from Version 1.12 with the other versions; version 1.12 output differed from that of Version 1.9 and 1.13 rain output. However, the runoff output from Version 1.12 nearly matches that of Version 1.9 and 1.13 runoff output. It is clear that the runoff is correct, but the outputting of rain rate in the time-dependent tabulation of results in Version 1.12 was messed up.

More importantly, the total rain for the event was correct; this is listed in the summary table at the bottom of the output file. An abstraction for runoff developed from Upper Split Wash by Woolhiser would only use the total rain for an event.

Therefore, in all the plots and comparisons, rain rates for Version 1.12 used rain from either other version. Below are four plots, one per event, comparing Versions 1.9, 1.12, and 1.13 runoff output.





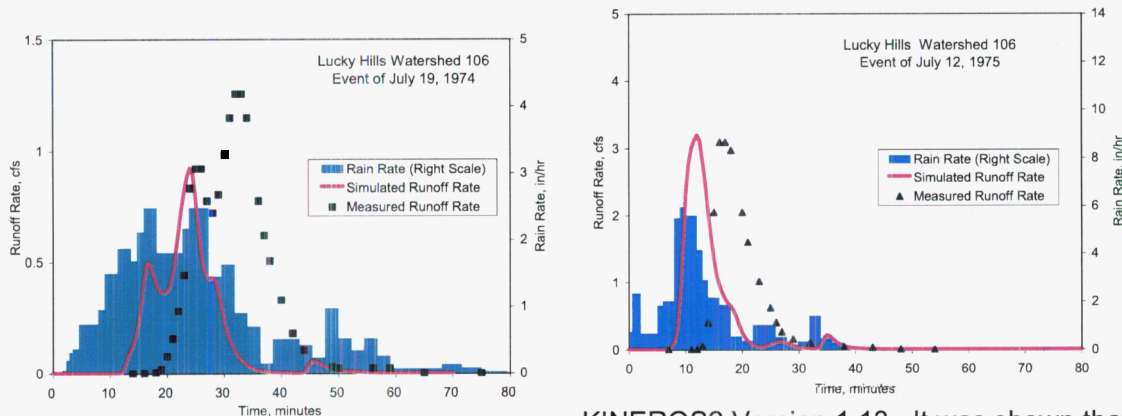
These 4 figures (above) were created in the spreadsheet called test5_v113.xls, worksheet "Compare Versions."

Generally speaking, runoff from Version 1.9 and 1.12 match closely. Version 1.13 runoff hydrographs exhibit slightly higher peaks for events 50 and 75, but match runoff from the other versions closely for events 62 and 63. The timing and pattern of runoff is otherwise identical for the KINEROS2 Versions 1.9, 1.12, and 1.13.

In terms of using Version 1.12 for Upper Split Wash at Yucca Mountain, the problematic rain output does not matter. The total rain for the event shown in the table at the bottom of each output file is correct. Only the infiltration and total rain were used for the runoff/runoff abstraction in TPA 5.1. The slightly higher peaks occasionally seen in the 4 events (not all peaks for exhibit Version 1.13 as being higher than the rest), means that infiltration may have been slightly under-estimated for Upper Split Wash at Yucca Mountain. The amount under-estimated is likely much smaller than the uncertainties for the runoff/runoff abstraction.

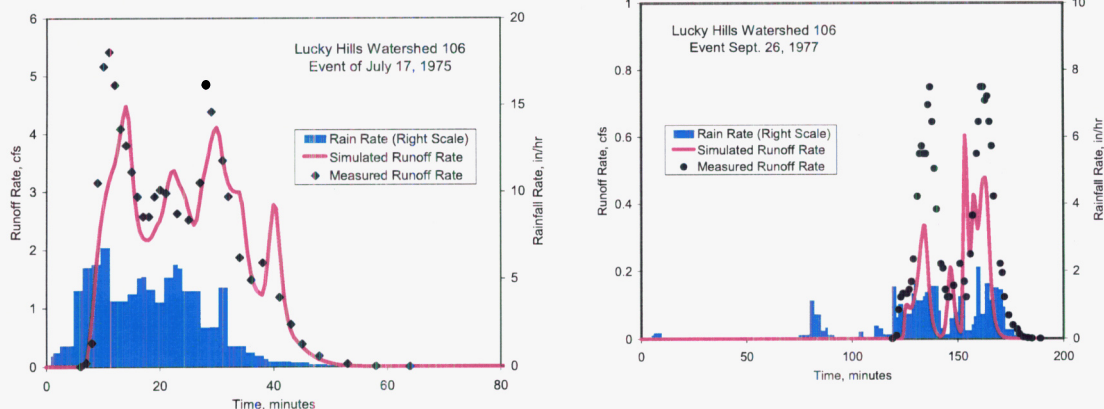
Plots and Analyses for Software Validation Report

Plots from the spreadsheet test5_v113.xls were put into the report. The actual figures were located as worksheets: "Plot Event 50," "Plot Event 62," "Plot Event 63," and "Plot Event 75" in the spreadsheet. These plots represent output from



KINEROS2 Version 1.13. It was shown that

Version 1.13 results were close, with minor differences in some of the peak flows, to results from Versions 1.9 and 1.12.



The timing of peaks is slightly shifted between simulated and measured for Events 50 and 62. A reason for this shift was discussed earlier and had to do with the direction of storm travel, and the timing of rain gage measurements versus the timing of when the watershed actually sees rain. Specification of initial conditions and calibration uncertainty of hydrological properties could also be factors. Remember that the watershed model was calibrated using a different set of events and KINEROS (an earlier version of KINEROS2) (Goodrich, 1990), and the properties were not further tuned for this modeling exercise.

The magnitude of peaks is underestimated in the simulations for Events 50, 63, and 75. The magnitude of runoff for Event 62 is well matched. The magnitudes could be off because of initial conditions, calibration uncertainty for hydrological properties, or how well the rain gages represent rain that falls over the watershed.

End May 27, 2008 RF

02/28/2005 RF

HYDRUS2D VERSION 2.01

As required for use in license application review, any software that produces data or conclusions that will be directly used in the license application review (i.e., safety evaluation report) must go through the TOP-018 software validation process. This process includes writing a software validation test plan and a software validation test results reports, both of which must go through the complete CNWRA review process.

Randall Fedors
Collaborators: None

Objective

spock: ~rfedors/SoftwareValidation/*
~rfedors/Bore/Analytic/analgwst.1/

bubo: E:\SoftwareValidation\HYDRUS2D*

Stripi code from the USGS

Previously used stripi for borehole dilution (scientific notebook 227).

The code was obtained from the U.S. Geological Survey, the compressed tar file is

spock: ~rfedors/Bore/Analytic/analgwst.1/analgwst.q.source.tar.gz

Stripi is run using a script in the local working directory. The script has the paths to the stripi executable (~rfedors/Bore/Analytic/analgwst.1/bin/stripi.exe) and to the Gauss-Legendre quadrature point file glq.pts. With the script and input file in the local working directory, the script may be run to reach an interactive prompt requesting the input file name, then the output file name (the name of the output file can default to base_filename.prt).

Notation for axes in stripi and HYDRUS2D: The xy plane in stripi corresponds to the zx plane in HYDRUS2D, except that the z-axis is positive upward in HYDRUS2D. Thus, the x-axis in stripi is flipped from the corresponding z-axis in HYDRUS2D, which just makes plotting comparisons slightly more difficult.

Confirmed that negative y-axis values can be used in stripi for the transverse axis by comparing results with from the two following input files

input file "sample7.dat"	original example problem 7 distributed by USGS in Wexler (1992) y-axis ranges from 0 to 1500 m with solute line from 635 to 865 m
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input file "sample7_yshift.dat"	shifted the y-axis locations to -750 m to +750 m with solute strip from -115 to +115 m on y-axis
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Results from sample7.dat and sample7_yshift.dat, when accounting for the translation, were identical.

HYDRUS2D Input Files

Input for transport parameters: "Disp.L" and "Disp.T" are dispersivities (α_L and α_T). Hence, to match the analytical solution that uses longitudinal dispersion = $0.1 \text{ m}^2/\text{d}$, the HYDRUS2D input should factor in the velocity (v) using the expression $D_L = v \cdot \alpha_L$. For a particle velocity of 0.1 m/d , which corresponds to a Darcy velocity of 0.03 m/d and a porosity of 0.3 , the $\alpha_L = 10 \text{ m/d}$ for the HYDRUS2D input. The particle velocity of $v = 0.1 \text{ m/d}$ and dispersion $D_L = 1 \text{ m}^2/\text{d}$ should be the input for the stripi analytical solution. Note, to confirm that HYDRUS2D is using the same particle velocity as the analytical solution, the plot of velocities in the graphical package should show a uniform value of "velocity" equal to 0.03 m/d ; this graphical package uses the term "velocity" to refer to the darcy velocity.

Comment in VS2DT documentation (Water-Resources Investigations Report 99-4130):

The most common occurrence of this apparent discrepancy is on the very first time step of a simulation when there is an inconsistency between initial and boundary conditions. Such an occurrence is manifested by a large mass balance error for the first time step. Users should be aware of this apparent discrepancy and should not be overly concerned about the mass balance error. NOTE, the same type of apparent discrepancy can occur in the Solute Mass Balance when fixed concentration boundaries are assigned in recharge periods.

RF 04/04/05

No mas (mgmt decided no validation was needed for HYDRUS).

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Entries made into Scientific Notebook #432E Volume XI for the period April 3, 2002 to June 10, 2008 have been made by Randall Fedors (June 10, 2008). RF

No original text or figures entered into this Scientific Notebook has been removed.

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ADDITIONAL INFORMATION FOR SCIENTIFIC NOTEBOOK NO. 432E

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