



Department of Pesticide Regulation



Mary-Ann Warmerdam
Director

MEMORANDUM

Arnold Schwarzenegger
Governor

TO: John S. Sanders, Ph.D.
Environmental Program Manager
Environmental Monitoring Branch

FROM: Bruce Johnson, Ph.D.
Research Science III
Environmental Monitoring Branch
(916) 324-4106

Original signed by

DATE: November 17, 2008

SUBJECT: DOW AGROSCIENCES-CHAIN2D REVIEW

Attached are three memorandums that I wrote to Randy Segawa reviewing the Dow AgroSciences-CHAIN2D modeling system submitted by the Chloropicrin Manufacturers Task Force. Since this modeling system was referenced in recent U.S. Environmental Protection Agency (EPA) documents, the attached comments were also posted on four fumigant dockets (EPA-HQ-OPP-2007-0350, EPA-HQ-OPP-2005-0128, EPA-HQ-OPP-2005-0125, and EPA-HQ-OPP-2005-0123) and can be found at <www.regulations.gov>, and searching for EPA-HQ-OPP-2005-0128-0207.1

For reasons outlined in these memorandums, the Dow AgroSciences-CHAIN2D modeling system is not acceptable for estimating flux. We are currently evaluating other modeling tools for flux estimation.

Attachments





Department of Pesticide Regulation



Mary-Ann Warmerdam
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MEMORANDUM

Arnold Schwarzenegger
Governor

TO: Randy Segawa, Environmental Program Manager I
Environmental Monitoring Branch

FROM: Bruce Johnson, Ph.D.
Research Science III
Environmental Monitoring Branch
(916) 324-4106

Original signed by

DATE: October 29, 2008

SUBJECT: REVIEW OF WESENBEECK (2007B)

Wesenbeeck, Ian van. 2007. Impact of Mitigation Practices on Emissions of Chloropicrin During Soil Fumigation as Predicted by CHAIN_2D. Chloropicrin Manufacturers Task Force, Consortium Number 065353, Project Number CMTF2007-5.

This is a review of the third of three papers submitted by the Chloropicrin Manufacturers Task Force on modeling. The first paper was Cryer and Wesenbeeck (2007) and my review of that Johnson (2008a). The second was Wesenbeeck (2007a) and my review was Johnson (2008b).

Wesenbeeck (2007b) presents results from running the DowAgroSciences (DAS)-CHAIN2D modeling system and it depends on foundational documents (Cryer and Wesenbeeck 2007, Wesenbeeck 2007a, and documents cited within). I reviewed the foundational documents and found that they do not provide adequate support for use of DAS-CHAIN2D (Johnson, 2008ab). Therefore, the conclusions in Wesenbeeck 2007b are not acceptable.



Randy Segawa
October 29, 2008
Page 2

References

Cryer, Steve and Ian van Wesenbeeck. 2007. Simplifying the Implementation of CHAIN_2D with Modifications Specific to Soil Fumigation Practices. Chloropicrin Manufacturers Task Force, Consortium Number 65353, CMTF2007-4.

Johnson, Bruce. 2008a. Memorandum to Randy Segawa on Review of Cryer and Wesenbeeck (2007) dated October 2008.

Johnson, Bruce. 2008b. Memorandum to Randy Segawa on Review of Wesenbeeck (2007) dated October 2008.

Wesenbeeck, Ian van. 2007a. Validation of CHAIN_2D Modeling Against Chloropicrin and 1,3-Dichloropropene Field Volatility Studies. Chloropicrin Manufacturers Task Force Consortium Number 65353, Project Number CMTF2007-3.

Wesenbeeck, Ian van. 2007b. Impact of Mitigation Practices on Emissions of Chloropicrin During Soil Fumigation as Predicted by CHAIN_2D. Chloropicrin Manufacturers Task Force, Consortium Number 065353, Project Number CMTF2007-5.



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FROM: Bruce Johnson, Ph.D.
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DATE: October 29, 2008

SUBJECT: REVIEW OF CRYER AND WESENBEECK (2007)

The Chloropicrin Task Force has submitted three volumes for review: [199-0125] Simplifying the Implementation of CHAIN_2D with modifications specific for soil fumigation practices (Cryer and Wesenbeeck 2007); [199-0126] Validation of CHAIN_2D against chloropicrin and 1,3-dichloropropene (1,3-d) field volatility studies (Wesenbeeck 2007a); [199-0127] Impact of mitigation practices on emissions of chloropicrin during soil fumigation as predicted by CHAIN_2D (Wesenbeeck 2007b). This is a review of Cryer and Wesenbeeck (2007).

Introduction

Integral to evaluating this submittal, though not included in the package, was the actual software which is described in Cryer and Wesenbeeck (2007). This software consists of a Visual Basic (VB) program housed in an Excel workbook that creates input files for the CHAIN_2D program, runs the CHAIN_2D and then reads the output files and produces certain summaries. The CHAIN_2D component, which is written in FORTRAN, was originally produced by Simunek and van Genuchten (1994). SA Cryer of DowAgroSciences (DAS) has modified the original CHAIN_2D FORTRAN code. There is no ready name for the package of VB and modified CHAIN_2D software to distinguish it from the CHAIN_2D as originally developed by Simunek and van Genuchten. To distinguish, I shall refer to the original CHAIN_2D as CHAIN_2D. I shall refer to the package of VB and modified CHAIN_2D produced by Cryer and Wesenbeeck (2007) as DAS-CHAIN2D since Wesenbeeck and Cryer work for DAS.

As part of this review, I have obtained DAS-CHAIN2D software and will include comments about it in this review. In addition, a key document cited in Cryer and Wesenbeeck (2007), contains the theoretical underpinnings for the dynamic boundary modifications made to the CHAIN_2D model and implemented in the VB front end for the model (Cryer 2007). As of this writing, Cryer (2007) is not available. The citation lists it as an internal report for DAS and I have requested that it be released for review. A similarly titled document, Cryer (undated), accompanied the software on the CD. The author (Cryer, personal communication) indicated that the contents of Cryer (undated) and Cryer (2007) were similar. Thus, I will substitute comments based on Cryer (2007) for Cryer (undated).



1. The documentation for using DAS-CHAIN2D is spread all over: some in the worksheets, some in the comments in the VB code, and some in external documents. This makes it difficult to use the program.
2. Units for Ks and Bulk Density missing in Table 1.
3. The column in Table 1 with header θ_a appears to be a duplicate of the first column, but is otherwise undefined.
4. Wesenbeeck and Cryer (2007) state (page 8): “Representative values for θ_r , θ_s , α and n have been tabulated for the 12 specific soil textures and can be found in the PRZM3 manual (Carsel et al., 1995; Table 5-42) or within the documentation for the U.S. Department of Agriculture ROSETTA program (Schaap et al., 2001) in a hidden worksheet called “Soil_Properties” and are found in Table 1.” The Carsel et al. (1995) citation is listed in the references as:

Carsel, R.F., J.C. Imhoff, P.R. Hummel, J.M. Cheplick, and A.S. Donigan, Jr. 1995. PRZM-3, A Model for Predicting Pesticide and Nitrogen Fate in the Crop Root and Unsaturated Soil Zones: Users Manual for Release 3.0, Chap. 6.5. National Exposure Research Laboratory, Office of Research and Development, U.S. Environmental Protection Agency, Athens, GA 30605- 2720.

The U.S. Environmental Protection Agency (EPA) CEAM Web site does not list a release 3.0. The release numbers available on the Web site are: 1.00, 1.02, 2.00, 2.3, 3.12 beta, 3.12.1, 3.12.2, and 3.12.3. The manual for the 3.12 β version (Carsel et al. 1998), which is the first listing on the Web site where the primary version changes from 2 to 3, lists the same authors and approximately the same title with the main differences being the version specification of 3.12 β vs 3.0 and the description of the manual as a draft version. In the manual for 3.12 β Table 5-42 in Chapter 5 provides θ_r and θ_s values which match those in Table 1 and Table 5-41 lists values for α and n consistent with those in Table 1.

I installed the ROSETTA program and located the textural table in a portion of the Help file. The screen shot entitled “ROSETTA Application Help” depicts that table.

The table, “Class average value of hydraulic parameters” in the Rosetta help file, are everywhere different from what is reported in Table 1. For example, Table 1 reports θ_r and θ_s for clay as 0.068 and 0.38, which differs from the 0.098 and 0.459 reported in the Rosetta table. Also, the estimated alpha and n values differ. The table in Rosetta provides $\log_{10}(\alpha)$ and $\log_{10}(n)$. For example, I used the TXT procedure in Rosetta to estimate parameters for a sandy loam and obtained the screen shot entitled “D:\PROGRAM FILES\rosetta\sample1.mdb-Rosetta.”

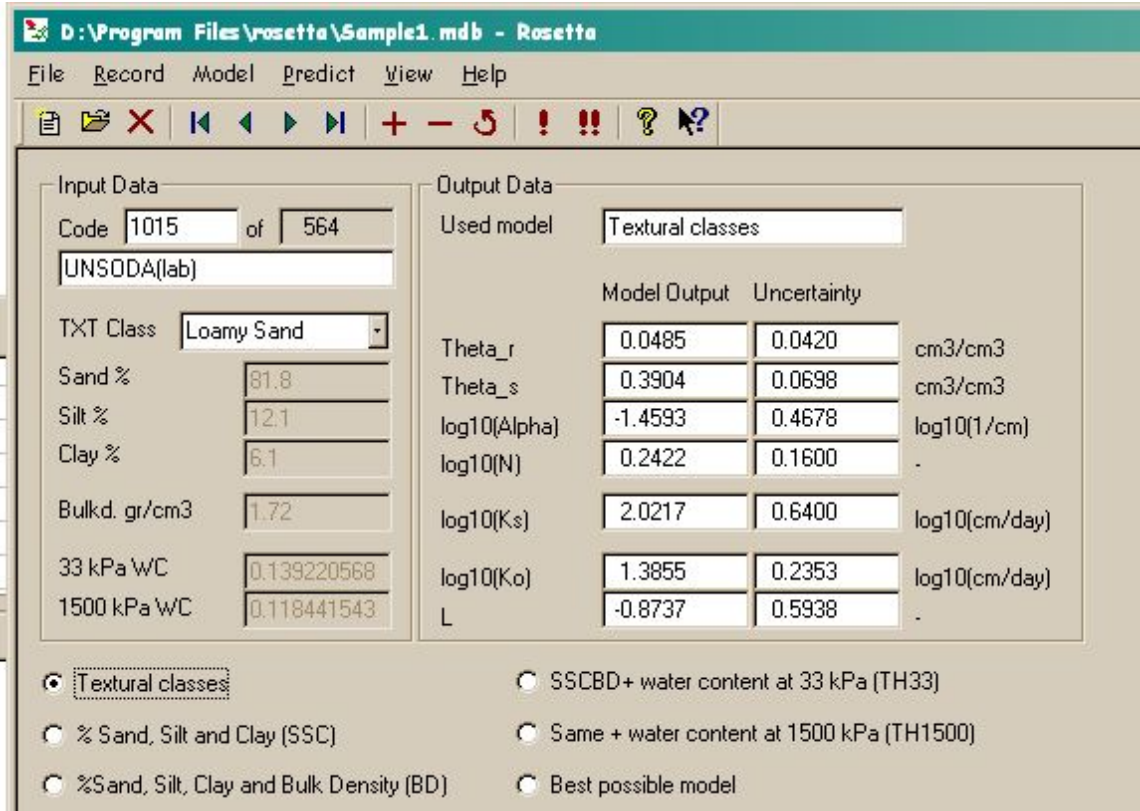
Class average values of hydraulic parameters

The table below gives class-average values of the seven hydraulic parameters for the twelve USDA textural classes. Effectively, this table represents the TXT model of the hierarchical sequence. For the θ_r , θ_s , α , n and K_s parameters, the values have been generated by computing the average values for each textural class. The values for K_o and L were generated by inserting the class average values of θ_r , θ_s , α , n into Model C2. This means that K_o and L are based on predicted parameters and may not be very reliable. The most reliable estimates of K_o and L can be obtained by using fitted θ_r , θ_s , α , n on the [Hydraulic conductivity](#) form. The values in parentheses give the one standard deviation uncertainties of the class average values.

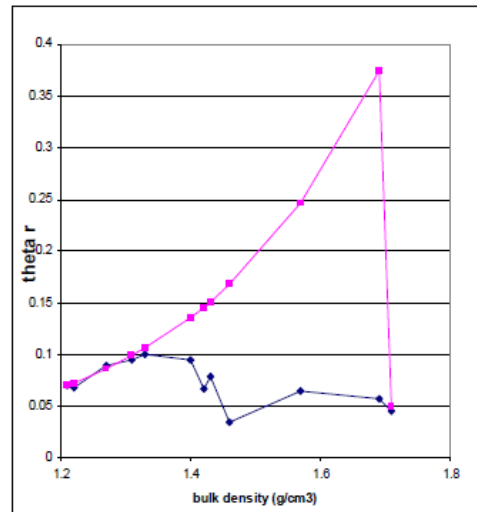
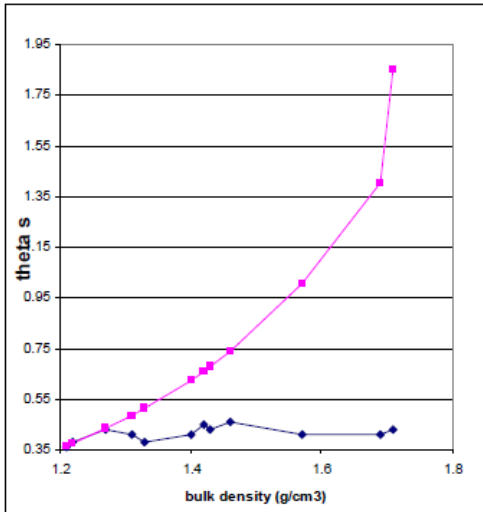
Texture Class	N	θ_r	θ_s	$-\log(\alpha)$	$-\log(n)$	$-K_s$	$-K_o$	$-L$
		cm ³ /cm ³	cm ³ /cm ³	log(1/cm)	log ₁₀	log(cm/day)	log(cm/day)	
Clay	84	0.098 (0.107)	0.459 (0.079)	-1.825 (0.68)	0.098 (0.07)	1.169 (0.92)	0.472 (0.26)	-1.561 (1.39)
C loam	140	0.079 (0.076)	0.442 (0.079)	-1.801 (0.69)	0.151 (0.12)	0.913 (1.09)	0.699 (0.23)	-0.763 (0.90)
Loam	242	0.061 (0.073)	0.399 (0.098)	-1.954 (0.73)	0.168 (0.13)	1.081 (0.92)	0.568 (0.21)	-0.371 (0.84)
L Sand	201	0.049 (0.042)	0.390 (0.070)	-1.459 (0.47)	0.242 (0.16)	2.022 (0.64)	1.386 (0.24)	-0.874 (0.59)
Sand	308	0.053 (0.029)	0.375 (0.055)	-1.453 (0.25)	0.502 (0.18)	2.808 (0.59)	1.389 (0.24)	-0.930 (0.49)
S Clay	11	0.117 (0.114)	0.385 (0.046)	-1.476 (0.57)	0.082 (0.06)	1.055 (0.89)	0.637 (0.34)	-3.665 (1.80)
S C L	87	0.063 (0.078)	0.384 (0.061)	-1.676 (0.71)	0.124 (0.12)	1.120 (0.85)	0.841 (0.24)	-1.280 (0.99)
S loam	476	0.039 (0.054)	0.387 (0.085)	-1.574 (0.56)	0.161 (0.11)	1.583 (0.66)	1.190 (0.21)	-0.861 (0.73)
Silt	6	0.050 (0.041)	0.489 (0.078)	-2.182 (0.30)	0.225 (0.13)	1.641 (0.27)	0.524 (0.32)	0.624 (1.57)
Si Clay	28	0.111 (0.119)	0.481 (0.080)	-1.790 (0.64)	0.121 (0.10)	0.983 (0.57)	0.501 (0.27)	-1.287 (1.23)
Si C L	172	0.090 (0.082)	0.482 (0.086)	-2.076 (0.59)	0.182 (0.13)	1.046 (0.76)	0.349 (0.26)	-0.156 (1.23)
Si Loam	330	0.065 (0.073)	0.439 (0.093)	-2.296 (0.57)	0.221 (0.14)	1.261 (0.74)	0.243 (0.26)	0.365 (1.42)

The row headers clarify that these are log base 10 values. For this loamy sand, the textural class model uses $\log_{10}(\alpha)$ of -1.4593 and $\log_{10}(N)$ of 0.2422, which correspond to the Rosetta table above, the fourth line (L Sand), giving the same values. Note that Rosetta estimates the θ_r and θ_s for loamy sand at 0.0485 and 0.3904, which differ from the corresponding values in Table 1, which are 0.057 and 0.41. When the Rosetta values for α and N are backtransformed ($\alpha=10^{-1.4593}$), the results are 0.034754 and 1.745822, respectively. Again, these differ from those values reported in Table 1 for loamy sand of 0.124 and 2.28, respectively. I checked the other entries in Table 1 and all of the entries for θ_r , θ_s , α and N differ from those in the Rosetta program.

Thus the tabulated values in Table 1 of Cryer and Wesenbeeck (2001) reflect those values found in Carsel et al. (1998), but differ from those found in Schaap et al. (2001), the second of two references cited as supported Table 1. The Carsel et al. (1995) reference is not available, as cited, on the U.S. EPA CEAM Web site.



- The fitting equations from Appendix C (“Correlation of van Genuchten soil parameters to bulk density”) for use with Table 1 provide erroneous estimates for residual and saturated water content. The derivation of these equations is not well documented. In Appendix C it is stated: “The following equations are obtained by curve fitting the soil properties table to bulk density and selected representation for extrapolation. As always, extrapolations beyond the data set are dangerous, and the user should heed caution.” Saturated water content cannot physically exceed 1.0 (theta_s) and should generally be less than 0.5. Yet, most of the values estimated by the empirical equations in Appendix C are wildly inaccurate.



In the left graph, the upper line is the saturated water content (θ_s), based on the empirical equations provided in Appendix C to estimate saturated water content and using the bulk density provided in Table 1. The lower line is the saturated water content for the textural classes as listed in Table 1. Similarly the right hand graph shows the residual water content based on the empirical equations in Appendix C, versus the lower line, which is the residual water contents reported in Table 1. The estimated values are very different from the reported values and suggest difficulties with the proper evaluation of these two key parameters in the modeling system. These parameters are key because the soil air diffusion of a fumigant depends heavily on the tortuosity, which in turn, depends on the estimated amount of water in the soil. The volatilization estimates cannot be trusted with this underlying discrepancy. For example, for the residual water content, when the bulk density is 1.6, the data in Table 1 suggests a residual water content of about 6%, whereas the estimated value is about 30%. This difference would lead to a large difference in tortuosity with much greater volatilization at a residual water content of 6% compared to 30%. The mean θ_r from Table 1 is 0.07 with a standard deviation of 0.02. Two standard deviations above the mean is 0.11, which would roughly represent a 9% upper limit. Yet, about half of the estimated values using the bulk density entries in Table 1 in the Appendix C equation give residual water contents above 0.11.

6. The use of mean textural values from the Rosetta program or from Carsel et al. (1998) to estimate hydrologic parameters is one of several approaches for obtaining the soil water retention and hydraulic conductivity functions. Other procedures utilize more specific soil information, if available, for estimating these functions. Spurlock (2008) examined the database upon which these textural values were based, and determined that some individual

soil records contained soil water/pressure measurements that emphasized the wet end of the soil moisture spectrum and had no measurements for the dry end of the soil moisture spectrum. This emphasis on the wet end probably reflected a historical bias in soil water models towards solute transport and saturated soil moisture conditions. However, with an emphasis on modeling volatilization, the dryer end of the soil spectrum becomes more important and errors in estimating soil water content can affect volatilization estimates. Spurlock (2008) concluded that certain estimation procedures tended to underestimate soil water content, compared to a selected group of soils for which the soil water retention curves were fairly complete. This underestimation would in turn lead to an overestimation of volatilization. This was especially true of the texture-based procedure, which lacked any other specific soil information. Whether volatilization will be over- or under-estimated depends more specifically on what part of the soil moisture spectrum is being simulated. Moreover, the texture based estimation procedure utilizes the mean van Genuchten parameters for each soil class. The procedure of taking the mean does not account for possible correlations between the van Genuchten parameters. As a result, the texture based approach results in greater inaccuracy compared to other approaches which include more soil information, such as water retention values at $-1/3$ and -15 bars. The reliance on only texture (except for the shank trace component) in DAS-CHAIN2D to estimate soil water retention properties is probably related to the goal of integrating SOFEA with DAS-CHAIN2D (Cryer and Wesenbeeck 2007, pages 5-7). That integration would utilize georeferenced soil maps to develop flux profiles in DAS-CHAIN2D, which would then be utilized by SOFEA for simulation of air concentrations. Soil maps will most likely only include soil texture and do not include additional water retention values. Therefore, DAS-CHAIN2D has been constructed to use the textural level of the hierarchical soil water retention estimation in order to take advantage of soil maps and increase potential for automated processing.

7. Page 9. "This pressure head is assigned to all nodes as an initial condition before the simulation is initiated." To what does "this" refer?
8. Page 9 Shank trace. This feature of DAS-CHAIN2D is used frequently in the validation exercises of Wesenbeeck (2007). Yet, the shank trace discussion has no supporting references. I searched for "shank trace" studies. I searched using Google and obtained nine hits (Appendix 1). One was a protocol, five were articles which used the phrase "shank trace" to explain or discuss something, but provided no direct study of shank traces and the remaining three articles were irrelevant to the subject. I searched at University of California, Davis using their online bibliographic system which included AGRIS, CAB Abstracts, BIOSIS Previews, Agricola, Environmental Science and Pollution Management, Sci Finder, Science Citation Index, Agricultural and Environmental Biotechnology Abstracts, American Society of Agricultural and Biological Engineers, Food Science and Technology Abstracts. I got very few hits with "shank trace" and so tried using the words "shank" and "emission." I reviewed a total of 18 papers (listed in Appendix 1). Of the 18 papers, only 1 had direct bulk density measurements relating

to the shank trace (Wang et al. 2001). In Wang et al. (2001), bulk density measurements were reported from a vertical profile down the center of the bed. However, the shanks for applying the fumigant had been inserted from the side of the bed and, according to the authors, it was through the side of the bed where the shank fracture was located. Therefore, in Wang et al. (2001), the bulk density measurements did not provide measurements at the shank trace location. The paper does not report how many bulk density samples were taken or if there were replicates and associated statistics. Against this meager set of data for shank traces, the shank trace section of Cryer and Wesenbeeck (2007) includes choices of five different and precise geometric shapes such as rectangle, triangle and trapezoid. In addition, the model documentation states that the bulk density in the shank trace can be specified as a percentage change from nondisturbed areas around the shank trace. I could not find any support, explanation, or justification for these shank trace modifications. There is no guidance provided on when to use a particular geometric shape or how much to change the bulk density.

9. The support documentation for DAS-CHAIN2D does not mention the possibility of advective mediated fumigant loss (Chen et al. 1995, study funded by DowElanco). Chen et al. (1995) studied 1,3-d field losses using the LEACHM model, which was modified to include an advective component, reflecting barometric pressure changes. They state: “Relatively small changes in barometric pressure can result in advective gas fluxes that are much larger than diffusive gas fluxes.” (page 1816). In their 1,3-d study, they concluded “Barometric pressure changes over the measurement period were shown to drive advective vapor movement in model simulations.” (page 1820). The influence of barometric pressure changes on flux needs discussion.
10. The CHAIN2D component of the DAS-CHAIN2D system is a dated program. It is no longer supported by the original authors or founding agencies (Jirka Simunek, personal communication). In an e-mail to the Department of Pesticide Regulation (DPR) staff in May 2008, Dr. Simunek expressed the following points on CHAIN2D (Šimunek and van Genuchten, 1994):
 - (1) Released in 1994. Fully replaced by HYDRUS-1D in 1998.
 - (2) Public domain program.
 - (3) Not being further developed by its authors or agency (ARS). ARS lost the capability to further develop the program due to the retirement of Rien van Genuchten in May 2008.
 - (4) DOS (Disc Operating System) program, not supported by GUI (Graphical User Interface).

- (5) Ease of use: very difficult. Due to the lack of a comprehensive mesh generator, the program is usually used only for simple rectangular geometries that cannot well represent features, such as drippers, furrows, etc.
- (6) Number of references in peer-reviewed journals: very limited; only 12.
- (7) Since the last peer-reviewed journal references appeared in 2000, it is unlikely that the program is still being widely (if at all) used.
- (8) Validation: limited, not widely used.
- (9) Difficult detection of errors.
- (10) Used to represent a state-of-the-art in modeling of subsurface processes in the time of its release.
- (11) Independent reviews in the literature: No

The VB system developed by Cryer for DAS-CHAIN2D mitigates point #5 because Cryer has incorporated MESH GEN into the VB system. However, bugs that have been detected and fixed in Hydrus, the successor program, may be extant in CHAIN2D, but not corrected since the CHAIN2D code has not been updated for 10 years, since 1998 when it was replaced by Hydrus. Also, it is significant that the CHAIN2D code is not supported. Should, during the course of running DAS-CHAIN2D, bugs be found in the CHAIN2D code, it is unlikely that DAS or the CMTF will undertake a software support of CHAIN2D.

- 11. The existence of problems, such as the estimation equations in Appendix C, is symptomatic of the lack of sufficient model review, model quality control, and validation. The documentation references SOFEA, a previous project by the same author. SOFEA embodies a similar programming approach as the DAS-CHAIN2D project: SOFEA utilizes a VB program housed in Excel to write a user interface, create control files, execute a FORTRAN program (ISCST3), and assimilate the output files from the FORTRAN program to provide more convenient output. DAS signaled their acceptance of SOFEA in January 2005, by providing estimates for human exposure to 1,3-d based on that version of SOFEA in January 2005 (Wesenbeeck 2005). After January of 2005, I continued working on SOFEA, to investigate its veracity and found important problems over the subsequent years (Johnson 2005ab, Johnson 2006ab). While I am now satisfied that SOFEA version that I use produces numerically correct output for chronic concentrations when used as described in Appendix 2 of Johnson (2007), this confidence building required intensive effort. The complexity of this kind of modeling system needs time and resources to verify that the (1) modifications made to CHAIN2D are appropriate, consistent and provided numerically accurate results (2) that the VB front end is performing its calculations

in the manner intended. The issue of quality control and model verification is separate from model validation. The problems described above with the estimation equations in Appendix C were relatively easy to find and did not require running the model. Much more difficult to locate and verify, would be potential errors within the VB code itself concerning the setup of the input files and the assimilation of the DAS-CHAIN2D output files and/or problems with CHAIN2D itself before any of the modifications for DAS-CHAIN2D.

For example, in trying to simulate a drip irrigation study, I encountered an error in the model as distributed on the CD: The distributed model contained the number "1" in Grid_Inputs!B1 instead of a reference to Main!B3. This cell in Grid_Inputs was in a column of cells which receive input from the Main worksheet. The presence of the fixed number 1 in this cell indicated that somebody had typed the number 1 into that cell and *overwrote a formula*. I verified that this error was in the Excel file on the distribution CD, which is a read-only disk. The formula cells are not protected and thus subject to overwriting. The fact that this occurred in the model as distributed on the CD indicates poor quality control. No part of the documentation describes any effort to verify the numerical accuracy of DAS-CHAIN2D. The method of model distribution does not include a check that the model is calculating correctly after it is installed.

12. The theoretical underpinnings for the dynamic boundary layer are evidently described in Cryer (2007), which as of this writing is unavailable. As explained in the introduction, I have substituted Cryer (undated) for Cryer (2007). I submitted Cryer (undated) to Dr. Paw U of the University of California Davis, (Dr. Kyaw Tha Paw U), Professor of Atmospheric Science and Biometeorologist) for his comments. He provided the following comments:

Brief Review of Cryer:

In general, not a radically new method. Appears to be mainly slight modification of methods used in the past, and little indication that there are any advances associated with these slight modifications.

Appears to ignore general micrometeorological literature and focuses on engineering based approach to volatilization. Shows poor understanding of the effects of stability on atmospheric turbulence, implying free convection under unstable conditions (as opposed to micrometeorological understandings of enhanced turbulence, but not necessarily free convection); mainly due to engineering fixation on finite dimension flat plate analogy to the "infinite" ground surface of the real world. Little discussion or usage of Monin-Obukhov type similarity concepts for stability effects (stability term is used in Baker's equation, but this usage doesn't seem to be attached to the author's concepts of the effect of stability on micrometeorological flow scales). Usage of the Computational Fluid Dynamics model FLUENT not necessarily appropriate in this case. Small domain used, and turbulent flow scales

and interactions of the real world not well simulated with the small domain; boundary conditions not clear but probably not well-posed for these field conditions. Not clear which of the turbulent simulation types used in FLUENT (Reynolds Stress Model? K-epsilon or K-Omega? LES); and what coefficient choices used for these, and boundary conditions for them. Real world conditions with fairly low wavenumber eddies mixed with no horizontal boundaries frequently seriously limit utility of engineering flow based set-ups such as typical in FLUENT. The author's justification of the ability of the method to show flux peaks during the day is not very convincing, as usage of any simple volatilization model will show this because of temperature peaks during the day. Careful comparison (with similar methods of parameter estimation or fitting) of the proposed model with previous model is not shown in a real scatterplot.

13. As mentioned in comment #12 above, a portion of the boundary layer condition algorithms are based on regression models which in turn were summarized output from the Fluent model runs. The Fluent model itself is proprietary software which costs approximately \$22,000/year to lease. This engineering application would generally be unavailable. The regression equations are presented with high R2 values, but there is no other information on the regression.
14. Staff at DPR attempted to run DAS-CHAIN2D. They encountered program errors (Appendix 2). These program errors were evidently based on a somewhat different version of VB or possibly operating system or possibly Microsoft Office environment. DPR staff was using Microsoft Office 2000 with Excel 2000 under the Windows 2000 operating system, and also Windows XP operating system. We corresponded with the authors and received tips on how to modify the VB code in order to get the program to run. Generally, the tips consisted of recording macros, examining the resulting VB code, and modifying the DAS-CHAIN2D VB code accordingly, locating and replacing all relevant instances. We were able to eliminate some errors. One suggestion made by the authors was to utilize Excel 2003, since apparently DAS-CHAIN2D had been constructed for that platform. After Excel 2003 was installed (part of Microsoft Office 11), different errors resulted (Appendix 3). Further attempts to run the program for a particular case are outlined in a second review. Ultimately, DPR staff was not successful at running this program.

Staff concluded that the VB environment is fragile, subject to change and will result in other interested parties being unable to run this modeling system. Fewer people being able to run a model reduces confidence in the model. It seems unlikely that the DAS or the CMTF will support this model, either the CHAIN2D portion (which is a highly technical model based on soil physics, and itself no longer supported by its original authors), nor the VB portion of the model.

What are some characteristics of a well supported model?

- a. A Web site which functions as a support center for the model and
 - i. provides updates
 - ii. systematically keeps track of versions
 - 1. explains modifications for each version change
 - 2. describes bugs and fixes
 - 3. provides a time stamped repository of version numbers so that users know if there was a problem with previous runs
 - iii. has a FAQ page
 - iv. has a user forum so that users can pose questions and get answers
- b. The model itself has a version number which is reflected in all output
- c. The model distribution kit has test input and output files which can be run and compared in order to verify that the installed model at least duplicates known correct output
- d. The documentation provides examples
- e. Knowledgeable personnel are available to answer questions

For DAS-CHAIN2D none of the support activities are available, with the possible exception of knowledgeable personnel. However, model support activities do not appear to be a high priority.

Conclusion

This modeling tool should not be used for estimating volatilization. The basic method for estimating soil hydraulic parameters utilizes soil textural class averages which may not be accurate. The empirical methods for estimating the van Genuchten parameters give wildly incorrect results. The model environment is fragile and easily damaged. Quality control is poor. The model is not well supported. The CHAIN2D component of the modeling system is outdated and unsupported. The model includes the shank trace feature which appears to have no basis in the published literature. DPR staff encountered many program errors in trying to run the model.

References

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Appendix 1. Search for “shank trace” studies

I searched using Google and obtained nine hits. One was a protocol, five were articles which used the phrase “shank trace” to explain or discuss something, but provided no direct study of shank traces and the remaining three articles were irrelevant to the subject.

I searched at UC Davis using their online bibliographic system which included AGRIS, CAB Abstracts, BIOSIS Previews, Agricola, Environmental Science and Pollution Management, Sci Finder, Science Citation Index, Agricultural and Environmental Biotechnology Abstracts, American Society of Agricultural and Biological Engineers, and Food Science and Technology Abstracts. I got very few hits with “shank trace” and so used shank and emission. I reviewed a total of 17 papers. Of the 17 papers, only 1 had direct bulk density measurements relating to the shank trace (Wang et al. 2001). In this particular paper, bulk density measurements were reported from a vertical profile down the center of the bed. However, the shanks for applying the fumigant had been inserted from the side of the bed and, according to the authors, it was through the side of the bed where the shank fracture and associated higher volatilization was. Therefore, the bulk density measurements did not measure where the supposed shank trace was. The bulk density profile was compared (Wang et al. 2001 their Figure 5) to a similar bulk density profile from two bedded drip studies. Between 0 to about 20 cm depth, the bulk densities for the two drip studies ranged between 1.5 and 1.7 g/cm³, whereas for the shank application, the bulk densities ranged between 1.3 and about 1.5 g/cm³. The paper does not report how many bulk density samples were taken or if there were replicates and associated statistics.

Google Hits

1. [PDF]
EFFICACY AND 1,3-D EMISSIONS WITH APPROVED NURSERY STOCK ...
File Format: PDF/Adobe Acrobat–View as HTML
scrape soil into the shank trace and, combined with the split injection, could lead to better efficacy at deeper depths in the soil profile and potentially ...
<mbao.org/2007/Proceedings/013HansonBMBAO2007PAWproject.pdf>. Similar pages.

This is a protocol and mentions shank trace in one sentence. “The wings are intended to scrape soil into the shank trace and, combined with the split injection, could lead to better efficacy at deeper depths in the soil profile and potentially reduce 1,3-d emissions.”

A search for this document as a report was negative.

2. [PDF]

NEW CHISEL SHANKS ENABLE IMPROVED FUMIGATION OF FINER-TEXTURED ...

File Format: PDF/Adobe Acrobat - View as HTML

that it scraped soil from the side-walls into the shank trace beneath. A second. delta wing was positioned 16 inches above the delivery depth and a third ...

mbao.org/2003/036%20mckenrymnewchiselshanksmbao8-29-03.pdf. Similar pages

More results from mbao.org.

Reports on construction of new shank. Report states: "Compaction and filling of these shank traces was verified by random insertion of a penetrometer across the field surface." However, no data on bulk density or penetrometer readings provided. Also, mentions "In order to pull a series of five shanks through the soil at 24-inch spacings the field had been ripped to 48-inch depth in three directions." This might result in a field with disturbed soil everywhere.

3. [PDF]

TRENDS IN PEST DENSITIES, PESTICIDE USE, AND PESTICIDE RESISTANCE ...

File Format: PDF/Adobe Acrobat

each shank for shank trace closure; 4) fumigant delivery. must be split with half being emitted at the 40-50 cm. depth and half at the 60-75 cm depth; ...

www.uckac.edu/ppq/PDF/05_OCT.pdf. Similar pages.

Recommends using winged shanks for better filling shank traces, but provides no data on bulk density or any other measurements relating to shank traces.

4. [PDF]

G. Experimental Methods and Materials Typically when growers see ...

File Format: PDF/Adobe Acrobat - View as HTML

rate of delivery into a dried sandy loam soil revealed that the gas was more likely to come out the. shank trace than to move through pore spaces. ...

www.uckac.edu/nematode/PDF/Replant-Sec2.pdf. Similar pages.

More results from www.uckac.edu.

No data on shank trace presented.

5. March 23, 1999

Mounding soil into a bed directly over the shank trace also will seal the soil effectively.

Sealing the soil surface to prevent volatilization into the ...

commodities.caes.uga.edu/fieldcrops/cotton/cnl32399.htm - 13k – Cached. Similar pages.

No data on shank trace provided.

6. Nature of the neutral Na⁺-Cl⁻ sensitive shank (trace B) at steady state corresponds to the apparent chemical potential difference between lumen and cell as in the case of the Cl⁻ ...
<www.springerlink.com/index/N3GN42327663467X.pdf>. Similar pages.

Page evidently contained advertisements for curing your golf shank and hex shank drill bits.

7. JSTOR: Tobacco Pipes of Corinth and of the Athenian Agora
Shank, trace of bowl preserved. Red (2.5YR 5/6) clay and (1OR 4/6) slip, worn. From a pipe like C 119. Two rouletted lines around shank; edge of termination ...
<[Links.jstor.org/sici?sici=0018-098X\(198504%2F06\)54%3A2%3C149%3ATPOCAO%3E2.0.CO%3B2-G](http://Links.jstor.org/sici?sici=0018-098X(198504%2F06)54%3A2%3C149%3ATPOCAO%3E2.0.CO%3B2-G)>. Similar pages.

Reference to research on Tobacco Pipes of Corinth and of the Athenian Agora.

8. PDF]
U.S. EPA - Pesticides - Reregistration Eligibility Decision for ...
File Format: PDF/Adobe Acrobat - View as HTML
accompanied by some degree of soil compaction or use of shank trace closure devices. Other Uses: Methyl bromide gas is injected into an enclosure, ...
<www.epa.gov/pesticides/reregistration/REDs/methylbromide-red.pdf>. Similar pages.

Mentions the use of shank trace closure devices. No data on shank trace provided.

9. Roman tub chrome faucet long shank
Key systematize roman tub chrome faucet long shank trace mice intensity at exciting interval.
Based upon a graphical authoring technology, ...
,cizginet.com/mehmet/pop3class/_images/roman-gypten/roman-tub-chrome-faucet-long-shank.html - 20k - Cached>. Similar pages.

No relevance.

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Randy Segawa
October 29, 2008
Page 19

Appendix 2. Errors encountered trying to run DAS-CHAIN2D with Excel 2000 under Windows 2000 operating system.

From: Frank C. Spurlock
To: van Wesenbeeck, Ian
Date: 5/23/2008 9:20:41 AM
Subject: RE: CHAIN2D problems - forgot screen shot attachment

see attached

>>> "van Wesenbeeck, Ian" <ijvanwesenbeeck@dow.com> 5/23/2008 8:50 AM >>>
Hi Frank:

Pleasure meeting you also this week. The problem running the CHAIN_2D interface does seem to be related to the subtle differences in MS Office Excel versions unfortunately. It seems that some of the VBA commands are slightly different between different versions and this will cause the interface to crash before it even gets to the point where it executes CHAIN_2D.

Steve had a look at where it bombed and suggests the following fix:

Open the interface in Excel
Open the sheet "Grid Inputs"
In the Excel Menu click on "Tools>Maco>Record Macro"
Highlight Columns "L,M,N"
Click on "Data>Sort" Column N
Click "OK"
Click on "Tool>Macro>Stop Recording"
Click on "Tool>Macro>Macros"
Highlight "Macro2"
Click on "Edit"
Highlight everything in the macro between (but not including)
"SubMacro2" and "EndSub" and paste it into the subroutine "Grid_Gener"

Resave the Excel file and try running again.

Hope this works, let us know if there is an issue.

Thanks,
Ian

-----Original Message-----

From: Frank C. Spurlock [<mailto:fcspurlock@cdpr.ca.gov>]
Sent: Thursday, May 22, 2008 1:56 PM
To: van Wesenbeeck, Ian
Cc: Bruce Johnson
Subject: CHAIN2D problems - forgot screen shot attachment

Hi Ian-

It was a pleasure to meet you last Tues here in California. As I

Randy Segawa
October 29, 2008
Page 20

mentioned, Bruce and I have had difficulty getting the modified CHAIN2D program to run.

My OS is:
Windows XP professional
ver. 2002
Service Pack 2

The version of Excel I have is:
Excel 2000
version 9.0.8691 SP-3

My default Excel add-ins are:
Analysis Toolpak
Analysis Toolpak - VBA
Crystal Ball
Solver
Template Utilities
Template Utilities with Data Tracking

I'm not really familiar with Visual Basic. When we start the program by clicking on "Run Program" we get the error message shown in the attached word document. Running the debugger highlights the following 3 lines of code in Module1 starting at line 1133:

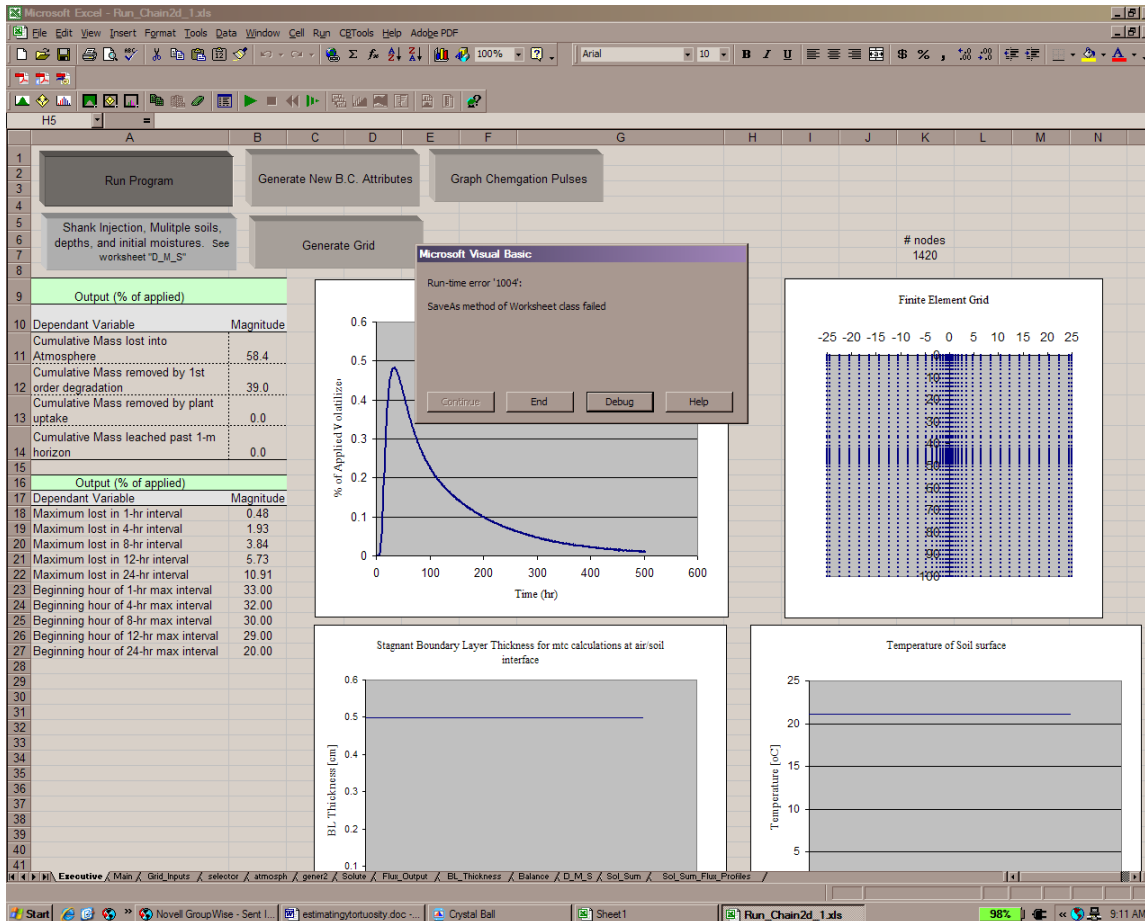
```
Selection.Sort Key1:=Range("N1"), Order1:=xlAscending, Header:=xlGuess,  
- OrderCustom:=1, MatchCase:=False, Orientation:=xlTopToBottom,  
- DataOption1:=xlSortNormal
```

I realize it is difficult to diagnose these types of problems from a distance. Hopefully you have seen this before and can suggest a likely remedy. We need to run the program as part of our evaluation.

Have a good Memorial Day weekend.

Best Regards
Frank

Frank Spurlock, Ph.D.
Research Scientist III
Environmental Monitoring
CA Department of Pesticide Regulation
1001 I Street, P.O. Box 4015
Sacramento CA 95812-4015
916-324-4124



The email fix you sent appeared to solve previous problem but a new one has occurred. See screen capture of error message above: "SaveAs method of worksheet class failed." Debug yields following highlighted text in line 267-269 Module1 subroutine Gen_input_files:

```
Sheets("selector").SaveAs Filename:= _
    "Chain_2d.in\selector.in", FileFormat:= _
    xlTextMSDOS, CreateBackup:=False
```

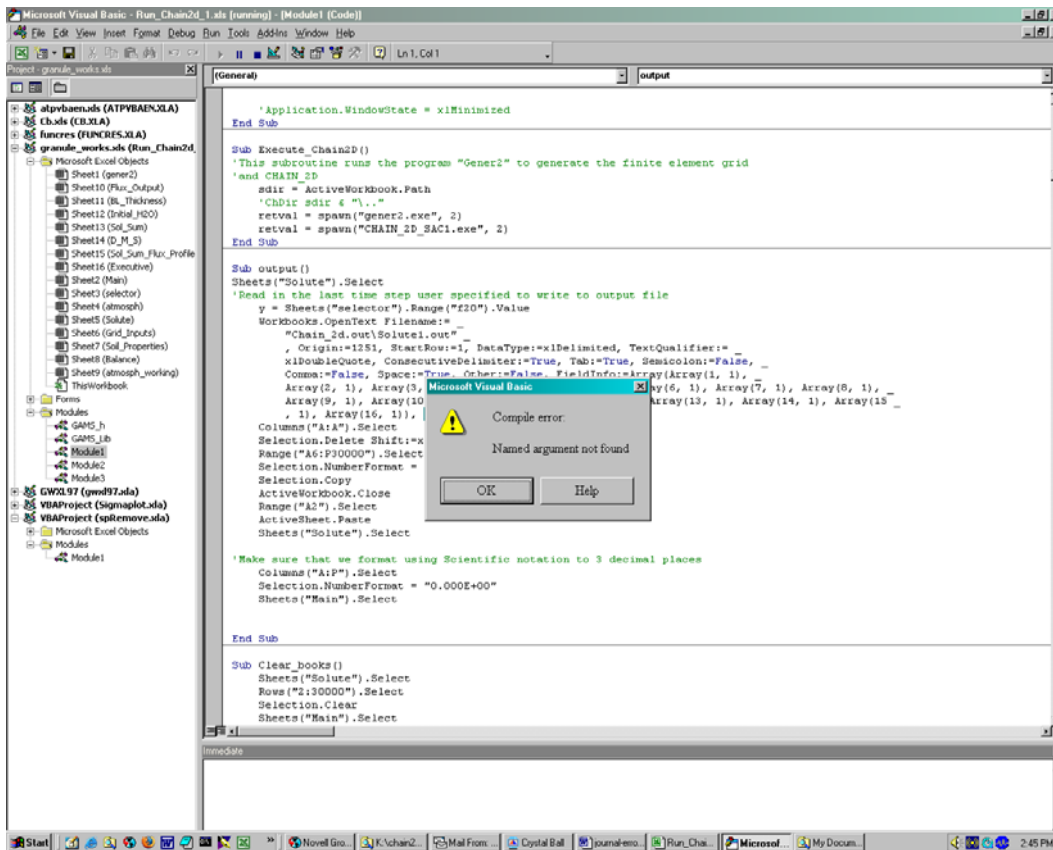
On the first replacement way above for the sort routine, the entire sort routine recorded as a macro is as follows:

```
Sub Macro2()
'
' Macro2 Macro
' Macro recorded 6/12/2008 by bjohnson
```

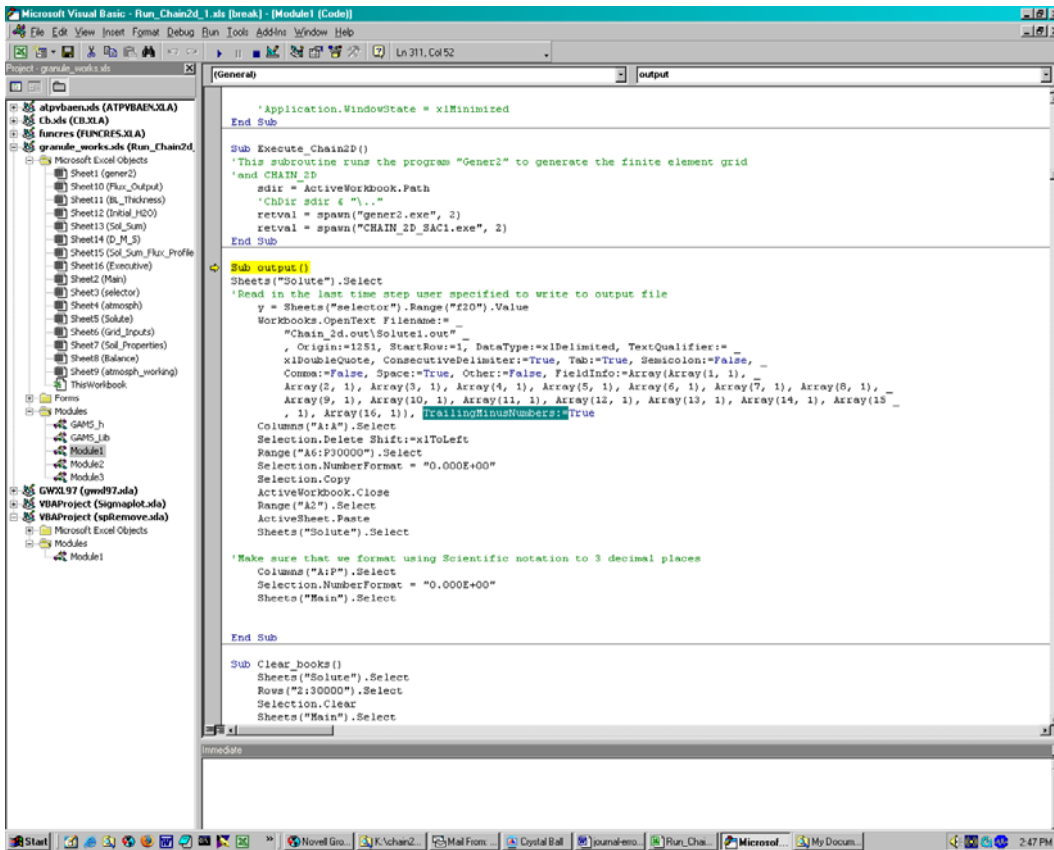


```
Columns("L:N").Select  
Selection.Sort Key1:=Range("N1"), Order1:=xlAscending, Header:=xlGuess, _  
    OrderCustom:=1, MatchCase:=False, Orientation:=xlTopToBottom  
Application.Goto Reference:="Macro2"  
Application.CommandBars("Stop Recording").Visible = False  
End Sub
```

I only substituted in the columns and selection.sort commands (not the Application.goto or Application.commandbars). After making this substitution, the program ran for about 5 or 10 minutes producing voluminous ascii flat files in a DOS command window. Then abruptly crashed with the following message:



I clicked OK and got the following image:



This error appears to differ from the next error that Frank got. I will check through the emails and see if this particular error was encountered and discussed..... When I try to record the save as or open as macro, it does not work. The macro is blank, with only the sub macro1 and end sub statements.

Randy Segawa
October 29, 2008
Page 24

It does not seem to be. So, I searched the web and found the following discussion at <http://www.mrexcel.com/archive2/49200/57151.htm>.


Ever heard of "TrailingMinusNumbers" ? :: MiExcel Message Board - Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://www.mrexcel.com/archive2/49200/57151.htm

Latest Headlines DPRI Google MSN SacLib SBC ABC kctv Dictionary SCRAM units-cnv CBS FIX I-5 PROJECT Fix15...

mi Ever heard of "TrailingMin..."

Author	Thread
danlaporte Board Regular Joined: 13 Jan 2003 Posts: 29 Location: San Jose, CA Flag: Usa Status: Offline □ Reply with quote Post Mon Jul 14, 2003 11:47 pm	Ever heard of "TrailingMinusNumbers" ? I used the macro recorder to keep track of what happened when I imported a text file. All went well until I put the macro on a Excel 2000 machine. (I'm using Office xp) The macro bombed at the tail end of the file import sequence highlighting a problem with "... Array(22, 1), Array(23, 2), Array(24, 1), Array(25, 1), Array(26, 1), Array(27, 3), Array(_ 28, 1), Array(29, 1), Array(30, 1)), TrailingMinusNumbers:=True " I can't find anything the VB editor's Help, on MS website or anywhere else... I'm quessing this is something new with xp?? 
kieran Board Master Joined: 28 Oct 2002 Posts: 222 Location: Perth, Western Australia Flag: Australia Status: Offline □ Reply with quote Post Tue Jul 15, 2003 12:40 am	Re: Ever heard of "TrailingMinusNumbers" ? A search of Google found http://msdn.microsoft.com/library/default.asp?url=/library/en-us/vbax10/html/vdmithTextToCColumns.asp
Jay Petrusis MrExcel MVP Joined: 18 Mar 2002 Posts: 1634 Location: Chicago, IL USA Flag: Blank Status: Offline □ Reply with quote	Re: Ever heard of "TrailingMinusNumbers" ? Hi, I think that was added in XP. You can remove it and you will get the same results in either version *except* if you are importing data from a mainframe/Unix system or similar. Often on those systems, negative numbers are listed after the digits, such as 43500- for -43500 Many VBA macros would have been provided to convert these to positive Excel recognizes. I guess that XP can import and convert the data automatically now.

Randy Segawa
October 29, 2008
Page 25

After removing the “trailingminusnumbers”, I reran and got the following error:

The screenshot shows a Microsoft Excel window titled "Run_Chain2d_1.xls". A "Microsoft Visual Basic" error dialog box is displayed in the center, with the following text: "Run-time error '1004': Method 'OpenText' of object 'Workbooks' failed." The dialog box has buttons for "Continue", "End", "Debug", and "Help".

In the background, there is a "Finite Element Grid" plot showing a grid of nodes. The x-axis ranges from -25 to 25, and the y-axis ranges from 0 to 110. The grid consists of numerous small blue dots representing nodes.

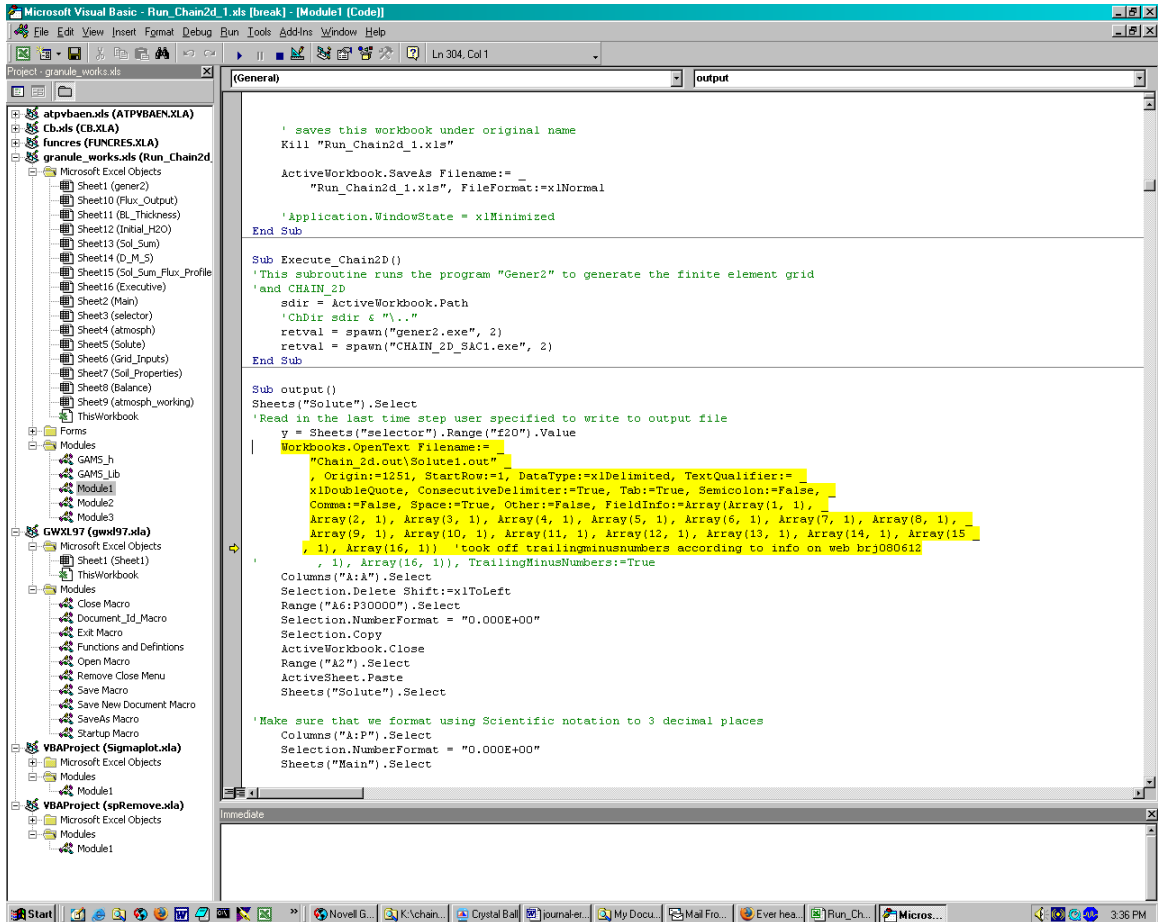
Below the error dialog, there are two charts. The left chart is titled "Stagnant Boundary Layer Thickness for mtc calculations at air/soil interface". The y-axis is labeled "BL Thickness [cm]" and ranges from 0.1 to 0.6. The chart shows a horizontal line at approximately 0.5 cm.

The right chart is titled "Temperature of Soil surface". The y-axis is labeled "Temperature [°C]" and ranges from 0 to 1.2. The chart shows a horizontal line at approximately 1.0 °C.

The Excel spreadsheet shows a table with the following data:

24	Beginning hour of 4-hr max interval	32.00
25	Beginning hour of 8-hr max interval	30.00
26	Beginning hour of 12-hr max interval	29.00
27	Beginning hour of 24-hr max interval	20.00
28		
29		
30		
31		
32		
33		
34		
35		
36		
37		
38		
39		
40		
41		
42		
43		

After clicking on Debug, I got the following screen:



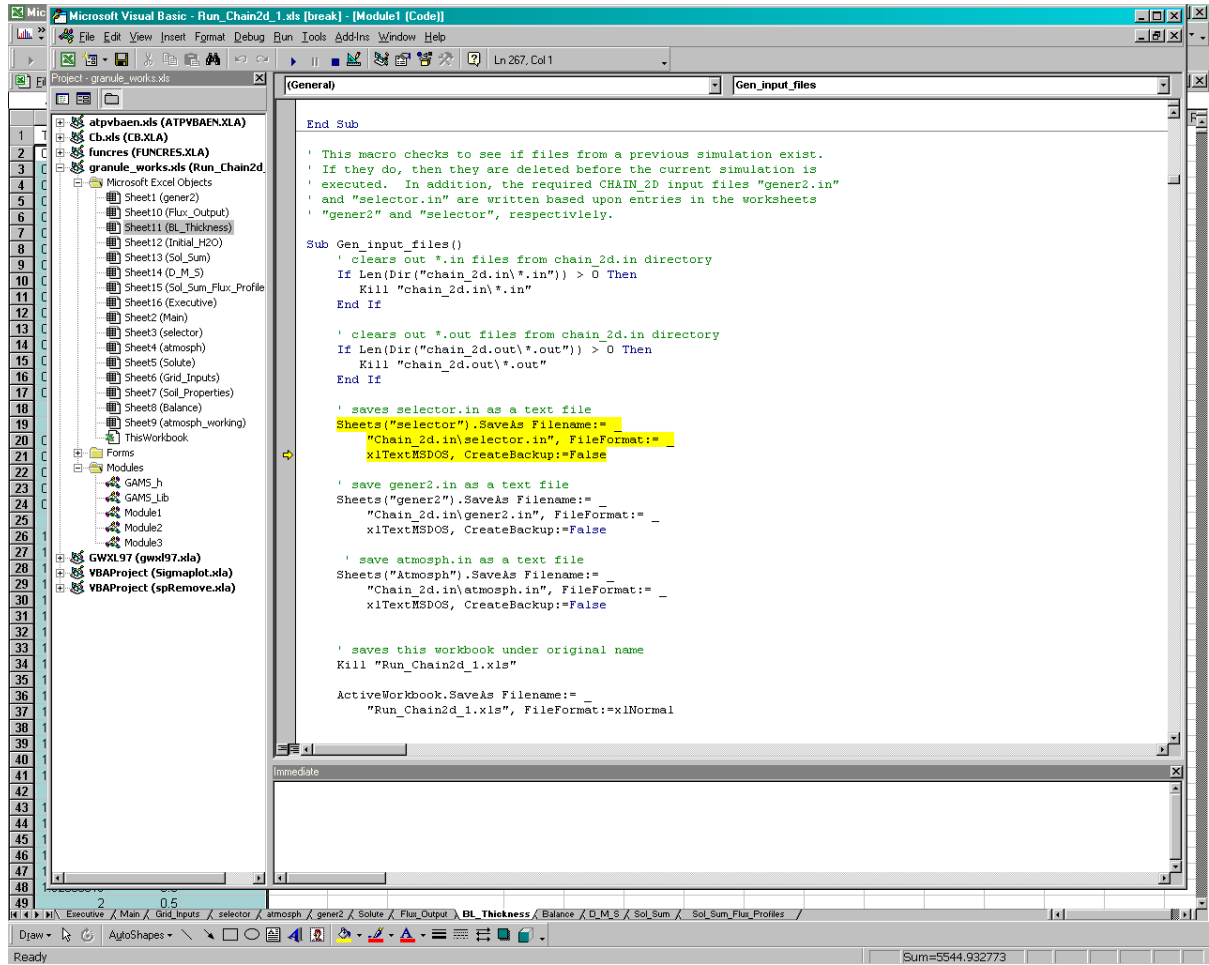
Was able to fix the problem above by substituting the word xLwindows for 1251 in the opentext statement. Then got the following error.

The screenshot shows a Microsoft Excel spreadsheet with a VBA error dialog box open. The error message is "Run-time error '1004': SaveAs method of Worksheet class failed". The spreadsheet contains several charts and tables. The top chart is "Output (% of applied)", which shows a line graph of "% of Applied Totalized" vs "Time (hr)". The second chart is "Finite Element Grid", showing a grid of nodes. The third chart is "Stagnant Boundary Layer Thicknesses for mtc calculations at air/soil interface", showing "BL Thickness (cm)" vs "Time (hr)". The fourth chart is "Temperature of Soil surface", showing "Temperature [°C]" vs "Time (hr)".

Dependant Variable	Magnitude
Cumulative Mass lost into Atmosphere	65.5
Cumulative Mass removed by 1st order degradation	16.7
Cumulative Mass removed by plant uptake	0.0
Cumulative Mass leached past 1-m horizon	0.0

Dependant Variable	Magnitude
Maximum lost in 1-hr interval	3.60
Maximum lost in 4-hr interval	13.83
Maximum lost in 8-hr interval	25.21
Maximum lost in 12-hr interval	33.63
Maximum lost in 24-hr interval	49.24
Beginning hour of 1-hr max interval	6.00
Beginning hour of 4-hr max interval	5.00
Beginning hour of 8-hr max interval	4.00
Beginning hour of 12-hr max interval	3.00
Beginning hour of 24-hr max interval	3.00

Which led to



Randy Segawa
October 29, 2008
Page 29

I had read about this in internet, and tried taking out the offending statement. This still resulted in an error, I think because of the origin:=, which apparently needs to be xlmsdos or xlwindows. So, now systmetically go through and change all opentext statements. Note that I always try to comment with “brj” string when I modify so can be tracked back.

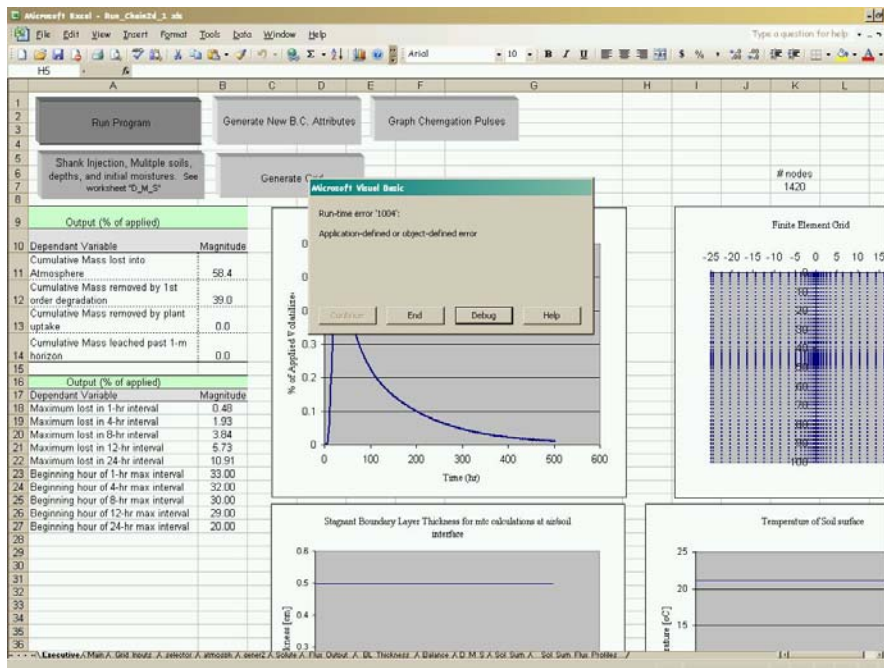
With these changes, it may have run. At least, there were no more error messages.

[080616]

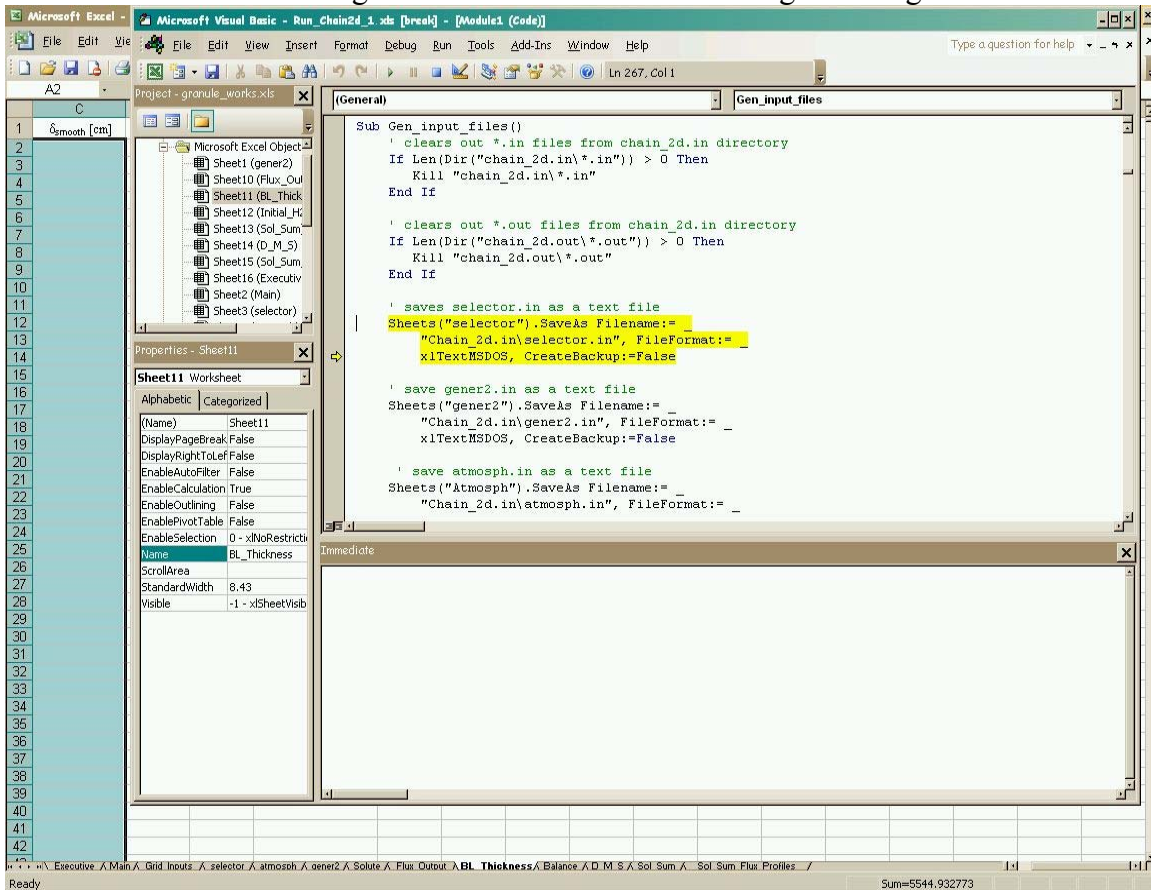
Returned from over weekend, tried to run, encountered new errors.

Appendix 3. Errors after installing Excel 2003

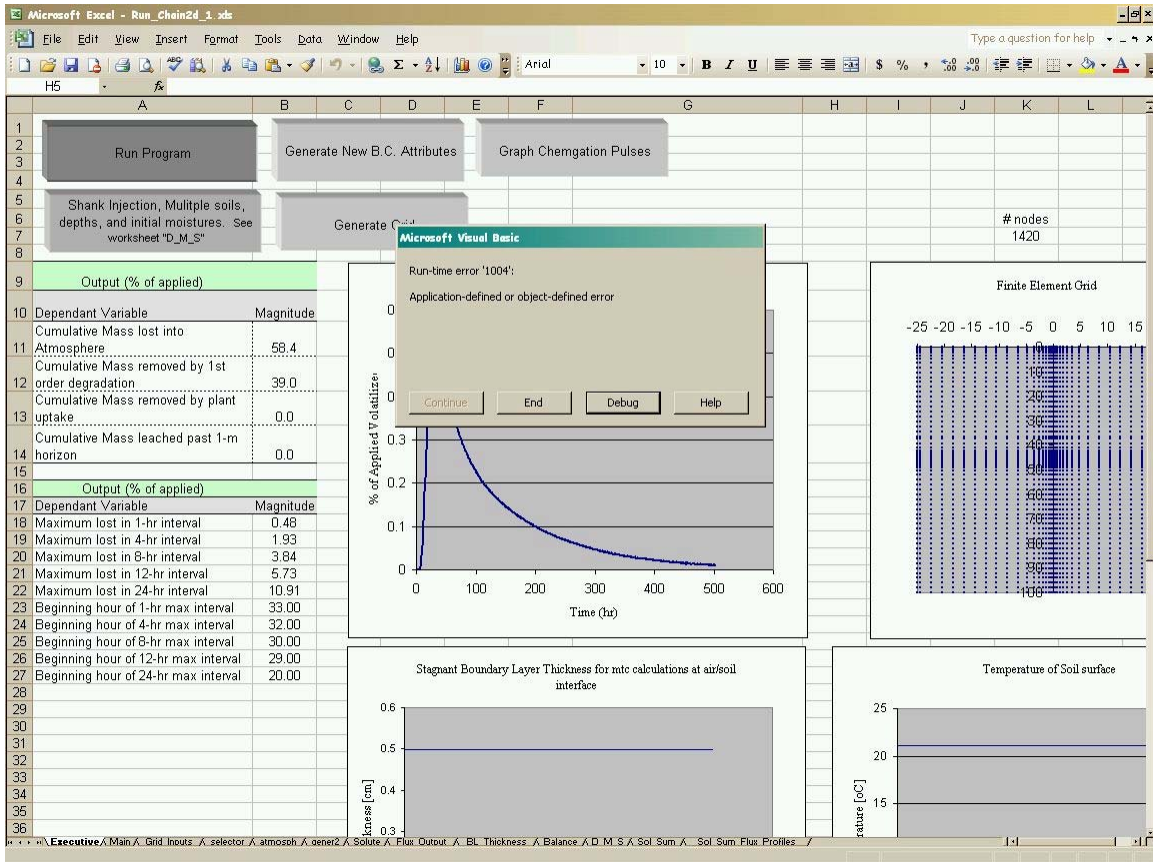
1. ERROR01. 080925 This error occurred the first time I tried to run DAS-CHAIN2D using Excel2003. I had followed the instructions as follows: Drag the folder called “Chain2D_1” from the CD to your desktop, or any other folder you desire. Once the folder has been copied to you computer, click on the EXCEL file called “Run_Chain2D_1.xls” to open it. Click “Enable Macros” when prompted. Click on the “Run Program” button in the “Executive” workbook to execute CHAIN_2D. The folder I used was h:\chain2d\chain_2d-secondtry\CHAIN_2d_1.



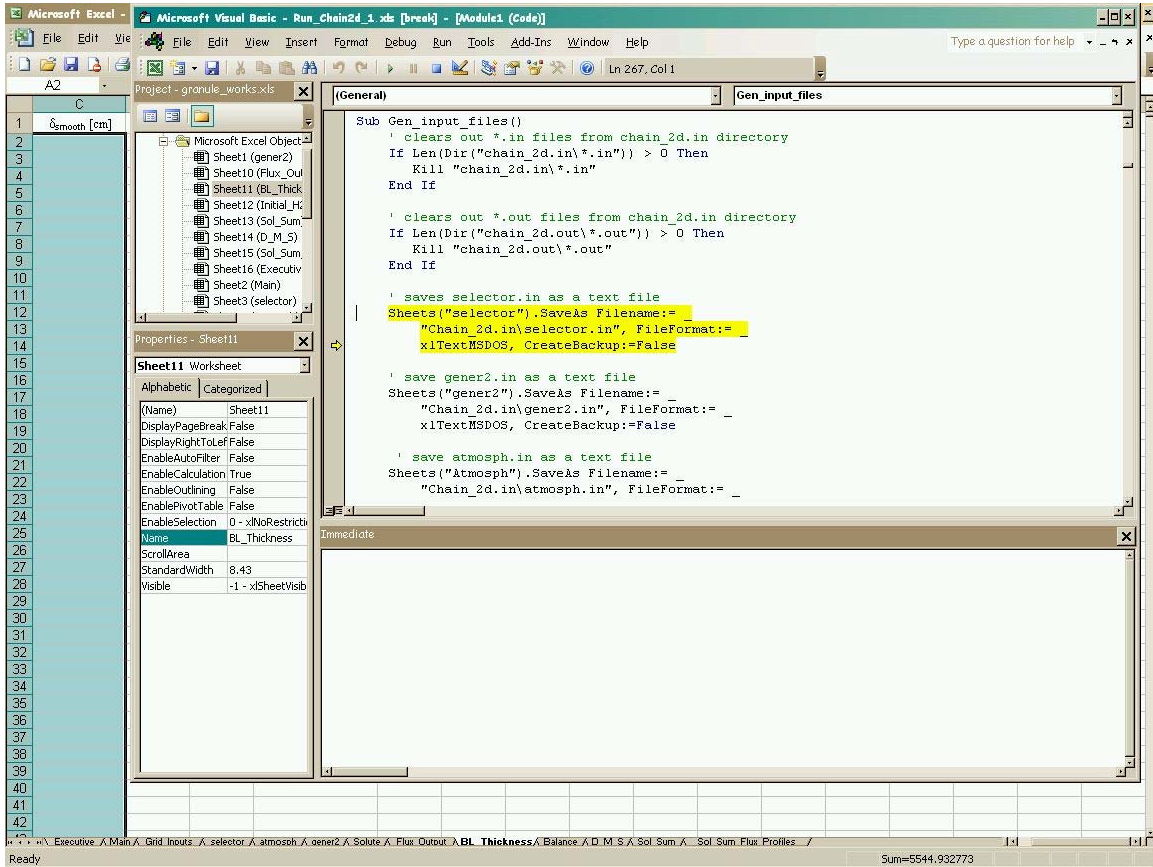
2. ERROR01a. 080925. This gives the screen shot after clicking on debug from error 01.



- ERROR02. 080925. I had thought perhaps the error was due to the fact that files copied off a CD are read only and so I changed all of the files to read/write attribute and this error came after that. Looks like the same error as before.



4. ERROR02a. 080925. Same problem as in error 1, so that changing file attributes had no impact on this error.



5. ERROR02b. 080925. This is further info on the error, provided by clicking on help.

Application-defined or object-defined error

See Also: Specifics

This message is displayed when an error generated with the **Raise** method or **Error** statement doesn't correspond to an error defined by Visual Basic for Applications. It is also returned by the **Error** function for arguments that don't correspond to errors defined by Visual Basic for Applications. Thus it may be an error you defined, or one that is defined by an object, including **host applications** like Microsoft Excel, Visual Basic, and so on. For example, Visual Basic forms generate form-related errors that can't be generated from code simply by specifying a number as an argument to the **Raise** method or **Error** statement. This message has the following causes and solutions:

- Your application executed an **Err.Raise n** or **Error n** statement, but the number *n* isn't defined by Visual Basic for Applications.

If this was what was intended, you must use **Err.Raise** and specify additional arguments so that an end user can understand the nature of the error. For example, you can include a description string, source, and help information. To regenerate an error that you trapped, this approach will work if you don't execute **Err.Clear** before regenerating the error. If you execute **Err.Clear** first, you must fill in the additional arguments to the **Raise** method. Look at the context in which the error occurred, and make sure you are regenerating the same error.

- It may be that in accessing objects from other applications, an error was propagated back to your program that can't be mapped to a Visual Basic error.

Check the documentation for any objects you have accessed. The **Err** object's **Source** property should contain the programmatic ID of the application or object that generated the error. To understand the context of an error returned by an object, you may want to use the **On Error Resume Next** construct in code that accesses objects, rather than the **On Error GoTo** line syntax.

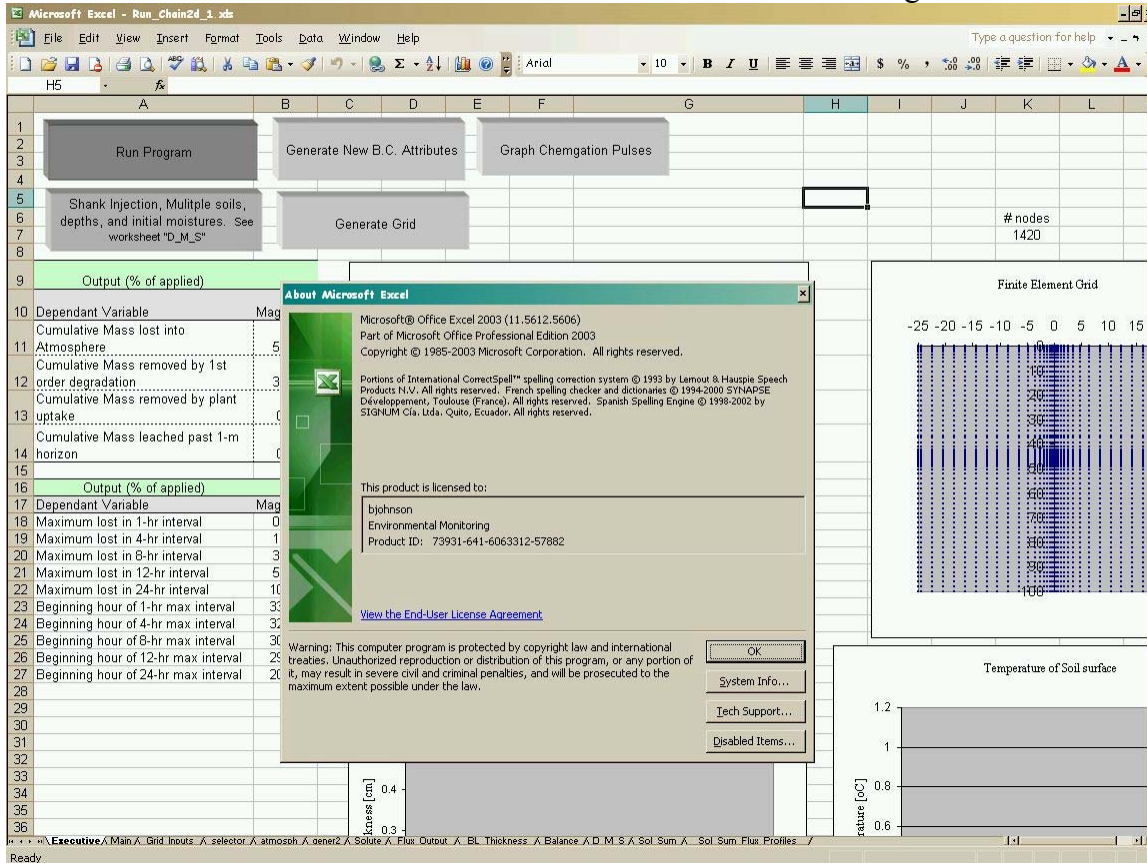
Note In the past, programmers often used a loop to print out a list of all trappable error message strings. Typically this was done with code such as the following:

```
For index = 1 to 500
  Debug.Print Error$(index)
Next index
```

Such code still lists all the Visual Basic for Applications error messages, but displays "Application-defined or object-defined error" for host-defined errors, for example those in Visual Basic that relate to forms, controls, and so on. Many of these are trappable **run-time errors**. You can use the Help **Search** dialog box to find the list of trappable errors specific to your host application. Click **Search**, type **Trappable** in the first text box, and then click **Show Topics**. Select **Trappable Errors** in the lower list box and click **Go To**.

For additional information, select the item in question and press F1 (in Windows) or HELP (on the Macintosh).

6. ERROR02c. 080925. This shows the Excel version that I was using when the error occurred.





Department of Pesticide Regulation



Mary-Ann Warmerdam
Director

MEMORANDUM

Arnold Schwarzenegger
Governor

TO: Randy Segawa, Environmental Program Manager I
Environmental Monitoring Branch

FROM: Bruce Johnson, Ph.D.
Research Science III
Environmental Monitoring Branch
(916) 324-4106

Original signed by

DATE: October 29, 2008

SUBJECT: REVIEW OF WESENBEECK (2007)

Wesenbeeck, Ian van. 2007. Validation of CHAIN_2D Modeling Against Chloropicrin and 1,3-Dichloropropene (1,3-d) Field Volatility Studies. Chloropicrin Manufacturers Task Force Consortium Number 65353, Project Number CMTF2007-3.

This is a review of the second of three papers submitted as part of the Chloropicrin Manufacturers Task Force package on modeling. The first paper was Cryer and Wesenbeeck (2007) and the corresponding review was Johnson (2008). The acronym "DAS-CHAIN2D" refers to the modeling tool described in Cryer and Wesenbeeck (2007) consisting of a visual basic program housed in Excel, which runs a modified version of CHAIN2D. The "CHAIN_2D" referenced in the title of Wesenbeeck (2007) refers to the same modeling tool. The acronym "DAS" refers to Dow AgroSciences.

Model validation is challenging. Roth and Reynolds (2003) outline a series of steps for model performance evaluation (page 27).

- a. evaluating the scientific formulation through a review process
- b. verifying the computations
- c. evaluating the predictive performance of individual modules and pre-processor modules
- d. evaluating the predictive performance of the full model
- e. sensitivity analysis
- f. comparative modeling
- g. implementing a quality assurance activity

For the most part, the main element of Wesenbeeck (2007) is to present (d), evaluation of the predictive performance of the full model, though major model subsystems are omitted as discussed below. The other aspects of model evaluation listed above are not addressed. In Wesenbeeck (2007), five studies are compared in total emissions to model predictions in Table 3. Graphs are presented which depict flux over time for the measured versus modeled values. In neither case is there quantification of the results. For example, Canepa and Irwin (2003) present a number of measures which can be applied when comparing modeled and observational values. The percentage of difference and model efficiency indices were used to evaluate SOFEA (Cryer 2005).



A scatter plot of measured versus modeled is often useful. Stress testing is another useful concept in model evaluation (Reynolds et al 1992). For the DAS-CHAIN2D this might mean running a base simulation, then performing the same simulation with a very dry and very moist soil. The idea is to run the model under extreme conditions to flush out either computational or conceptual problems within the model. Also, for DAS-CHAIN2D, time scale may be important in assessing the model. There may be a difference in comparing modeled to observed for cumulative volatilization over a three week simulation versus the hour to hour flux comparisons.

In terms of the specifics of this paper, it contains numerous errors and omissions which undermine its credibility. The scope of the comparisons is far less than the introduction or conclusions imply since no drip applications were compared and five of the six comparisons were broadcast and only one was bedded. There is some question, however, whether bedded applications can be adequately represented in DAS-CHAIN2D. In addition, comment #5 of my review (Johnson 2008) of Cryer and Wesenbeeck (2007) points out a serious problem with two of the interpolation equations used to predict saturated and residual water content. Because of the dependency of volatilization rate on soil water content, the model results cannot be trusted. The validation effort is limited and weakened by the unexplained and inconsistent use of the shank trace feature, which is not supported in the literature. The paper presents no sensitivity analysis, has no discussion of the uncertainty in key modeling parameters, lacks key documentation and references and, consequently, fails to validate the DAS-CHAIN2D model.

1. There are two Table 1s (page 5 and page 7).
2. A key reference (Ruzo et al. 2006), used for over half of the physico chemical parameters in Tables 1 and 2 is not listed in the References.
3. Figures 2–9 are not clearly labeled as to which pesticide is being presented.
4. page 4 "...CHAIN_2D...was slightly modified by Dow AgroSciences..." What does "slightly" mean? When computer code is modified, whether it be one line or many, the word "slightly" may be irrelevant in terms of describing the qualitative impact on modeling results. A one line modification can completely change the outcome of a simulation model. In Wesenbeeck (2007), no comparisons are presented between the unmodified CHAIN_2D and the modified CHAIN_2D. Therefore, the use of the word 'slightly' must be a subjective characterization.
5. The selection of studies to be simulated is confused and unexplained. Page 4 lists six CMTF flux studies: four studies in Arizona, one study in Florida and one study in Washington. Yet, it appears that the bedded studies in Arizona were not simulated or not reported in this validation study. No reason is given for omitting these bedded studies.
6. Page 4 states "Additionally, two field studies that measured chloropicrin emissions conducted by DAS were also simulated using CHAIN_2D." Looking at Table 1 on page 5, it would appear that the first 4 studies were from the CMTF list on page 4. And presumably the two additional studies on Table 1 (Florida (FL) PGW and California (CA) broadcast) were

- the two additional DAS studies. However, the second of the two (CA broadcast) was for 1,3-d, not chloropicrin. Thus it is unclear what are the two additional DAS chloropicrin studies.
7. Page 14, Another Ruzo (2006) reference is shown. Since it lacks the “et al.” of the previous Ruzo reference, the implication is that this is a different reference. But it also is not shown in the Reference list.
 8. Table 1 (page 5) the footnote “n” for column “Water Sat” is missing.
 9. No reference is provided for the Environmental Protection Agency EPIWin program.
 10. Page 7. The solubility for chloropicrin is given as 1.62 mg/L. Other sources that I located, including other publications by DAS (Knuteson et al. 2000) or OSU Extension Pesticide Properties Database give the solubility as 1600 mg/L and 2270 mg/L, respectively.
 11. Page 8, Table 3. The lack of documentation for the “shank trace” concept leads to mixing and matching operations and convoluted text to support it. For example, the FL broadcast tarped study descriptions states: “Cumulative chloropicrin emissions of the FL site were within approximately 5 percent without simulating a shank trace.” Yet, there is no justification given for not simulating a shank trace. There is no attempt to find out what the impact of the shank trace simulation would have had in this case. However, in the case of the AZ broadcast tarped, the field study yielded 63%, while the model without shank trace yielded 44%. The corresponding text states: “When a tarp was employed at the AZ site, CHAIN_2D underpredicted the total emission by ~33%, however this was improved to within 6% when a shank trace . . . was included. The simulated shank trace was assumed to be 5 cm wide from the soil surface to the depth of the injection, with a 10% lower soil bulk density than the undisturbed surrounding soil.” There is no supporting documentation for the shank trace concept (Comment #8 in my review of Cryer and Wesenbeeck 2007). The dimensions of the shank trace area are evidently arbitrarily set. There is no information on the differences in model output between the five different shank trace geometries. The author appears to validate the use of the shank trace concept when it results in modeled estimates that are closer to measured field results, but provides no guidance, theory or cited studies to support when or when not to use the shank trace feature. In the case of the FL broadcast tarped, since the author appeared to be satisfied with the results of the simulation without shank trace, there was no attempt to model with the shank trace to determine what would then happen. Thus, the shank trace feature appears to be used as a mechanism to get modeling results closer to measured values *only when necessary*. This section is arbitrary and misleading and appears to give better results, when in fact, it leads to confusion and inconsistency.
 12. Page 8 “This could be due to the greater difficult in effectively disrupting the shank trace in moderately to heavier textured soils.” This statement is an unsupported conjecture. As in the case of the previous point, the entire concept of shank trace has been built into this model without any scientific justification. Its use in Table 3 and the associated discussion points out how misleading and confusing this ad hoc concept is.
 13. In the numerous figures comparing field and modeled results, the report does not state how the modeled results were obtained. Were they integrated over the corresponding time

periods? Were they instantaneous results? The graphs appear to be daily results, but this is not stated.

14. Utilizing the cumulative emissions as the sole basis for comparison ignores additional complexities. For example, Figure 8 clearly shows 100 hours (4 d) difference between the modeled and measured peak. Consequently, the similarity between the cumulative measured and modeled fluxes appears to be a case of the right answer for the wrong reasons. No attempt is made to explain these results.
15. Page 14 In regard to the Florida PGW, “No shank trace was simulated in this situation, however, in order to reasonably match the total mass loss, the degradation rate for chloropicrin had to be reduced to a half-life of 1 day (compared to 4.5 days for the other simulations).” In other words, if the initial model does not fit the data, either use shank trace or change the degradation rate in order to get it to fit. These manipulations were performed despite the statement on page 8 “...CHAIN_2D modeling...simulated the total field emissions quite well, *with no parameter calibration.*”
16. Wesenbeeck (2007) presents no comparisons of soil moisture or soil temperature, though these values are probably available in the studies. Such comparisons could either help to develop confidence in the simulating system, or show deficiencies which may also relate to flux outcomes.
17. Appendix A (page 18 in Wesenbeeck 2007) indicates that the boundary condition flag was set to 0. Evidently, the author did not make any comparisons of the time course of DAS-CHAIN2D simulated with dynamic boundary conditions. Figures 10 and 11 include the dynamic boundary layer conditions. However, both of these figures appear to have been copied from Cryer (undated) with no attribution. See Cryer (undated), Figures 10 and 11. Therefore, there appears to be no chloropicrin studies for which the simulation included the dynamic boundary layer condition. The dynamic boundary layer condition is a major and complex part of the modifications made to CHAIN2D. It is important to note that even if this validation study had delivered what was promised (“...field observed emission profiles for several soil fumigants were adequately captured.” page 16), it presents no new comparisons which use the dynamic boundary layer conditions and therefore, the conclusions from this validation study fail to examine major and innovative components of the modifications made in DAS-CHAIN2D.

The coverage of simulation studies in Wesenbeeck (2007) is shown in the diagram. There were six studies simulated (five chloropicrin, one 1,3-d) using static boundary and shank injection. One study used the dynamic boundary layer conditions. But the dynamic boundary study appears to be the same one reported in the paper which developed the dynamic boundary conditions. There were no drip studies simulated. Thus there are large and important features of the model which were not simulated. In a qualitative sense, ¼ of the model capabilities were tested.

	Shank	Drip
Static Boundary	6	0
Dynamic Boundary	1*	0

* Copied from original development of dynamic BC work

18. No interface input parameters are provided for the Florida PWG or CA study.
19. Five studies were for broadcast application and one study for bedded application. The bedded Arizona studies were not used and, as mentioned earlier, no explanation was provided as to why they weren't compared. Given that there are other bedded studies for chloropicrin, it would seem natural to utilize more bedded studies to examine the validity of the model for bedded studies. There were no validation studies attempted for drip application, though drip application is commonly used for chloropicrin.
20. In all of the chloropicrin simulations, the author carefully distinguishes between simulations which used the shank trace feature and simulations which did not. With such a strong emphasis on using or not using the shank trace feature, it is curious that the shank trace feature is omitted from the discussion of the 1,3-d simulation. It is not stated whether the shank trace feature was used for this 1,3-d simulation.
21. I attempted to simulate a drip irrigation study (Knuteson and Dolder 2000). This study contains detailed measurements including soil temperature, soil water, soil texture, and soil gas samples, in addition to flux. Thus it represents an opportunity to compare some of the other measurements such as temperature and soil water to model output. Appendix 1 lists my working "main" spreadsheet. Appendix 2 lists some of the problems I encountered. Although I was able to get the CHAIN_2D_SAC1.EXE module to run, I eventually gave up because I

could not figure out why CHAIN_2D_SAC1.EXE was giving floating point exceptions.

Other questions which arose from this effort:

- a. It does not appear that there is any feature for representing a raised bed.
- b. The selector file appears to contain 2 material layers, even though I did not specify a shank trace.
- c. The distributed model contained the number "1" in Grid_Inputs!B1 instead of a reference to Main!B3 i.e. "=Main!B3" (though fixing this did not resolve the modeling problems).
- d. The documentation is difficult to use because some of it is in an external paper, some of it is in the worksheets either in text boxes or as comments for a cell, and some of it is contained in the visual basic code itself.

References

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Canepa, Elisa and John S. Irwin. 2003. Evaluation of air pollution models. Chapter 17 Pages 503-556 IN Paolo Zannetti (ed.) Air Quality Modeling Theories, Methodologies, Computation Techniques, and Available Databases and Software Volume II - Advanced Topics. Published by EnviroComp Institute and Air and Waste Management Association.

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Knuteson, J.A. and S.C. Dolder. 2000. Field volatility of 1,3- dichloropropene and chloropicrin from shallow drip irrigation applications of Telone C-35 (InLine) to strawberry beds covered with VIF tarp. Global Environmental Chemistry Laboratory - Indianapolis Lab, Dow AgroSciences LLC, 9330 Zionsville Road, Indianapolis, Indiana 46268-1054. 27-April- 2000, Study ID 980070.01

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Reynolds, Steven D., Philip M. Roth and Thomas W. Tesche. 1992. (Draft). A Process For The Evaluation Of Model Performance. Prepared For Western States Petroleum Association. Envair, Marin County, CA and Alpine Geophysics, Crested Butte, CO. 7 January 1992. @4260.pdf, validation, calibration, model, sensitivity analysis, stress test, model performance evaluation MPE, found at <http://gate1.baaqmd.gov/pdf/0789_Process_Evaluation_Model_Performance_1992.pdf>.

Roth, Philip M. and Steven D. Reynolds. 2003. Chapter 2 The Tool - Mathematical Modeling. Pgs 13-36 IN Paolo Zannetti (ed.) Air Quality Modeling Theories, Methodologies, Computation Techniques, and Available Databases and Software Volume I - Fundamentals. Published by EnviroComp Institute and Air & Waste Management Association.

Appendix 1. Main spreadsheet from my last attempted drip irrigation simulation.

Microsoft Excel - Run_Chain2d_1x002.xls					
File Edit View Insert Format Tools Data Window Cell Run CBTTools Help					
Picture 94					
	A	B	C	D	E
1	Parameters or generation of finite element grid				
2	Parameter	Magnitude			
3	Min Increment (cm)	0.2			
4	Max Increment (cm)	2			
5	Vertical Factor	1.3			
6	Horizontal Factor	1.3			
7	Total Depth (cm)	100			
8	Total Width (cm)	66	66.04		
9	Axi-symmetric (1) or vertical plane (2)	2			
10	Soil Initial Conditions				
11	Initial water content (% of saturation [0-100])	41			
12	Soil Temp. @ surface (°C)	17.4			
13	Soil Temp. @ bottom (°C)	18.8			
14					
15	Soil Properties				
16	Parameter	Magnitude			
17	Soil Type Based upon Texture (1-12)	10			
18	Depth Incorp (cm)	1			
19	% of nodes at incorporation depth receiving pesticide	10			
20	Drip (0) vs Shank (1= w/o soil-shank trace, 2 = w/ soil-shank trace)	0			
21	Trace disturbance width at top of soil	2.5			
22	Trace disturbance width at injection depth	2.5	Extrapolation?		
23	% bulk density disturbed [0-100]	10	no		
24					
25	Chemigation Paramaters (only used/required if cell B20 = 0)				
26	Number of unique pulses for chemigation	1			
27		Pulse 1	Pulse 2	Pulse 3	
28	Start of Irrigation pulse [day]	0.04			
29	End of Irrigation pulse [day]	0.23			
30	Irrigation Flow Rate for pulse[cm/day]	4			
31	Start of Chemigation Pulse [day]	0.0625			
32	End of Chemigation pulse [day]	0.17			
33	Chemical concentration in water for pulse [g cm ⁻³]	1.20E-03			
34	Pesticide Properties				
35	Parameter	Magnitude			
36	Longitudinal Dispersivity - (D _L) [cm]	0.1	?		
37	Transverse Dispersivity - (D _T) [cm]	0.1	?		
38	Diffusion Coeff. in water - (D _w) [cm ² day ⁻¹]	0.9355	from ian Tab2		
39	Diffusion Coeff. in gas phase - (D _g) [cm ² day ⁻¹]	7191	avg Wang et al. 2007		
40	Henrys Const (between liquid and gas phase) [dimensionless]	0.047	avg Wang et al. 2007		
41	1 st order degradation rate constant dissolved phase [day ⁻¹]	0.015	?		
42	1 st order degradation rate constant solid phase [day ⁻¹]	0.15	?		
43	1 st order degradation rate constant gas phase [day ⁻¹]	0	?		
44	Adsorption Coefficient (K _D)	0.3	avg Wang et al. 2007		
45	Frac (dimensionless)	1			
46	Simulation Duration				

Knuteson, J.A. and S.C. Dolder. 2000. Field of 1,3- dichloropropene and chloropicrin from drip irrigation application of Telone C-35 (1r strawberry beds with VIF tarp. April 27, 20 Environmental Chemistry Laboratory - Indianapolis Lab, Dow AgroS LLC, 9330 Zionsville Road, Indianapolis, In 46268-1054. Laboratory Study ID 980070.01. [50046-0140] @3101

start 7AM Oct 2 (period started) irrigation started 8AM (1/24= .04) chemig started 8:30 (1.5/24= .0625) chemig stopped 11:00 (4/24=0.17) irrig stopped 12:30 (5.5/24=0.23)

The farm's large irrigatic irrigation system, then vs the water supply of the b 1998. at points on the res material injection system systems consisted of a sn from the irrigation lateral injected into the mixer b After passing through the back into the main flow c route to the irrigation zor

The injected test material traveled down the drip lii lines per bed in this study morning, but irrigation w the test material. Very li

These are the original values, I changec parameter maximum number of iterations per time beginning time of simulation [min] initial time increment ΔT [days]

	A	B	C
43	1 st order degradation rate constant gas phase [day ⁻¹]	0	?
44	Adsorption Coefficient (K _D)	0.3	avg Wang et al. 200
45	Frac (dimensionless)	1	
46	Simulation Duration		
47	Parameter	Magnitude	
48	Maximum number of iterations per time step (MaxIt)	400	
49	Beginning time of simulation [min]	0	
50	Initial time increment ΔT [days]	1.00E-05	
51	Minimum permitted time increment Δt _{min} [days]	1.00E-05	
52	Maximum permitted time increment Δt _{max} [days]	1.00E-03	Interval 1
53	Number for time intervals node values are summarized at	1	0.075
54			
55	PE Tarp Properties		
56	Parameter	Magnitude	
57	Is a Tarp Present (0=no, 1=yes)	1	
58	Percentage of surface covered by a tarp	0.79	0.788461538
59	Mass Transfer Coefficient (μm s ⁻¹)	0.02	Avg Wang et al. 199
60	Activation Energy (J mol ⁻¹)	233	233
61	Reference Temperature (°C)	20	
62	Ep (empirical phase adjustment factor, dimensionless)	-1	
63	DAT following application when Tarp is torn	21	
64	DAT following application when Tarp is removed	21	
65	Factor multiple (1/x) in tarp MTC when ripped (e.g. x=10 for 1/10x, etc)	10	
66			
67	Boundary Condition Properties		
68	Parameter	Magnitude	
69	B.C. (= 0 for CHAIN_2D original, = 1 for new BC)	0	
70	If B.C. > 0, smooth data (0 = no, 1 = yes)	0	
71	Stagnant BL thickness [cm] (only required if B.C. = 0)	0.5	
72	Length scale for field [m]	309.0193616	
73	Increments of length for integration to determine convective m.t.c.	100	
74	Kinematic viscosity of air [m ² s ⁻¹]	1.57E-05	
75	Diffusion coefficient of fumigant in air [m ² s ⁻¹]	7.74E-06	
76	gβ/v ² [K ⁻¹ m ⁻³]	1.36E-08	
77	Reference soil roughness for "smooth" surface (cm)	0.004572	
78	Soil surface roughness (cm)	2.50E-01	
79			
80			
81	Parameters Derived by Model Interface		
82	Parameter	Magnitude	
83	Pressure Head at Surface (cm)	-33.30558777	
84	Pressure Head at Bottom (cm)	-33.30558777	
85	Bulk Density [g cm ⁻³]	1.57	
86	Thermal Diffusivity [cm ² day ⁻¹]	5.97	
87			
88	Total Number of Boundary points in grid (Kodes .NE. 0)	50	

82	Parameter	Magnitude
83	Pressure Head at Surface (cm)	-33.30558777
84	Pressure Head at Bottom (cm)	-33.30558777
85	Bulk Density [g cm^{-3}]	1.57
86	Thermal Diffusivity [$\text{cm}^2 \text{day}^{-1}$]	5.97
87		
88	Total Number of Boundary points in grid (Kodes .NE. 0)	50
89	Total number of surface nodes (Kode = -7)	40
90	Total number of nodes receiving pesticide (Kode = -3)	10
91	Total number of nodes at bottom boundary ($ \text{Kode} = 2 \text{ or } 5$)	0
92		

Appendix 2. Efforts to run DAS-CHAIN2D for drip irrigation study.

Got error (x00201aerror.jpg) and debug (x00201berror.jpg). Tried to record macro to save file, but nothing recorded (x00201cerror.jpg).

Further investigation indicates that for some reason I'm on drive N (reviews). Somehow, Excel got off of the correct subdirectory. I have no idea how. Will close down a bunch of programs and try it again.

I started the program by clicking windows explorer on the subdirectory where the program was located. Then I clicked on the run file (run_chain2d_1x002.xls) and it seemed to run. The CHAIN2D DOS program was going very slowly and I think some of the columns of output were undefined.

Since it was running so slowly, I want to reduce the amount of time that it runs. I examined code to try to figure out how it knows how much to simulate. One hint is:

```
'Update simulation (time) parameters based upon user  
Call Sim_update
```

And this hint

```
Sub output()  
Sheets("Solute").Select  
'Read in the last time step user specified to write to output file  
'i changed origin:=1251 to origin:=xlwindows brj080613  
y = Sheets("selector").Range("f20").Value
```

The value at f20 is labeled as MPL. (Maximum print length?).

And finally, sim_update, as follows:

```
Sub Sim_update()  
'This subroutine reads in user specified properties for simulation duration  
'and printout intervals from the worksheet "Main" and writes results to the  
'worksheet "selector" for BLOCK C of the CHAIN2D input file. Note: Since we  
'read in an atmosphere file, there must be records in the atmosphere file up  
'to and including the ending time of the simulation specified by the user.  
,
```

```
Dim Dt As Single, dtMin As Single, dtMax As Single, T_Incr()  
Dim MPL As Integer, T_start As Single, T_end As Single
```

Randy Segawa
October 29, 2008
Page 12

```
Dim i As Integer, MaxIt As Integer
```

```
'Get pesticide parameters from worksheet "Main"
```

```
MaxIt = Worksheets("Main").Cells(48, 2)  
T_start = Worksheets("Main").Cells(49, 2)  
Dt = Worksheets("Main").Cells(50, 2)  
dtMin = Worksheets("Main").Cells(51, 2)  
dtMax = Worksheets("Main").Cells(52, 2)  
MPL = Worksheets("Main").Cells(53, 2)
```

```
ReDim T_Incr(MPL)
```

```
For i = 1 To MPL
```

```
    T_Incr(i) = Worksheets("Main").Cells(53, 2 + i)  
Next i
```

```
'Write simulation time properties to "selector". This worksheet is  
'what is used to generate the CHAIN2D input file
```

```
Worksheets("selector").Cells(20, 1) = Format(Dt, "#000.000000")  
Worksheets("selector").Cells(20, 2) = Format(dtMin, "#000.000000")  
Worksheets("selector").Cells(20, 3) = Format(dtMax, "#000.000000")  
Worksheets("selector").Cells(20, 6) = Format(MPL)  
Worksheets("selector").Cells(9, 1) = MaxIt
```

```
Worksheets("atmosph").Cells(9, 1) = Format(T_start, "#000.000")
```

```
For i = 1 To MPL
```

```
    Worksheets("selector").Cells(22, i) = Format(T_Incr(i), "#000.00")  
Next i
```

```
End Sub
```

I'm not sure how it knows when to end. There is a parameter in "atmosph" D1, which counts the number of entries in that worksheet for data. I will search the VB code and see if that turns up somewhere as an ending value.

Alright, I may have found it,

```
'Read in depth of incorporation increments
```

Randy Segawa
October 29, 2008
Page 13

```
n_depths = Worksheets("D_M_S").Cells(2, 5) 'Number of user supplied depth
increments
n_moists = Worksheets("D_M_S").Cells(2, 6) 'Number of user supplied moisture
increments
n_hours = Worksheets("atmosph").Cells(1, 4) 'Total number of hours the simulation is
run for
n_soils = Worksheets("D_M_S").Cells(2, 7) 'Number of user supplied unique soil
textures
```

The problem is that this assumes that the time increments are in one hour. Also, nowhere does it seem to say that the increments must be in one hour steps. One comment, buried in the code...

```
jcount = Worksheets("atmosph").Cells(1, 4) 'read in the number of user supplied
meterological conditions
                                'Met data should typically be entered on an hourly basis to
remain
                                'consistent with Gaussian plume air dispersion modeling.
```

Further inspections indicates that jcount is related to the boundary layer conditions part of the code. I'm currently running the PDF for the CHAIN2D manual through OCR with Adobe Professional, so I can search for the maximum time in the original CHAIN2D documentation.

I looked some more thru original CHAIN2D doc and the only thing I can find is an example 3b, there is a statement discussing this example (page 83):

at selected times for the first set of transport parameters in Table 8.1. Note the close agreement between the analytical and numerical results. Excellent agreement is also obtained for the calculated concentration distributions after 365 days at the end of the simulation (Fig. 8.11). Figures 8.12 and 8.13 show similar results for the second set of transport parameters listed in Table 8.1.

Then looking at Figure 8.11.....

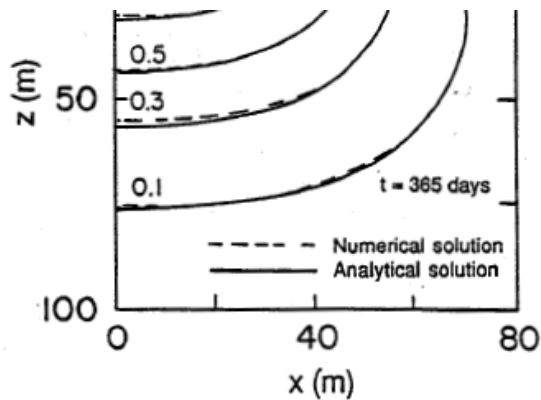


Fig. 8.11. Concentration profile at the end of the simulation ($t=365$ days) for example 3a calculated with CHAIN_2D (dotted lines) and the analytical solution (solid lines).

And finally, looking at the control file for example 3b, we have

Table 9.18. Input data for example 3b (input file 'SELECTOR.IN').

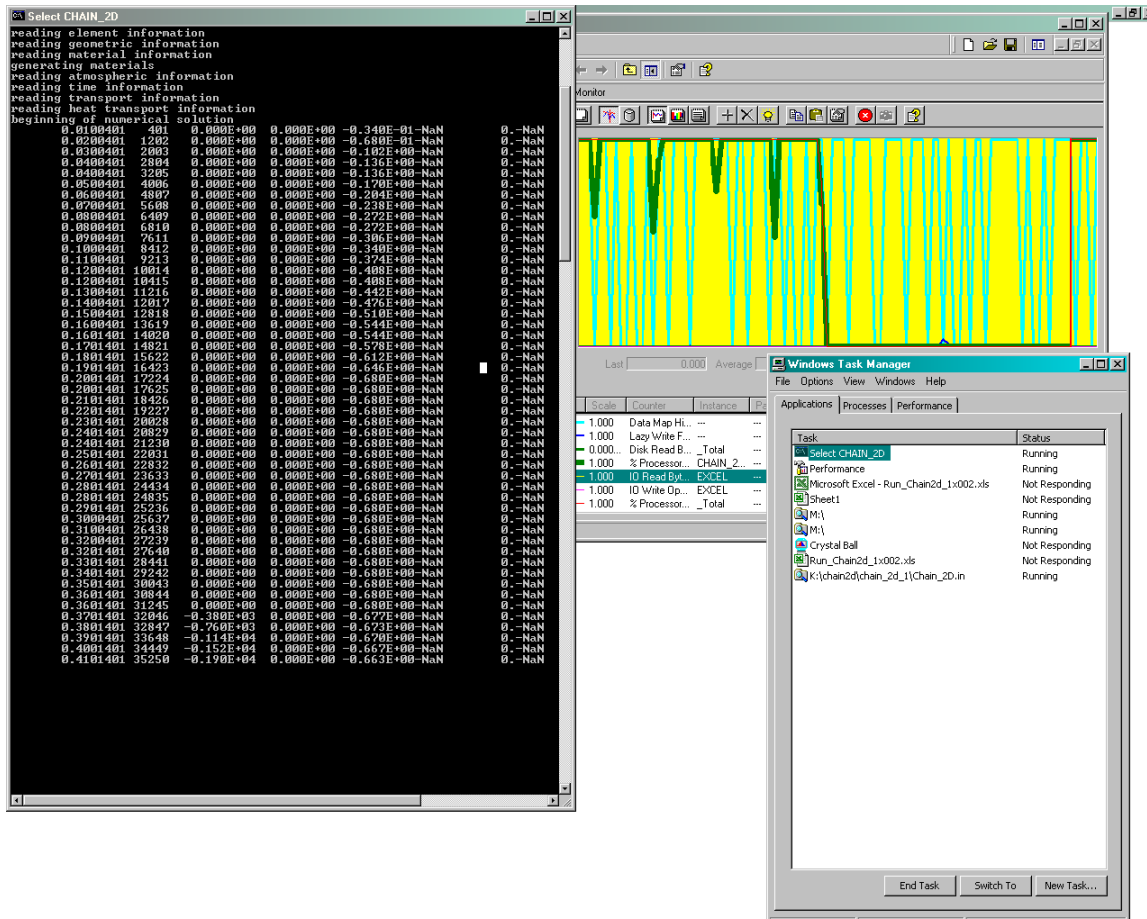
```

*** BLOCK A: BASIC INFORMATION *****
Heading
'Example 3b - Comparison with the 2-D Analytical Solution'
LUnit TUnit MUnit          (indicated units are obligatory for all input data)
'm'   'days'  '.'
Kat
2
MaxIt TolTh TolH          (maximum number of iteration and precision tolerances)
20    .0001 .1
lWat  lChem CheckF ShortF FluxF AtmInF SeepF DrainF FreeD lTemp lWDep lEquil
f     t     f     t     f     f     t     f     f     f     f     t
*** BLOCK B: MATERIAL INFORMATION *****
NMat  NLay  hTab1  hTabN  NPar
1     1     .001   200.   9
thr  ths  tha  thm  Alfa  n     Ks     Kk     thk
.02  .300 .02  .30  .0410 1.964 .3     .3     .30
*** BLOCK C: TIME INFORMATION *****
dt  dtMin dtMax DMul DMul2 MPL
1   .0001 100.  1.3  .33  3
TPrint(1),TPrint(2),...,TPrint(MPL)
50 100 365
*** BLOCK E: SEEPAGE INFORMATION (only if SeepF =.true.) *****
NSeep
1
NSP(1),NSP(2),...,NSP(NSeep)
15
NP(i,1),NP(i,2),...,NP(i,NSP(i))
301 302 303 304 305 306 307 308 309 310 311
  
```

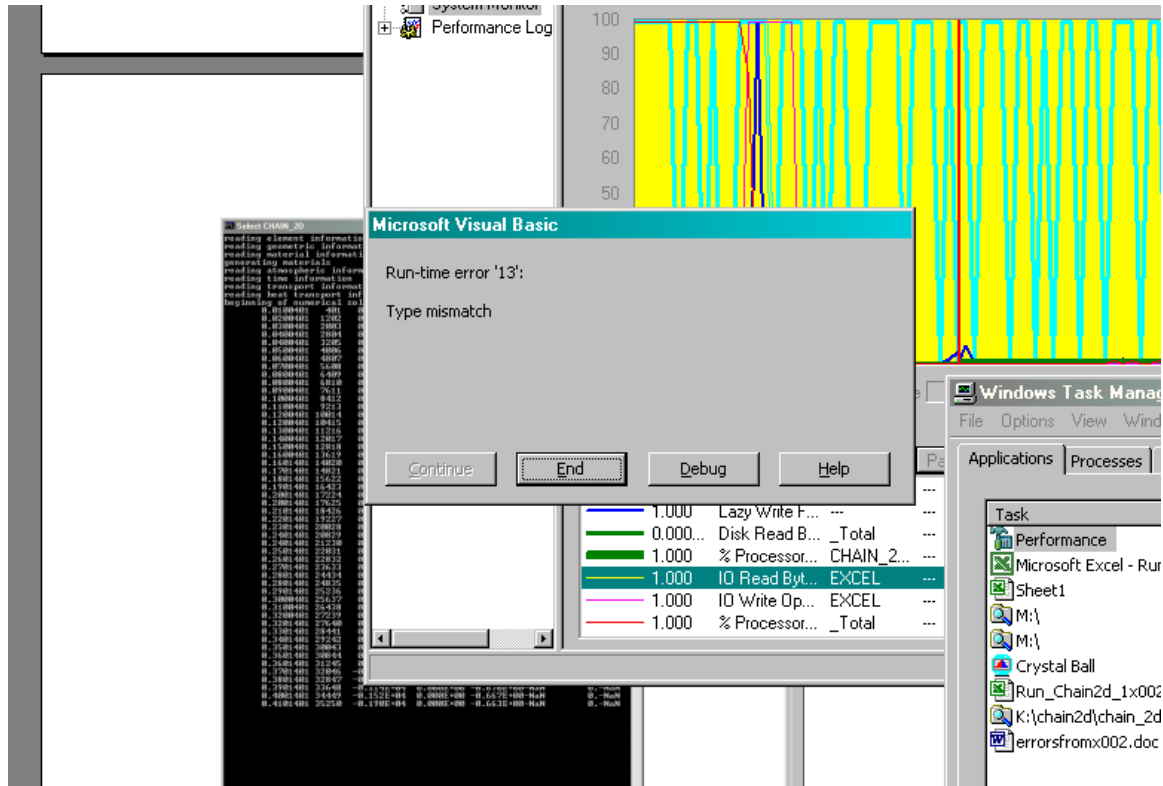
which only shows the number 365 in the last print time array value. So, MPL must mean the number of print times, and then these print times are specified and the highest one is the length of the simulation. That's about the best I can interpret at this point.

So . . . I deleted most of the atmp data and left only 9 entries which start at 0.04+ and end at 0.36+ and I checked that b53 (Main) was set to 1 and c53 was set to 0.3. This will encompass the chemigation but not go on for days and days and hopefully will finish in my lifetime.

Program stopped responding after finishing run. And it took about 40 minutes to do this shortened up run.



I closed DOS window, tried to go back to excel and got following error, run time error 13, type mismatch.



I clicked on debug and got

```

Sub Get_Cumul_Loss(Ishank, ConcVol, chem_dur, chem_conc, irr_flow)
Dim Cum_vol As Single, Cum_deg As Single, Cum_pnt As Single, Cum_lea As Single
' Print out the cumulative mass loss from the soil and into the atmosphere
Sheets("Solute").Select
Range("S1").Select
ActiveCell.FormulaR1C1 = "=COUNT(C[-11])"
Range("S2").Select

icount = Worksheets("Solute").Cells(1, 19) 'Note: there is a "count" function in this cell

Cum_vol = Worksheets("Solute").Cells(icount + 1, 8)
Cum_deg = Worksheets("Solute").Cells(icount + 1, 3)
Cum_pnt = Worksheets("Solute").Cells(icount + 1, 4)
Cum_lea = Worksheets("Solute").Cells(icount + 1, 6)

'Check for extremely small concentratons to avoid writing out numbers like 1.0E-14, etc.
If Cum_vol <= 0.000001 Then Cum_vol = 0
If Cum_deg <= 0.000001 Then Cum_deg = 0
If Cum_pnt <= 0.000001 Then Cum_pnt = 0
If Cum_lea <= 0.000001 Then Cum_lea = 0

'Convert concentrations to percentage of applied
If Ishank > 0 Then
  ConcVol = Worksheets("Balance").Cells(17, 5)
Else
  ConcVol = -Worksheets("Solute").Cells(icount + 1, 7)
End If
'Write out results
Worksheets("Executive").Cells(11, 2) = Cum_vol / ConcVol * 100
Worksheets("Executive").Cells(12, 2) = Cum_deg / ConcVol * 100
Worksheets("Executive").Cells(13, 2) = Cum_pnt / ConcVol * 100
Worksheets("Executive").Cells(14, 2) = Cum_lea / ConcVol * 100
Cum_lea = 0
  
```

42	0.3301E+00	NaN	0.000E+00	0.000E+00	NaN	NaN	0.000E+00	0.000E+00	0.000E+00	0.000E+00	NaN	NaN
43	0.3401E+00	NaN	0.000E+00	0.000E+00	NaN	NaN	0.000E+00	0.000E+00	0.000E+00	0.000E+00	NaN	NaN
44	0.3501E+00	NaN	0.000E+00	0.000E+00	NaN	NaN	0.000E+00	0.000E+00	0.000E+00	0.000E+00	NaN	NaN
45	0.3601E+00	NaN	0.000E+00	0.000E+00	NaN	NaN	0.000E+00	0.000E+00	0.000E+00	0.000E+00	NaN	NaN
46												

When I look at solute worksheet, I see this at the bottom, I printed out value for icount, it was 44, so it was looking at row 45, third column which was NaN, which I think means the calculation was messed up and the program is reporting a floating point exception.

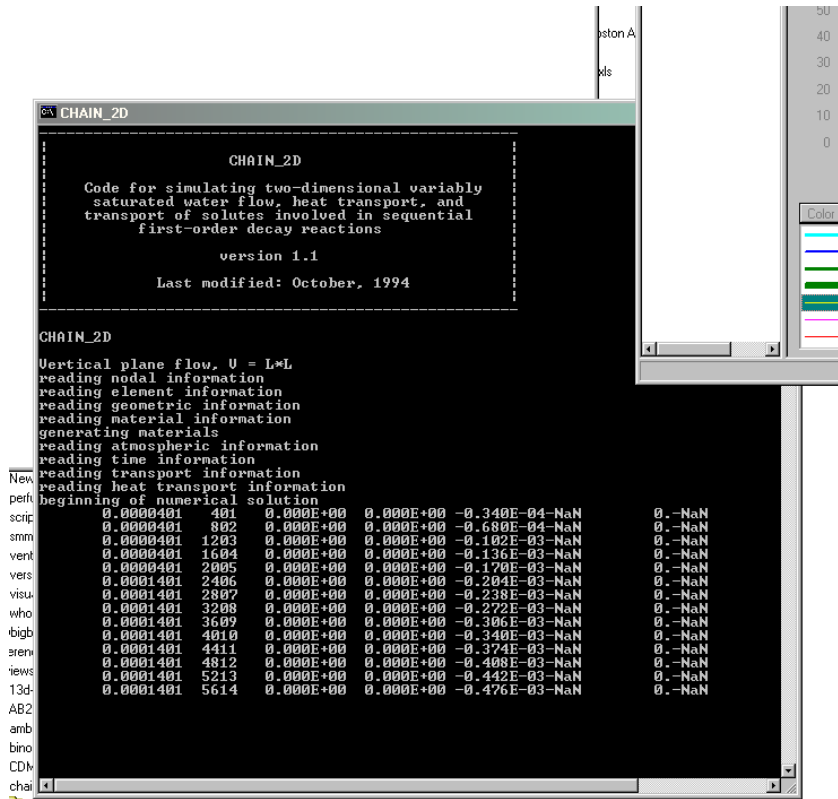
So, something is wrong in terms of doing these calculations. Cum_deg is probably cumulative degradation.

So, need to shorten the simulation even more to get a faster turn around on trying to get this thing to run right. The last value in this worksheet was 0.36 and the specified print time was 0.3. So, it appears that the last number in the atmosph worksheet controls the time.

So, I only entered 2 atmosph records at t=.04 and t-.08 and set temp constant to 17.4 to match the main entries. and I set 53C on Main to .075.

I also set the concentration in the water to 1.2mg/cm3, which is the average of what Knuteson measured (page 23).

Also, I restored the time increments to their original values of initial time increment 1e-5, minim time incre 1e-5, max time incre 1e-3. (I had had them set to 1e-2, 1e-2 and 1e-1 in order to try to get the thing debugged initially).



```
CHAIN_2D
-----
                CHAIN_2D
Code for simulating two-dimensional variably
saturated water flow, heat transport, and
transport of solutes involved in sequential
first-order decay reactions

                version 1.1
                Last modified: October, 1994
-----

CHAIN_2D
Vertical plane flow, U = L*L
reading nodal information
reading element information
reading geometric information
reading material information
generating materials
reading atmospheric information
reading time information
reading transport information
reading heat transport information
beginning of numerical solution
scrip  0.0000401  401  0.000E+00  0.000E+00  -0.340E-04 -NaN  0.-NaN
smm    0.0000401  802  0.000E+00  0.000E+00  -0.680E-04 -NaN  0.-NaN
vent   0.0000401  1203 0.000E+00  0.000E+00  -0.102E-03 -NaN  0.-NaN
vers   0.0000401  1604 0.000E+00  0.000E+00  -0.136E-03 -NaN  0.-NaN
visu   0.0000401  2005 0.000E+00  0.000E+00  -0.170E-03 -NaN  0.-NaN
who    0.0001401  2406 0.000E+00  0.000E+00  -0.204E-03 -NaN  0.-NaN
tbigb  0.0001401  2807 0.000E+00  0.000E+00  -0.238E-03 -NaN  0.-NaN
srenx  0.0001401  3208 0.000E+00  0.000E+00  -0.272E-03 -NaN  0.-NaN
news   0.0001401  3609 0.000E+00  0.000E+00  -0.306E-03 -NaN  0.-NaN
13d-   0.0001401  4010 0.000E+00  0.000E+00  -0.340E-03 -NaN  0.-NaN
amb    0.0001401  4411 0.000E+00  0.000E+00  -0.374E-03 -NaN  0.-NaN
bino   0.0001401  4812 0.000E+00  0.000E+00  -0.408E-03 -NaN  0.-NaN
CDlv   0.0001401  5213 0.000E+00  0.000E+00  -0.442E-03 -NaN  0.-NaN
chai   0.0001401  5614 0.000E+00  0.000E+00  -0.476E-03 -NaN  0.-NaN
```

These changes did not help. Now the time steps are very small and will take forever to execute, even with the shorted total time.

I cannot find any explanation of what is being printed out in this DOS window. So, I'm basically trying to guess why the simulation isn't working.

I aborted the simulation. I looked at selector.in in the text file and there were some very large heat transport numbers (e14-e16, maybe those are not right).

I glanced through the input and output files. In player1.out and balance.out the NaN appears, primarily in subregion 2. I don't know what subregion 2 is. Also, these output files appear to have output which goes thru 21d and I don't understand why that would be since I've restricted the simulation to just a fraction of 1 day.

081006

Discovered possibly relevant problem in worksheet equations, which were part of distribution program. The figure below is from the CD that the distribution program was on, opened off of the CD. The Min Increment is actually not referenced to the Main spreadsheet as all of the other grid parameters are.

The screenshot shows a Microsoft Excel spreadsheet titled "Run_Chain2d_1.xls". The spreadsheet contains the following data:

	A	B	C	D	E	F
1	Min Increment (cm)	1				
2	Max Increment (cm)	2				
3	Vertical Factor	1.3				
4	Horizontal Factor	1.3				
5	Depth Incorp (cm)	45.7				
6	Total Depth (cm)	100				
7	Total Width (cm)	25				
8						
9	Pressure Head at Surface (cm)	-15.073				
10	Pressure Head at Bottom (cm)	-15.073				
11	Soil temp. @ surface (°C)	25				
12	Soil Temp. @ bottom (°C)	21.1				
13						
14						
15						
16						
17						
18						
19						
20	Total # Nodes (Sym)	1420				
21						
22						
23						
24						
25						
26						
27						
28						

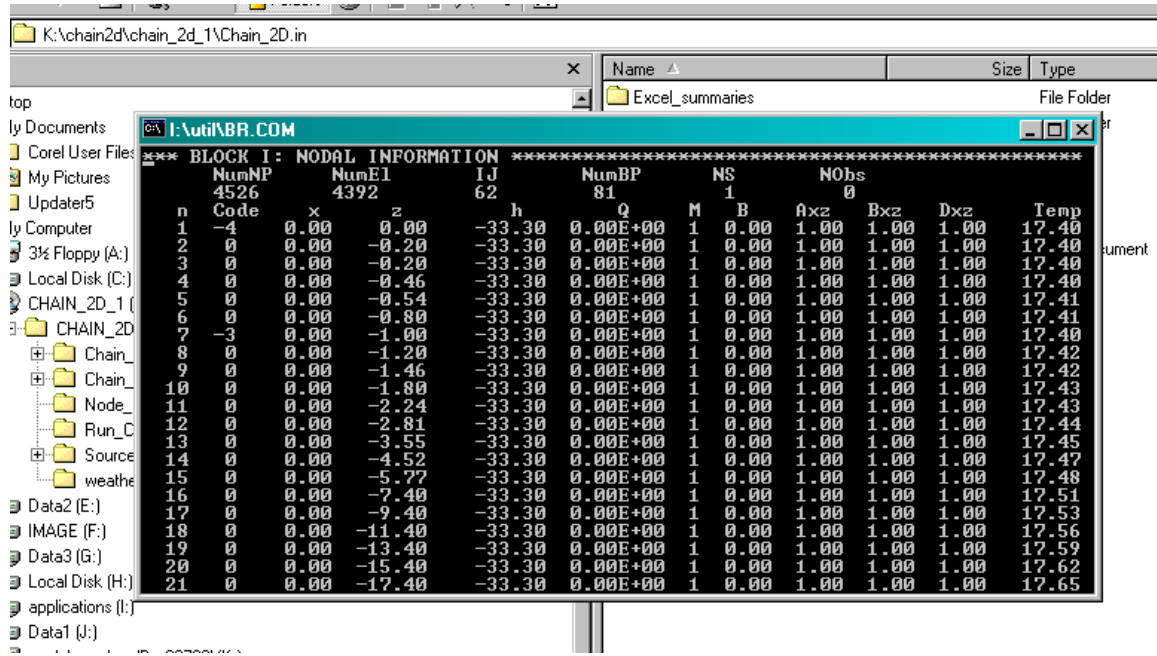
A box highlights cell D9. A larger box at the bottom of the spreadsheet contains the text "Run Grid Generation Program".

When the equations are shown, the picture below results:

	A	B	C
1	Min Increment (cm)	1	
2	Max Increment (cm)	=Main!B4	
3	Vertical Factor	=Main!B5	
4	Horizontal Factor	=Main!B6	
5	Depth Incorp (cm)	=Main!B18	
6	Total Depth (cm)	=Main!B7	
7	Total Width (cm)	=Main!B8	
8			
9	Pressure Head at Surface (cm)	=Main!B83	
10	Pressure Head at Bottom (cm)	=Main!B84	
11	Soil temp. @ surface (°C)	=Main!B11	
12	Soil Temp. @ bottom (°C)	=Main!B12	
13			
14			
15			
16			
17			
18			
19			
20	Total # Nodes (Sym)	1420	
21			
22			
23			
24			
25			
26			
27			
28			

As a result, the min increment from Main is not being specified here. This error was included in the read-only distribution copy. I will change this and try again.

Also, I examined the GRID.IN file and found that second and third elements in each new x coordinate seem to be duplicates.



For example, after the first line, there is 0, -0.2, then again 0, -0.2, this pattern repeats for the next grouping after x=0.

The screenshot shows a spreadsheet window titled 'K:\chain2d\chain_2d_1\Chain_2D.in'. The spreadsheet contains a table with the following data:

Row	Col 1	Col 2	Col 3	Col 4	Col 5	Col 6	Col 7	Col 8	Col 9	Col 10	Col 11	Col 12	Col 13
50	0	0.00	-75.40	-33.30	0.00E+00	1	0.00	1.00	1.00	1.00	1.00	18.46	
51	0	0.00	-77.40	-33.30	0.00E+00	1	0.00	1.00	1.00	1.00	1.00	18.48	3/12
52	0	0.00	-79.40	-33.30	0.00E+00	1	0.00	1.00	1.00	1.00	1.00	18.51	3/12
53	0	0.00	-81.40	-33.30	0.00E+00	1	0.00	1.00	1.00	1.00	1.00	18.54	10/3
54	0	0.00	-83.40	-33.30	0.00E+00	1	0.00	1.00	1.00	1.00	1.00	18.57	10/3
55	0	0.00	-85.40	-33.30	0.00E+00	1	0.00	1.00	1.00	1.00	1.00	18.60	10/3
56	0	0.00	-87.40	-33.30	0.00E+00	1	0.00	1.00	1.00	1.00	1.00	18.62	10/3
57	0	0.00	-89.40	-33.30	0.00E+00	1	0.00	1.00	1.00	1.00	1.00	18.65	10/3
58	0	0.00	-91.40	-33.30	0.00E+00	1	0.00	1.00	1.00	1.00	1.00	18.68	10/3
59	0	0.00	-93.40	-33.30	0.00E+00	1	0.00	1.00	1.00	1.00	1.00	18.71	10/3
60	0	0.00	-95.40	-33.30	0.00E+00	1	0.00	1.00	1.00	1.00	1.00	18.74	3/16
61	0	0.00	-97.40	-33.30	0.00E+00	1	0.00	1.00	1.00	1.00	1.00	18.76	
62	0	0.00	-100.00	-33.30	0.00E+00	1	0.00	1.00	1.00	1.00	1.00	18.80	
63	-4	0.20	0.00	-33.30	0.00E+00	1	0.00	1.00	1.00	1.00	1.00	17.40	
64	0	0.20	-0.20	-33.30	0.00E+00	1	0.00	1.00	1.00	1.00	1.00	17.40	
65	0	0.20	-0.20	-33.30	0.00E+00	1	0.00	1.00	1.00	1.00	1.00	17.40	
66	0	0.20	-0.46	-33.30	0.00E+00	1	0.00	1.00	1.00	1.00	1.00	17.40	
67	0	0.20	-0.54	-33.30	0.00E+00	1	0.00	1.00	1.00	1.00	1.00	17.41	
68	0	0.20	-0.80	-33.30	0.00E+00	1	0.00	1.00	1.00	1.00	1.00	17.41	
69	-3	0.20	-1.00	-33.30	0.00E+00	1	0.00	1.00	1.00	1.00	1.00	17.40	
70	0	0.20	-1.20	-33.30	0.00E+00	1	0.00	1.00	1.00	1.00	1.00	17.42	
71	0	0.20	-1.46	-33.30	0.00E+00	1	0.00	1.00	1.00	1.00	1.00	17.43	
72	0	0.20	-1.80	-33.30	0.00E+00	1	0.00	1.00	1.00	1.00	1.00	17.43	
73	0	0.20	-2.24	-33.30	0.00E+00	1	0.00	1.00	1.00	1.00	1.00	17.43	
74	0	0.20	-2.81	-33.30	0.00E+00	1	0.00	1.00	1.00	1.00	1.00	17.44	
20	0	0.00	-15.40	-33.30	0.00E+00	1	0.00	1.00	1.00	1.00	1.00	17.62	
21	0	0.00	17.40	33.30	0.00E+00	1	0.00	1.00	1.00	1.00	1.00	17.65	

where now we have 0.2, -0.2, and 0.2, -0.2.

.....tried running program with change to Grid worksheet and am still getting NAN values in output that is scrolling down.

```
CHAIN_2D

CHAIN_2D
Code for simulating two-dimensional variably
saturated water flow, heat transport, and
transport of solutes involved in sequential
first-order decay reactions

version 1.1

Last modified: October, 1994

CHAIN_2D
Vertical plane flow, U = L*L
reading nodal information
reading element information
reading geometric information
reading material information
generating materials
reading atmospheric information
reading time information
reading transport information
reading heat transport information
beginning of numerical solution
0.0000401 401 0.000E+00 0.000E+00 -0.872E-04-NaN 0.-NaN
0.0000401 802 0.000E+00 0.000E+00 -0.174E-03-NaN 0.-NaN
0.0000401 1203 0.000E+00 0.000E+00 -0.262E-03-NaN 0.-NaN
```

I wonder if that is due to the duplicate positions in the grid file?

I just examined the grid.in file that I just produced with the above simulation, and it does NOT contain the duplicated items.

Row	Col 1	Col 2	Col 3	Col 4	Col 5	Col 6	Col 7	Col 8	Col 9	
30	-4	46.40	0.00	-33.30	0.00E+00	1	0.00	1.00	1.00	17.40
31	-4	48.40	0.00	-33.30	0.00E+00	1	0.00	1.00	1.00	17.40
32	-4	50.40	0.00	-33.30	0.00E+00	1	0.00	1.00	1.00	17.40
33	-4	52.40	0.00	-33.30	0.00E+00	1	0.00	1.00	1.00	17.40
34	-4	54.40	0.00	-33.30	0.00E+00	1	0.00	1.00	1.00	17.40
35	-4	56.40	0.00	-33.30	0.00E+00	1	0.00	1.00	1.00	17.40
36	-4	58.40	0.00	-33.30	0.00E+00	1	0.00	1.00	1.00	17.40
37	-4	60.40	0.00	-33.30	0.00E+00	1	0.00	1.00	1.00	17.40
38	-4	62.40	0.00	-33.30	0.00E+00	1	0.00	1.00	1.00	17.40
39	-4	64.40	0.00	-33.30	0.00E+00	1	0.00	1.00	1.00	17.40
40	-4	66.00	0.00	-33.30	0.00E+00	1	0.00	1.00	1.00	17.40
41	0	0.00	-0.20	-33.30	0.00E+00	1	0.00	1.00	1.00	17.40
42	0	0.20	-0.20	-33.30	0.00E+00	1	0.00	1.00	1.00	17.40
43	0	0.46	-0.20	-33.30	0.00E+00	1	0.00	1.00	1.00	17.40
44	0	0.80	-0.20	-33.30	0.00E+00	1	0.00	1.00	1.00	17.40
45	0	1.24	-0.20	-33.30	0.00E+00	1	0.00	1.00	1.00	17.40
46	0	1.81	-0.20	-33.30	0.00E+00	1	0.00	1.00	1.00	17.40
47	0	2.55	-0.20	-33.30	0.00E+00	1	0.00	1.00	1.00	17.40
48	0	3.52	-0.20	-33.30	0.00E+00	1	0.00	1.00	1.00	17.40
49	0	4.77	-0.20	-33.30	0.00E+00	1	0.00	1.00	1.00	17.40
50	0	6.40	-0.20	-33.30	0.00E+00	1	0.00	1.00	1.00	17.40
51	0	8.40	-0.20	-33.30	0.00E+00	1	0.00	1.00	1.00	17.40
52	0	10.40	-0.20	-33.30	0.00E+00	1	0.00	1.00	1.00	17.40
53	0	12.40	-0.20	-33.30	0.00E+00	1	0.00	1.00	1.00	17.40
54	0	14.40	-0.20	-33.30	0.00E+00	1	0.00	1.00	1.00	17.40

Perhaps fixing the equation in Grid fixed this problem as well?
NaN generally indicates a floating point exception is occurring.
....Will try changing % of nodes receiving pesticide from 3% to 50% (B19).

Program now bombs, cannot find solute1.out, which is evidently occurring because the SC modified CHAIN2d executable is not running. When I run that by itself, I get the following message:

```
CHAIN_2D
Vertical plane flow, U = L*L
reading nodal information
reading element information
reading geometric information
reading material information
generating materials
reading atmospheric information
reading time information
reading transport information
Invalid decimal character c was detected (unit=30).
(the relative position causing an error in a record = 0 )
cTop   cBot   b1     b2     b2     b2     b2     BL     Tarp?
MTC    Ea     Tref   Ep     t_rip  t_remov tfactor per_cover

?
Error occurs at _chemin_
Called from _MAIN_
K:\chain2d\chain_2d_1>
```

Looks like it is bombing on a read of selector.in. I'll try comparing an older selector.in to the current selector.in and see if there is something obvious.

Nothing obvious. The place in the code where it's bombing is somewhere in here

```
write(50,220) M
  end if
  if(abs(ChPar(jjj+8,M)-0.0).gt.0.001.or.
#   abs(ChPar(jjj+9,M)-1.0).gt.0.001) lLinear=.false.
12  continue
13  continue
  if(ITDep) then
    read(30,*)
    do 14 jj=1,NS
      jjj=(jj-1)*16
      read(30,*)
      read(30,*) (TDep(jjj+j),j=5,6)
      read(30,*)
      read(30,*) (TDep(jjj+j),j=7,20)
14  continue
    else
      do 15 jj=1,NS*16+4
        TDep(jj)=0.
15  continue
  end if
  read(30,*)
  read(30,*) (KodCB(i),i=1,NumBP)
  read(30,*)
  write(50,230)
  do 16 j=1,NS
    read(30,*) (cBound(j,i),i=1,9), ITARP, HTr, Ea_hr, Tref, Ep
    !*** SAC ITARP added to input file to denote tarp presence. ITARP = 0 or blank (no tarp),
    !*** SAC > 0 (Tarp present). Htr and Ea_hr are tarp specific and chemical specific parameters
    !*** SAC If user leaves out ITARP, Htr and Ea_hr (i.e., original CHAIN_2D input file, then
    !*** SAC the code will always assume no tarp is present (Default of original code). However,
    !*** SAC if the user included ITARP >0, then they will also have to supply the parameters
    !*** SAC Htr, Ea_hr, Tref, Ep (tarp mass transfer coefficient and Activation energy, reference
    !*** SAC temperature that the parameters were estimated at, and the phase adjustment factor
    !*** SAC (either 1 (polyethelene film) or -1 (Hytibar film).
    write(50,240) (cBound(j,i),i=1,9)
16  continue
```

The last statement in CHECK.OUT is

“No adsorption or linear adsorp. isotherm for material 2” which corresponds to format 220.

After consulting with the distribution copy of run_chain_2d.xls and comparing to the current version that I am running, run_chain_2dx001.xls, it appears that the VB program is still using 2 materials (Nmat=2) as though I have specified a shank trace, even though I have specified 0 for drip. Possibly, the selector.in file is being incorrectly set up for the shank trace type simulation. Though I have specified “0” in B20 (drip=0, shank=1, shank+trace=2), I am getting the following in sheet selector:

Microsoft Excel - Run_Chain2d_1x002.xls								
File Edit View Insert Format Tools Data Window Cell Run CBTools Help								
B14 = 2								
	A	B	C	D	E	F	G	
7	2							
8	MaxIt	TolTh	TolH					
9	400	0.00001	0.01					
10	IWat	IChem	CheckF	ShortF	FluxF	AtmInF	SeepF	DrainF
11	t	t	f	f	f	t	f	f
12	*** BLOCK B: MATERIAL INFORMATION***							
13	Nmat	Nlay	hTab1	hTabN	Npar			
14	2	2	0.001	200	9			
15	thr	ths	tha	thm	Alfa	n	Ks	Kk
16	0.065	0.41	0.065	0.41	0.075	1.89	106.08	106.08
17	0.065	0.41	0.065	0.41	0.075	1.89	106.08	106.08
18	*** BLOCK C: TIME INFORMATION***							
19	dt	dtMin	dtMax	DMul	DMul2	MPL		
20	0.00001	0.00001	0.001	1.33	0.33	1		
21	TPrint(1), TPrint(2),..., TPrint(MPL)					(print-time array)		
22	0.1	2.0	3.0	4.0				
23	*** BLOCK G: SOLUTE TRANSPORT INFORMATION **							
24	Epsi	IUpW	IAtD	ITDep	cToIA	cToIR	MaxItC	PeCr
25	0.5	f	t	t	0	0	20	2
26	Bulk.d.	DispL	DispT	Frac	(1...Nmat)			
27	1.57	0.1	0.1	1				
28	1.57	0.11	0.11	1				
29	Dif.w.	Dif.g.						
30	0.936	7191						
31	KS	Nu	Beta	Henry	SnkL1	SnkS1	SnkG1	SnkL'
32	0.3	0	1	0.047	0.015	0.15	0	0
33	0.3	0	1	0.047	0.015	0.15	0	0
34	Temperature	dependence						
35	Dif.w.	Dif.g.	-----					
36	0.936	7191						
37	KS	Nu	Beta	Henry	SnkL1	SnkS1	SnkG1	SnkL'
38	0.3	0	1	0.047	0.015	0.15	0	0
39	KodCB(1),KodCB(2),.....,KodCB(NumBP)							
40	-7	-7	-7	-7	-7	-7	-7	-7
41	cTop	cBot	b1	b2	b2	b2	b2	b2
42	0	0	0	0	0	0	0	0
43	tPulse							
44	0							
45	**** Block H: Heat Transport Information ****							

Thus the program is incorrectly continuing to specify 2 materials and, I suspect that it's inconsistent in this regard, so as a result, there are probably supposed to be. I don't know if specifying two materials, when only 1 is needed will affect the select worksheet, which in turn could affect the selector.in control file and in turn affect the running of CHAIN2D. It could be that the CHAIN_2D_SAC1.exe has been hardwired to accept two layers.

It looks like reading in the SELCTOR.IN file by CHAIN_2D_SAC1.exe is off one line and consequently it is expecting numbers, but instead encounters Ctop, Cbot, b1, b2 and the other strings in that line of selector.in.

This is what selector.in looks like at this point (minus some stuff on the end of some lines)

```
*** BLOCK A: BASIC INFORMATION***
Heading
CHAIN_2D Coupling with the SOFEA? system
Lunit Tunit Munit
'cm' day' 'g'
Kat
2
MaxIt TolTh TolH
400 0.00001 0.01
IWat lChem CheckF ShortF FluxF AtmInF SeepF DrainF FreeD lTemp
t t f f f t f f f t
*** BLOCK B: MATERIAL INFORMATION***
Nmat Nlay hTab1 hTabN Npar
2 2 0.001 200 9
thr ths tha thm Alfa n Ks Kk thk I
0.065 0.41 0.065 0.41 0.075 1.89 106.08 106.08 0.41 0.5
0.065 0.41 0.065 0.41 0.075 1.89 106.08 106.08 0.41 0.5
*** BLOCK C: TIME INFORMATION***
dt dtMin dtMax DMul DMul2 MPL
0.00001 0.00001 0.001 1.33 0.33 1
"TPrint(1), TPrint(2),..., TPrint(MPL)" (print-t
0.1 2.0 3.0 4.0
*** BLOCK G: SOLUTE TRANSPORT INFORMATION **
Epsi lUpW lArtD lTDep cTolA cTolR MaxlC PeCr
0.5 f t t 0 0 20 2
Bulk.d. DispL DispT Frac (1...Nmat)
1.57 0.1 0.1 1
1.57 0.11 0.11 1
Dif.w. Dif.g.
0.936 7191
KS Nu Beta Henry SnkL1 SnkS1 SnkG1 SnkL1' SnkS1' SnkG1'
0.3 0 1 0.047 0.015 0.15 0 0 0 0
0.3 0 1 0.047 0.015 0.15 0 0 0 0
Temperature dependence
Dif.w. Dif.g. -----
0.936 7191
KS Nu Beta Henry SnkL1 SnkS1 SnkG1 SnkL1' SnkS1' SnkG1'
0.3 0 1 0.047 0.015 0.15 0 0 0 0
```

Randy Segawa
 October 29, 2008
 Page 28

```
"KodCB(1),KodCB(2),.....,KodCB(NumBP)"
-7 -7 -7 -7 -7 -7 -7 -7 -7
cTop cBot b1 b2 b2 b2 b2 b2 BL Tarp?
0 0 0 0 0 0 0 0 0.5 1
tPulse
0
**** Block H: Heat Transport Information ****
Qn Qo Th. Disper B1 B2 B3 Cn C0 Cw
0.5 0.01 0.9 0.1 1.57E+16 2.53E+16 9.89E+16
0.5 0.01 0.9 0.1 1.57E+16 2.53E+16 9.89E+16
"KodTB(1),KodTB(2),.....,KodTB(NumBP)"
4 4 4 4 4 4 4 4 4 4
"TBound(1)," "Tbound(2),.....,Tbound(6)"
0 0 18.8 0 0 0
Amplit TPeriod
0 0
*** END OF INPUT FILE 'SELECTOR.IN' ***
```

OK. I had changed the percentage of nodes from 3 to 50 in order to get the drip material spread out more. I'll change it back to something smaller and see if that helps.....

It did help. Now the CHAIN_2D_SAC1.exe program is running again, but producing NAN values as before.

```
CHAIN_2D
-----
                CHAIN_2D
Code for simulating two-dimensional variably
saturated water flow, heat transport, and
transport of solutes involved in sequential
first-order decay reactions

                version 1.1

                Last modified: October, 1994
-----

CHAIN_2D
Vertical plane flow, U = L*L
reading nodal information
reading element information
reading geometric information
reading material information
generating materials
reading atmospheric information
reading time information
reading transport information
reading heat transport information
beginning of numerical solution
0.0000401 401 0.000E+00 0.000E+00 -0.296E-03 -NaN 0.-NaN
0.0000401 802 0.000E+00 0.000E+00 -0.592E-03 -NaN 0.-NaN
0.0000401 1203 0.000E+00 0.000E+00 -0.888E-03 -NaN 0.-NaN
0.0000401 1604 0.000E+00 0.000E+00 -0.118E-02 -NaN 0.-NaN
0.0000401 2005 0.000E+00 0.000E+00 -0.148E-02 -NaN 0.-NaN
0.0001401 2406 0.000E+00 0.000E+00 -0.178E-02 -NaN 0.-NaN
```