SCIENTIFIC NOTE BOOK # 518E
(Work performed for TEF)

by

Stefan Mayer

Southwest Research Institute
Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas

July 24, 2002

TABLE OF CONTENTS

0. INITIAL ENTRIES

Scientific Note Book:	# 518E
Issued to:	Stefan Mayer
Issue Date:	May 6, 2002
Printing Period:	05/06/2002 - 07/24/2002
Project Title:	TEF
Project Staff:	Stefan Mayer
Project Manager:	Asadul Chowdhury
Principal Investigator:	Randy Fedors
Cross-Reference:	Randy Fedors maintains independent SN432E for TEF.

By agreement with the CNWRA QA, this notebook is to be printed at approximate semi-annual intervals. This computerized Scientific Notebook is intended to address the criteria of CNWRA QAP-001.

[Stefan Mayer, May 7, 2002]

1. GENERAL

1.1 Objectives

Objectives are to document details of scientific work performed to support TEF.

1.2 Computers, Computer Codes, and Data Files

Flow3D to be used for CFD simulations related to cold trap effect. Currently, Flow3D license and software resides on Div. 18 HP-UX machine. Possible that in future, will have software and license on Div. 20 unix workstation.

Software loaded on PC lemur can be used (e.g. excel, powerpoint, adobe illustrator, mathematica).

Table 1-1. Computer, operating system, and compiler used in the tests.

Machine Name	Machine Type	Operating System	Compiler	Location
lemur	PC	Windows NT	none used	Bldg. 189
amadala	HP unix workstation	HP-UX	pre-compiled commercial software	Div. 18

2. Compare Flow3D and Fluent

CNWRA intends to use the CFD code Flow3D to simulate heat and mass flow related to the cold trap effect.

DOE intends to use FLUENT to simulate the same.

A basic comparison of the theories, mainly the equations solved by these codes is performed.

2.1 Flow3D

Solves the complete mass continuity equation (see p. 105, Flow Science manual), momentum equations (pp. 106-107), fluid energy equation (p. 111), tracks the evolution of fluid interfaces or free surfaces if needed (p. 110).

The aspect particular to the equations used is the use of the FAVOR method, by which all "equations are formulated with area and volume porosity functions" (p. 104). All terms are multiplied by the fractional volume or the fractional area open to flow, as appropriate (p. 105).

Fluid configurations are defined using a volume of fluid (VOF) function (p. 110). This spatial distribution function for the interface is tracked, allowing for an accurate representation of the evolution of the interface.

A number of auxiliary models are available, for example the homogeneous bubble model (pp. 118-120), which allows for phase changes at its surface to be computed (condensation, evaporation); wall heat transfer (pp. 120-124), which is needed to model heat sources or sinks; buoyant flow model (pp. 124-125), which is needed to model temperature dependent density changes.

Numerical approximations are presented on pp. 141-214. The code uses a finite-difference mesh (p. 145). First- and second-order accurate solutions algorithms offered are essentially explicit. Emphasis is on robustness, with potentially stringent requirements on time-stepping to preserve stability (Courant number). Simultaneous over-relaxation (SOR) and an alternating-direction-implicit scheme (SADI) are algorithm options to compute pressure distributions (p. 165).

Note that a multi-block grid option is available, which allows for local higher resolution of flow (Ch.5, p. 76).

2.2 Fluent 6.0

No complete reference manual was available from Fluent 6.0. However, an overview manual and slides from a Fluent training workshop were available. This material sufficiently describes what equations Fluent solves.

Fluent solvers are based on the finite volume method. All conservation equations (continuity, momentum, energy) are expressed as integrals over the finite control volume and are discretized into algebraic equations (slide A2).

A substantial difference to Flow3D is the ability of Fluent to used unstructured, solution-adaptive grids (p. 2-3).

Natural convection is modeled using the Boussinesq model (slide F-13).

Fluent handles multiphase flow using several optional approaches, among which is the VOF method. Mass

transfers due to evaporation and condensation can also be modeled (slide 18).

2.3 Comparison

The basic equations solved by both codes are similar. While Flow3D solves the differential forms of the conservation equations, with terms scaled and included as required by the FAVOR and VOF methods, and uses a finite difference, structured mesh numerical approach, Fluent solves the integral forms of the conservation equations for each finite volume and uses the finite volume, unstructured mesh numerical approach.

Both codes use the Boussinesq approximation to simulate natural convection due to temperature effects.

Given the approximations that are made during numerical simulations, it is possible that both codes, when used to simulate the same problem, give differing results in detail. However, overall they should predict same cold trap flow and temperature distributions since the fundamental equations are the same, and only the implementation methods are different.

3. Cold Trap experiment: Ambient temperature evolution

In preparation of a lab scale cold trap experiment, ambient temperature distributions are analyzed. Thermocouples were installed to measure temperature distributions in the drift, in the wet sand, and outside the experiment for ambient conditions.

Figure 3-1 shows select plots over time of the diurnal fluctuations (solid lines with large fluctuations), of temperature fluctuations in the wet sand (symbols only, no lines, intermediate set of curves, small fluctuations), and of temperature fluctuations in the drift model (solid lines, lower average values, small fluctuations).

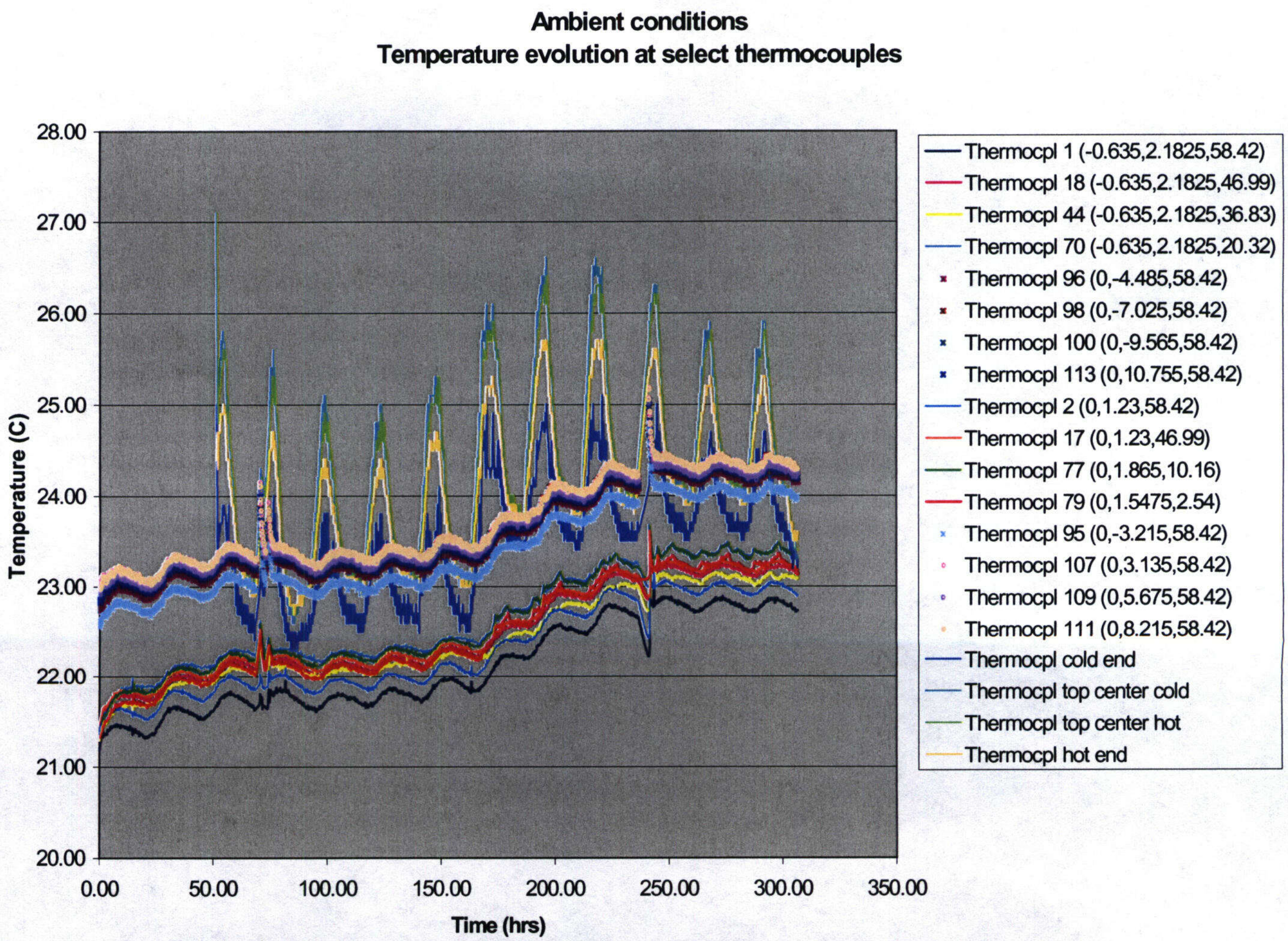

Figure 3-1: Thermocouple data for ambient temperature fluctuations.

The diurnal effect is obvious.

Plotted are a number of thermocouple data from:

a) inside the drift, along the axis (solid lines, small diurnal)

b) select locations in the wet sand at the z=58.42 cm cross-section (symbols only, no line)

c) the 4 provided ambient conditions outside the insulation material (solid line, larger diurnal oscillation)

An unvoluntary, but useful addition to this preliminary test:

Someone imposed a near-stepfunction change in the ambient temps at about 160 hrs. (Note that the lower, nighttime temps are more consistent than the daytime temps).

Preliminary observations:

1) Temperature oscillations in the wet sand are significantly damped compared to the ambient ones.

2) No substantial temperature gradient across the wet sand is observed.

3) On average, temperatures in wet sand appear slightly lower than ambient (will calculate and provide numbers later)

4) There is a time lag of approximately 6 hrs between the sand temp fluctuations and the ambient fluctuations

5) There is a time lag of approximately 3 - 4 days of the average sand temp response to ambient temp step function

6) The temps inside the drift are significantly lower than inside the wet sand.

7) No noticeable time lag between wet sand temp oscillation and drift temp oscillations.

Questions to answer:

1) Infer heat transfer from ambient to wet sand from damping and time shift of oscillations and from asymptotic approach to ambient step function

2) Infer heat transfer required from drift to heat sink to justify for lower temperatures in drift (only potential I can think of: evaporation or heat loss out the sides)

3) Why does the thermocouple on the outside at the "cold" end indicate lower ambient temps?

4) Why do select thermocouples inside the drift indicate temps similar to wet sand (e.g. thmcpl 83 and 90)?

5) What is the reason for the two "spikes" of temperature (at about 70 hrs and 240 hrs) in wet sand and drift, but not in ambient temp thmcpls?

Other observations:

The temperature differences observed are very small. But they are well within the resolution of the thermocouples. However, before inferring any local trends from the data, a specialized calibration

needs to be performed to ensure that the indicated temperatures are accurate within the allowed tolerances.

4. Cold Trap experiment: Regression curves from calibration of thermocouples

All thermocouples have undergone dedicated calibration, by direct comparison of their readings to reading of a precise (0.1 °C), calibrated thermometer.

Regression curves are inferred for all thermocouples from this comparison.

A simple FORTRAN code must be written to compute the needed linear regression parameters *a* and *b*. The equations used are obtained from Press et al., 1986 (Numerical Recipes, Cambridge University Press, pp. 504–505.

Y := actual temperature
x := thermocouple measured temperature
y=a+bx :=linear regression curve fit to transform measured (x) onto calibrated (y) temperature
(a,b) := linear regression parameters
σ_i := individual measurement error (a priori not known)

$$a = \frac{S_{xx}S_y - S_x S_{xy}}{\Delta},$$

$$b = \frac{SS_{xy} - S_x S_y}{\Delta},$$

where:

$$\Delta = SS_{xx} - (S_x)^2$$

$$S = \sum_{i=1}^{N} \frac{1}{\sigma_i^2}, \quad S_x = \sum_{i=1}^{N} \frac{x_i}{\sigma_i^2}, \quad S_y = \sum_{i=1}^{N} \frac{y_i}{\sigma_i^2}$$

$$S_{xx} = \sum_{i=1}^{N} \frac{x_i^2}{\sigma_i^2}, \quad S_{xy} = \sum_{i=1}^{N} \frac{x_i y_i}{\sigma_i^2}$$

Since the individual measurement errors σ_i are not known, Press et al. (1986, p. 507) suggest to assume:

$$\sigma_i = \sigma$$

whence the term cancels from the estimates for a and b.

$$\tilde{S} = \frac{1}{\sigma^2}\sum_{i=1}^{N} 1 = \frac{N}{\sigma^2}, \quad \tilde{S}_x = \frac{1}{\sigma^2}\sum_{i=1}^{N} x_i, \quad \tilde{S}_y = \frac{1}{\sigma^2}\sum_{i=1}^{N} y_i$$

$$\widetilde{S}_{xx} = \frac{1}{\sigma^2}\sum_{i=1}^{N} x_i^2 \,,\; \widetilde{S}_{xy} = \frac{1}{\sigma^2}\sum_{i=1}^{N} x_i y_i \,.$$

$$\widetilde{\Delta} = \widetilde{S}\widetilde{S}_{xx} - \left(\widetilde{S}_x\right)^2 = \frac{1}{\sigma^4}\left(N\sum_{i=1}^{N} x_i^2 - \left(\sum_{i=1}^{N} x_i\right)^2 \right),$$

$$a = \frac{\widetilde{S}_{xx}\widetilde{S}_y - \widetilde{S}_x\widetilde{S}_{xy}}{\widetilde{\Delta}},$$

$$b = \frac{\widetilde{S}\widetilde{S}_{xy} - \widetilde{S}_x\widetilde{S}_y}{\widetilde{\Delta}} \,.$$

5. Natural convection fluid simulations with Flow3D

To run Flow3D, an account on a Div. 18 Unix machine is required. This allows access to the license. Possibly, in the future, a separate license can be purchased for direct installation and running of the code inside Div. 20.

During remote login using a secure shell window, only text can be edited, but no graphics requiring e.g. an X-window can be displayed on the local (Div. 20) PC. This is most likely due to the firewall.

Input files were edited remotely from the Div. 20 PC lemur, and the file structure of the Div. 18 unix account was accessed to manipulate files as needed.

Instead of directly viewing the simulation result graphics on the screen (not possible due to firewall), the plot option of the Flow3D package was used to store the graphics results into PostScript files. These files were then transferred using secure shell ftp to the local PC, and results were viewed locally using Acrobat Illustrator, and printed as needed.

Again due to the firewall restrictions, the graphical user interface for flow3D could not be used. The input files were edited directly, and runs were submitted from the command line.

Note that for proper execution, a number of lines needed to be included in the .cshrc and .tcshrc files. By way of example, a copy of these files that I have used, and which allowed for proper execution from command line, are included here.

Sample .cshrc file used on unix workstation:

```
#
# Default user .cshrc file (/usr/bin/csh initialization).

# Usage:  Copy this file to a user's home directory and edit it to
# customize it to taste.  It is run by csh each time it starts up.

# Set up default command search path:
#
# (For security, this default is a minimal set.)

      set path=( $path \
                 /bin \
                 /usr/local/bin \
                 /usr/bin/X11 \
                 /lib \
                 /rusr/Flow3d/local )

# Set up C shell environment:

      if ( $?prompt ) then          # shell is interactive.
          set history=20            # previous commands to remember.
          set savehist=20           # number to save across sessions.
          set system='hostname'     # name of this system.
          set prompt = "$system \!: "     # command prompt.

          # Sample alias:
```

```
          alias   h     history

          # More sample aliases, commented out by default:

          # alias d     dirs
          # alias pd    pushd
          # alias pd2   pushd +2
          # alias po    popd
          # alias m     more
      endif
```

Sample .tcshrc file used:

```
# .tcshrc

# User specific aliases and functions

alias rm 'rm -i'
alias cp 'cp -i'
alias mv 'mv -i'
alias ls 'ls -F'

setenv PATH "/sbin:`cat /etc/PATH`"
setenv F3D_HOME /rusr/Flow3d

set prompt="\n%B[%n@%m]%b (%~)\ntcsh:{!}%# "

source ~/.cshrc
```

CFD: computational, fluid dynamics

The default commands were used. These are described in the Flow3D manual, Section 1.4.2 ("Running Flow3D from the command line"). Note that, without additional settings:
- The input file must be called prepin.inp
- The input file to each run needs to be preprocessed. Use the line command: runpre.
- To check the output of the preprocessor, including the gridding and the initial distribution of parameters, run the plot command: pltfsi. The plot command will ask for which file to use. The default is the file prpplt.dat.
- To run the simulation, use the line command: runhyd. Intermediate execution controls will be flushed to the screen as specified in the input file. If the run should be in the background, make sure to redirect the screen output to a file, using the complete line command: runpre > screendump.dat &.
- The results of the simulation must be postprocessed, using the line command: runpost.
- To view the graphics, run pltfsi. The default file containing the output of the completed simulation is flsplt.dat.

5.1 Sample Run: Numerical solution to natural convection flow in a square cavity

The problem was executed on amadala.div18.swri.edu. The input and output files are transferred and stored on lemur in D:\smayer\Tef_kti\ColdTrap\Flow3DSimulations\AnalyticalSquareCavity.

The simulation is for normalized variables, with normalized temperature T=1 imposed at the left boundary wall,

and T=0 imposed at the right wall. The resulting circular natural convection flow pattern, as well as the isothermal contours in the cavity are clearly seen on the graphic output of the results. Sample printouts are attached to the printout of this electronic notebook, at the end of this section.

5.2 Sample Run: Numerical solution to natural convection flow in a rectangular cavity

This simulation is fairly similar to the one discussed in 5.1. It is for a rectangular cavity of aspect ratio 10:1. The heated wall (normalized temperature = 1) is now on the right side, instead of the left. The problem was executed on amadala.div18.swri.edu. The input and output files are transferred and stored on lemur in D:\smayer\Tef_kti\ColdTrap\Flow3DSimulations\AnalyticalRectangularCavity.

The results suggest the development of two convection cells, one near each of the cold and the hot wall. This was not predicted by the simplified theory. The result needs to be checked. The initially separate cells are a transient state, and they appear to connect at higher times. The same run will be resubmitted over twice the duration, to check for convergence and to obtain a steady state result.

[Stefan Mayer, 07/24/02]

Entries into Scientific Notebook No. 518E for the period 05/06/2002 to 07/24/2002 and for the entire notebook (all pages) have been made by Stefan Mayer and no original text entered into this Scientific Notebook has been removed.

Stefan Mayer/ Stefan Mayer /July 24, 2002

No data quality or traceability issues will arise from the data and plots presented in this notebook, as all Stefan's work was/is supplanted by work in sci ntbk #432e and #536e. Stefan's work was exploratory in nature. R. Fedors 10/4/02

I have reviewed this scientific notebook and find it in compliance with QAP-001. There is sufficient information regarding procedures used for conducting tests, acquiring and analyzing data so that another qualified individual could repeat the activity.

[signature] 10-3-02
MGFE