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

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

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

DATE: October 29, 2008

SUBJECT: REVIEW OF WESENBEECK (2007B)


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.
References


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

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

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 $\theta_a$ appears to be a duplicate of the first column, but is otherwise undefined.

4. Wesenbeeck and Cryer (2007) state (page 8): “Representative values for $\theta_r$, $\theta_s$, $\alpha$ 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:


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$\beta$ 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$\beta$ vs 3.0 and the description of the manual as a draft version. In the manual for 3.12$\beta$ Table 5-42 in Chapter 5 provides $\theta_r$ and $\theta_s$ values which match those in Table 1 and Table 5-41 lists values for $\alpha$ 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 $\theta_r$ and $\theta_s$ 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.”
The row headers clarify that these are log base 10 values. For this loamy sand, the textural class model uses log10(α) of -1.4593 and log10(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 θr and θs 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 (α=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 θr, θs, 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.
5. 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 (\( \theta_s \)), 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 \( \theta_r \) 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 (Šimůnek and van Genuchten, 1994):

(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


Johnson, Bruce. 2006b. Memorandum to Tobi Jones on Interim statewide caps risk analysis for 1,3-dichloropropene with Soil Fumigant Exposure Assessment System computer code corrected for proper buffer zone calculations dated March 10, 2006.
Johnson, Bruce. 2007. Memorandum to Tobi Jones on Simulation of concentrations and exposure associated with Dow AgroSciences-proposed township caps for Ventura County for 1,3-Dichloropropene dated March 27, 2007. Available at: <http://www.cdpr.ca.gov/docs/emon/pubs/ehapreps/analysis_memos/ventur_telone.pdf>.


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, SciFinder, 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 ...

   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
   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. ... 
   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 \( \text{Na}^{+} - \text{Cl}^{-} \) sensitive shank (trace B) at steady state corresponds to the apparent chemical potential difference between lumen and cell as in the case of the C1-- ... 

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 (10R 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>. 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. OtherUses: Methyl bromide gas is injected into an enclosure, ...

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, ...

No relevance.

Search at UC Davis online reference


3. Hanson, B.D., S. Gao, M. McKenry, J. Gerik, D. Wang, K. Klonsky, D. Cox, B. Correiar, and S. Yates. 2007. Efficacy of 1,3-d emissions with approved nursery stock certification treatments applied with two shank designs.


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 lan-

It was a pleasure to meet you last Tues here in California. As I
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.inselector.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.
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>.
After removing the “trailingminusnumbers”, I reran and got the following error:
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.
Which led to
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 systematically 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 your 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.
3. 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

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 forms-related errors that can be generated from code simply by providing a number as an argument to the Raise method or Error statement. This message has the following form:

Error n: Error Description

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

If this is what was intended, you must use Error 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 ErrorClear before regenerating the error, if you execute ErrorClear first, you must fill in the additional arguments to the Error 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 ErrorSource 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 Do Error GoTo line.

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

```
For i = 1 To 500
    Debug.Print ErrSource(i)
Next i
```

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

For additional information, refer the item in question and press F1 (In Windows) or F1 (In Macintosh).
6. ERROR02c, 080925. This shows the Excel version that I was using when the error occurred.
MEMORANDUM

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

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

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.


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.” page16), 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.
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

<table>
<thead>
<tr>
<th>Static Boundary</th>
<th>Shank</th>
<th>Drip</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dynamic Boundary</td>
<td>6</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>1*</td>
<td>0</td>
</tr>
</tbody>
</table>

* Copied from original development of dynamic BC work
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


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


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

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Parameter</strong></td>
<td><strong>Magnitude</strong></td>
<td><strong>No. of unique pulses</strong></td>
<td><strong>Pesticide Properties</strong></td>
</tr>
<tr>
<td>Parameters or generation of finite element grid</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Parameter</strong></td>
<td><strong>Magnitude</strong></td>
<td><strong>Pulse 1</strong></td>
<td><strong>Pulse 2</strong></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td><strong>Pulse 3</strong></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Soil Type Based upon Texture (1-10)</td>
<td>10</td>
<td>3</td>
<td>2</td>
</tr>
<tr>
<td>Soil Incorp (cm)</td>
<td>1</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>% of soil moisture at incorporation depth reaching pesticide</td>
<td>10</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>Drip Spacing (1 = w/ soil-shank trace, 2 = w/o soil-shank trace)</td>
<td>0</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>Trickle disturbance width at top of soil</td>
<td>2.5</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>% bulk density disturbed (1-100)</td>
<td>10</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>Chemical Parameters (only used if cell C00 = 0)</td>
<td>1</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>Number of unique pulses for chemigation</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pesticide Properties</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The farm's large irrigation system, which is 13 miles per hour, is designed for the water supply of the irrigation system. The system consisted of a main valved line, which was passed through the main flow to the irrigation area. The injected test material traveled down the drip line to the irrigation area, and irrigation was taking place. Very little irrigation was taking place, and the material was very easy to see. These are the original values, including changes to the storage tank.
<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
<th>C</th>
</tr>
</thead>
<tbody>
<tr>
<td>1st order degradation rate constant gas phase [day^(-1)]</td>
<td>0</td>
<td>?</td>
</tr>
<tr>
<td>Adsorption Coefficient (K_d)</td>
<td>0.3</td>
<td>avg Wang et al. 200</td>
</tr>
<tr>
<td>Frac (dimensionless)</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Simulation Duration</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Parameter</td>
<td>Magnitude</td>
<td></td>
</tr>
<tr>
<td>Maximum number of iterations per time step (MaxIt)</td>
<td>400</td>
<td></td>
</tr>
<tr>
<td>Beginning time of simulation [min]</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Initial time increment ΔT [days]</td>
<td>1.00E-05</td>
<td></td>
</tr>
<tr>
<td>Minimum permitted time increment Δt_{min} [days]</td>
<td>1.00E-05</td>
<td></td>
</tr>
<tr>
<td>Maximum permitted time increment Δt_{max} [days]</td>
<td>1.00E-03</td>
<td>interval 1</td>
</tr>
<tr>
<td>Number for time intervals node values are summarized at</td>
<td>1</td>
<td>0.075</td>
</tr>
</tbody>
</table>

PE Tarps Properties

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Magnitude</th>
</tr>
</thead>
<tbody>
<tr>
<td>Is a Tar present? (0=no, 1=yes)</td>
<td>1</td>
</tr>
<tr>
<td>Percentage of surface covered by a tarp</td>
<td>0.79</td>
</tr>
<tr>
<td>Mass Transfer Coefficient (μm s^{-1})</td>
<td>0.02 avg Wang et al. 199</td>
</tr>
<tr>
<td>Activation Energy (J mol^{-1})</td>
<td>233</td>
</tr>
<tr>
<td>Reference Temperature (°C)</td>
<td>20</td>
</tr>
<tr>
<td>Ep (empirical phase adjustment factor, dimensionless)</td>
<td>-1</td>
</tr>
<tr>
<td>DAT following application when Tarps is torn</td>
<td>21</td>
</tr>
<tr>
<td>DAT following application when Tarps is removed</td>
<td>21</td>
</tr>
<tr>
<td>Factor multiple (1/x) in tarps MTC when ripped (e.g. x=10 for 1/10x, etc)</td>
<td>10</td>
</tr>
</tbody>
</table>

Boundary Condition Properties

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Magnitude</th>
</tr>
</thead>
<tbody>
<tr>
<td>B.C. (= 0 for CHAIN, 2D original, = 1 for new EC)</td>
<td>0</td>
</tr>
<tr>
<td>If B.C. &gt; 0, smooth data (0=no, 1=yes)</td>
<td>0</td>
</tr>
<tr>
<td>Stagnant EL thickness [cm] (only required if B.C. = 0)</td>
<td>0.5</td>
</tr>
<tr>
<td>Length scale for field [m]</td>
<td>303.0139616</td>
</tr>
<tr>
<td>Increment of length for integration to determine convective m.t.c.</td>
<td>100</td>
</tr>
<tr>
<td>Kinematic viscosity of air [m^2 s^{-1}]</td>
<td>1.57E-05</td>
</tr>
<tr>
<td>Diffusion coefficient of fumigant in air [m^2 s^{-1}]</td>
<td>7.74E-06</td>
</tr>
<tr>
<td>g β (K^1 m^{-3})</td>
<td>1.36E-03</td>
</tr>
<tr>
<td>Reference soil roughness for &quot;smooth&quot; surface (cm)</td>
<td>0.004572</td>
</tr>
<tr>
<td>Soil surface roughness (cm)</td>
<td>2.50E-01</td>
</tr>
</tbody>
</table>

Parameters Derived by Model Interface

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Magnitude</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure Head at Surface (cm)</td>
<td>-33.30559777</td>
</tr>
<tr>
<td>Pressure Head at Bottom (cm)</td>
<td>-33.30559777</td>
</tr>
<tr>
<td>Bulk Density [g cm^{-3}]</td>
<td>1.57</td>
</tr>
<tr>
<td>Thermal Diffusivity [cm^2 day^{-1}]</td>
<td>5.97</td>
</tr>
<tr>
<td>Total Number of Boundary points in grid (Kocos, NE, 0)</td>
<td>50</td>
</tr>
<tr>
<td>Parameter</td>
<td>Magnitude</td>
</tr>
<tr>
<td>---------------------------------------------------------------------------</td>
<td>--------------------</td>
</tr>
<tr>
<td>Pressure Head at Surface (cm)</td>
<td>-33.30558777</td>
</tr>
<tr>
<td>Pressure Head at Bottom (cm)</td>
<td>-33.30558777</td>
</tr>
<tr>
<td>Bulk Density [g cm(^{-3})]</td>
<td>1.57</td>
</tr>
<tr>
<td>Thermal Diffusivity [cm(^2) day(^{-1})]</td>
<td>5.97</td>
</tr>
<tr>
<td>Total Number of Boundary points in grid (Kodes .NE. 0)</td>
<td>50</td>
</tr>
<tr>
<td>Total number of surface nodes (Kode = -7)</td>
<td>40</td>
</tr>
<tr>
<td>Total number of nodes receiving pesticide (Kode = -3)</td>
<td>10</td>
</tr>
<tr>
<td>Total number of nodes at bottom boundary (</td>
<td>Kode</td>
</tr>
</tbody>
</table>
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
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 “atmosp” 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
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........
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 (horizontal plane, 1:axi-symmetric vertical flow, 2:vertical plane)
MaxIt TolTh TolH (maximum number of iteration and precision tolerances)
20 .0001 .1
LList lChem CheckF ShortF FluxF AtminF SeepF DrainF FreeD lTemp lDep lEquil
f t f t f t f f f t

*** BLOCK B: MATERIAL INFORMATION **********************************************************

NMat NLay hTab1 hTabM NPer
1 1 .001 200 9
thr ths the thm Alfa n Ks Kk thk
.02 .300 .02 .30 .0410 1.964 .5 .5 .30

*** BLOCK C: TIME INFORMATION ***************************************************************

dt cmin cMax DNu1 DNu2 MPl
1 1 .0001 100 1.3 .33 3
TPrint(1),TPrint(2),...,TPrint(MPl) (print-time array)
50 100 365

*** BLOCK E: SEEPAGE INFORMATION (only if SeepF = true.) **************************************

NSeep
1
NSP(1),NSP(2),...,NSP(NSeep) (number of nodes in each seepage faces)
15
NP(1,1),NP(1,2),...,NP(1,NP(1)) (nodal number array of 1-th seepage faces)
301 302 303 304 305 306 307 308 309 310 311

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).
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 atmosp 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

[ ]
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 \(10^{-5}\), \(10^{-5}\), \(10^{-3}\). (I had had them set to \(10^{-2}\), \(10^{-2}\) and \(10^{-1}\) in order to try to get the thing debugged initially).

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 (\(10^{14}\)–\(10^{16}\), maybe those are not right).

I glanced through the input and output files. In blayer1.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.

![Microsoft Excel - Run_Chain2d_1.xls](image-url)

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>Min Increment (cm)</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Max Increment (cm)</td>
<td>2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Vertical Factor</td>
<td>1.3</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Horizontal Factor</td>
<td>1.3</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Depth Incorp (cm)</td>
<td>45.7</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total Depth (cm)</td>
<td>100</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total Width (cm)</td>
<td>25</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pressure Head at Surface (cm)</td>
<td>-15.073</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pressure Head at Bottom (cm)</td>
<td>-15.073</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Soil temp. @ surface (°C)</td>
<td>25</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Soil Temp. @ bottom (°C)</td>
<td>21.1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total #Nodes (Sym)</td>
<td></td>
<td>1420</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Run Grid Generation Program
When the equations are shown, the picture below results:

<table>
<thead>
<tr>
<th></th>
<th>A</th>
<th>B</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Min Increment (cm)</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>Max Increment (cm)</td>
<td>=MainB4</td>
</tr>
<tr>
<td>3</td>
<td>Vertical Factor</td>
<td>=MainB5</td>
</tr>
<tr>
<td>4</td>
<td>Horizontal Factor</td>
<td>=MainB6</td>
</tr>
<tr>
<td>5</td>
<td>Depth Incorp (cm)</td>
<td>=MainB18</td>
</tr>
<tr>
<td>6</td>
<td>Total Depth (cm)</td>
<td>=MainB7</td>
</tr>
<tr>
<td>7</td>
<td>Total Width (cm)</td>
<td>=MainB8</td>
</tr>
<tr>
<td>8</td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>Pressure Head at Surface (cm)</td>
<td>=MainB83</td>
</tr>
<tr>
<td>10</td>
<td>Pressure Head at Bottom (cm)</td>
<td>=MainB84</td>
</tr>
<tr>
<td>11</td>
<td>Soil temp. @ surface (°C)</td>
<td>=MainB11</td>
</tr>
<tr>
<td>12</td>
<td>Soil Temp. @ bottom (°C)</td>
<td>=MainB12</td>
</tr>
<tr>
<td>13</td>
<td></td>
<td></td>
</tr>
<tr>
<td>14</td>
<td></td>
<td></td>
</tr>
<tr>
<td>15</td>
<td></td>
<td></td>
</tr>
<tr>
<td>16</td>
<td></td>
<td></td>
</tr>
<tr>
<td>17</td>
<td></td>
<td></td>
</tr>
<tr>
<td>18</td>
<td></td>
<td></td>
</tr>
<tr>
<td>19</td>
<td></td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>Total # Nodes (Sym)</td>
<td>1420</td>
</tr>
</tbody>
</table>

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.
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.
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.
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:

```
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

```fortran
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(lTDep) then
read(30,*)
do 14 jj=1,NS
jjj=(jj-1)*16
read(30,*) (TDep(jjj+j),j=5,6)
read(30,*) (TDep(jjj+j),j=7,20)
14      continue
else
continue
end if
read(30,*)
read(30,*) (TDep(jjj),j=1,NS)
TDep(jjj)=0.
15     continue
end if
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 includeds 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 (Hytabar 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:
<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
<th>F</th>
<th>G</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Maxt</td>
<td>ToTh</td>
<td>ToH</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>Maxt</td>
<td>ToTh</td>
<td>ToH</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>400</td>
<td>0.0001</td>
<td>0.01</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>Nmat</td>
<td>Chem</td>
<td>CheckF</td>
<td>ShortF</td>
<td>FluxF</td>
<td>AtmInF</td>
</tr>
<tr>
<td>11</td>
<td>t</td>
<td>t</td>
<td>f</td>
<td>f</td>
<td>f</td>
<td>t</td>
</tr>
<tr>
<td>12</td>
<td>*** BLOCK B: MATERIAL INFORMATION ***</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>Nmat</td>
<td>Nlay</td>
<td>hTab1</td>
<td>hTabN</td>
<td>Npar</td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>2</td>
<td>2</td>
<td>0.001</td>
<td>200</td>
<td>9</td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>thr</td>
<td>th</td>
<td>thm</td>
<td>Alfa</td>
<td>n</td>
<td>KG</td>
</tr>
<tr>
<td>16</td>
<td>0.065</td>
<td>0.41</td>
<td>0.065</td>
<td>0.41</td>
<td>0.075</td>
<td>1.89</td>
</tr>
<tr>
<td>17</td>
<td>0.065</td>
<td>0.41</td>
<td>0.065</td>
<td>0.41</td>
<td>0.075</td>
<td>1.89</td>
</tr>
<tr>
<td>18</td>
<td>*** BLOCK C: TIME INFORMATION ***</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>19</td>
<td>dt</td>
<td>dtMin</td>
<td>dtMax</td>
<td>DMul</td>
<td>DMul2</td>
<td>MPL</td>
</tr>
<tr>
<td>20</td>
<td>0.0001</td>
<td>0.0001</td>
<td>0.001</td>
<td>1.33</td>
<td>0.33</td>
<td>1</td>
</tr>
<tr>
<td>21</td>
<td>TPrint(1), TPrint(2),...., TPrint(MPL)</td>
<td>(print-time array)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>22</td>
<td>0.1</td>
<td>2.0</td>
<td>3.0</td>
<td>4.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>23</td>
<td>*** BLOCK G: SOLUTE TRANSPORT INFORMATION **</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>24</td>
<td>Epsi</td>
<td>IUW</td>
<td>IARfD</td>
<td>ITRfD</td>
<td>cTorA</td>
<td>cToR</td>
</tr>
<tr>
<td>25</td>
<td>0.5</td>
<td>f</td>
<td>t</td>
<td>t</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>26</td>
<td>Bulk d.</td>
<td>DispL</td>
<td>DispT</td>
<td>Frac</td>
<td>(1...Nmat)</td>
<td></td>
</tr>
<tr>
<td>27</td>
<td>1.57</td>
<td>0.1</td>
<td>0.1</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>28</td>
<td>1.57</td>
<td>0.11</td>
<td>0.11</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>29</td>
<td>Dif w.</td>
<td>Dif g.</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>0.936</td>
<td>7191</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>31</td>
<td>KS</td>
<td>Nu</td>
<td>Beta</td>
<td>Henry</td>
<td>SnkL1</td>
<td>SnkS1</td>
</tr>
<tr>
<td>32</td>
<td>0.3</td>
<td>0</td>
<td>1</td>
<td>0.047</td>
<td>0.015</td>
<td>0.15</td>
</tr>
<tr>
<td>33</td>
<td>0.3</td>
<td>0</td>
<td>1</td>
<td>0.047</td>
<td>0.015</td>
<td>0.15</td>
</tr>
<tr>
<td>34</td>
<td>Temperature dependence</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>35</td>
<td>Dif w.</td>
<td>Dif g.</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>36</td>
<td>0.936</td>
<td>7191</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>37</td>
<td>KS</td>
<td>Nu</td>
<td>Beta</td>
<td>Henry</td>
<td>SnkL1</td>
<td>SnkS1</td>
</tr>
<tr>
<td>38</td>
<td>0.3</td>
<td>0</td>
<td>1</td>
<td>0.047</td>
<td>0.015</td>
<td>0.15</td>
</tr>
<tr>
<td>39</td>
<td>KodCB(1),KodCB(2),.....,KodCB(NumBP)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>-7</td>
<td>-7</td>
<td>-7</td>
<td>-7</td>
<td>-7</td>
<td>-7</td>
</tr>
<tr>
<td>41</td>
<td>cTop</td>
<td>cBot</td>
<td>b1</td>
<td>b2</td>
<td>b2</td>
<td>b2</td>
</tr>
<tr>
<td>42</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>43</td>
<td>tPulse</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>44</td>
<td>0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>45</td>
<td>*** Block H: Heat Transport Information ******************</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
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
lWat lChem CheckF ShortF FluxF AtmInF SeepF DrainF FreeD ITemp
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 lDep cToA cToR MaxItC PeCr
0.5 f t t 0 0 20 2
Bulk.d. DispL DispT Frac (1...Nmat)
1.57 0.1 0.1
1.57 0.11 0.11
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
0.3 0 1 0.047 0.015 0.15 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
"KodCB(1),KodCB(2),.....,KodCB(NumBP)"
-7      -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 ************************
<table>
<thead>
<tr>
<th>Qn</th>
<th>Qo</th>
<th>Th.</th>
<th>Disper</th>
<th>B1</th>
<th>B2</th>
<th>B3</th>
<th>Cn</th>
<th>C0</th>
<th>Cw</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>0.01</td>
<td>0.9</td>
<td>0.1</td>
<td>1.57E+16</td>
<td>2.53E+16</td>
<td>9.89E+16</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.5</td>
<td>0.01</td>
<td>0.9</td>
<td>0.1</td>
<td>1.57E+16</td>
<td>2.53E+16</td>
<td>9.89E+16</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
"KodTB(1),KodTB(2),.....,KodTB(NumBP)"
| 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.