

**Original Page Numbering Retained.**

This research project has been devoted to developing numerical models for addressing two-phase flow and phase separation in NaCl-H<sub>2</sub>O hydrothermal systems. The goal has been to develop numerical modeling capabilities for understanding seafloor hydrothermal systems, nearly all of which show evidence of either current or past phase separation processes. The research has involved four separate steps: (1) development of an equation of state for NaCl-H<sub>2</sub>O fluids in the PTX range useful for simulation of seafloor hydrothermal systems; (2) development of a new numerical simulator (called FISHERS—Fully Implicit Seafloor Hydrothermal Event Simulator) incorporating the equation of state; (3) testing this code on sample problems and comparing the results to those generated by other numerical algorithms; and (4) using the code to investigate scenarios two-phase flow processes in seafloor hydrothermal systems, with particular emphasis on hydrothermal fluids from the Main Endeavour Field on the Juan de Fuca Ridge.

The major educational activity has been the training of a female Ph.D. graduate student, Kayla Lewis. Kayla successfully defended her thesis on August 31, 2007 and will officially graduate in December, 2007. When testing and documentation of the new code is complete it will be made available for general use—most likely through placement on the PI's hydrothermal website that is under construction at Virginia Tech.

**Findings: (See PDF version submitted by PI at the end of the report)**

#### **Training and Development:**

The graduate student, Kayla Lewis, has become familiar with the complex numerical code GTHSW and has learned about multi-phase multi-component flow processes in porous media. She has developed a thorough understanding of the phase diagram of NaCl-water. Students in my course Fluids in the Earth's Crust at Georgia Tech and Virginia Tech have learned about the complexities of multi-phase multi-component flow.

The graduate student has learned to create her own numerical modeling schemes (FISHERS), using the control volume technique, how to numerically implement equations of state, and has a deeper understanding of multi-phase multi-component flow processes in porous media. She is now ready to enter the scientific community as an accomplished fluid dynamicist and numerical modeler. Two of my current graduate students will be using FISHERS in their MS and Doctoral research.

#### **Outreach Activities:**

#### **Journal Publications**

#### **Books or Other One-time Publications**

Lowell, R.P., B.W. Crowell, K.C. Lewis, and L. Liu, "Modeling multiphase, multi-component processes at oceanic spreading centers: Magma to microbe", (2007). Book, Accepted

Editor(s): Robert P. Lowell, Jeff Seewald, Michael Perfit, and Anna Metaxas

Collection: Modeling Hydrothermal Processes at Oceanic Spreading Centers: Magma to Microbe

Bibliography: American Geophysical Union, Washington, DC

Kayla C. Lewis, "Numerical Modeling of Two-Phase Flow in the Sodium Chloride-Water System with Applications to Seafloor Hydrothermal Systems", (2007). Thesis, Accepted

Bibliography: Doctoral Dissertation, Georgia Institute of Technology, Atlanta

#### **Web/Internet Site**

#### **Other Specific Products**

#### **Product Type:**

**Software (or netware)**

**Product Description:**

The numerical Code FISHERS with the new equation of state is being tested and documentation is being prepared. When these items are finished, the code will be made available for community use.

**Sharing Information:**

When completed, a link will be placed on the hydrotherm website so that interested users can download the program and pertinent documentation.

**Contributions**

**Contributions within Discipline:**

Multi-phase multi-component flow in porous media is a very difficult subject that must be investigated numerically. The codes we have developed are among the first of its kind and will hopefully be used by others in the community. Phase separation in ridge crest hydrothermal systems is of fundamental importance to the RIDGE 2000 Initiative at NSF

**Contributions to Other Disciplines:**

Multi-phase, multi-component flow has applications to methane gas hydrate evolution, oil formation and reservoir dynamics, and in other science and engineering disciplines.

**Contributions to Human Resource Development:**

This research project has helped train a female scientist who is entering the teaching/research profession upon completion of her degree. The code developed by this graduate student is being used by other graduate students in the PI's research program.

**Contributions to Resources for Research and Education:**

**Contributions Beyond Science and Engineering:**

**Categories for which nothing is reported:**

Organizational Partners

Activities and Findings: Any Outreach Activities

Any Journal

Any Web/Internet Site

Contributions: To Any Resources for Research and Education

Contributions: To Any Beyond Science and Engineering

Initial findings from this research project have been presented at the Ridge Theoretical Institute 2006 meeting “Modeling Hydrothermal Processes at Oceanic Spreading Centers: Magma to Microbe” [Lewis *et al.*, 2006]. Two papers are currently being prepared for submission to peer-reviewed journals. One will highlight the development of the equation of state and the FISHERS code; the other will use the code to understand the salinity and temperature of black smoker fluids at Main Endeavour Field. Some of this material is also in Lowell *et al* [2007]. The material below is taken from Kayla Lewis’ Doctoral Dissertation entitled “Numerical Modeling of Two-Phase Flow in the Sodium Chloride-Water System with Applications to Seafloor Hydrothermal Systems”

### (1) *The Equations of State*

The densities, salinities, and enthalpies as functions of  $P$ - $T$ - $X$  are evaluated via linear interpolation between values in thermodynamic lookup tables. These tables are valid for pressures between 85 bars and 1 kbar, temperatures between 0° and 800° C, and salinities between 0 and 100 wt% NaCl. For the bulk densities above 300°C as well as for values of the salinity and density on the upper boundary of the two-phase region above this temperature, these tables were compiled using a computer program developed by A. Anderko, which is based upon the theoretical free energy framework presented in Anderko [1993]. This framework is only valid for temperatures between 300° and 800°C; however, the two-phase region does not exist below 300°C and pressures above 85 bars, because the critical curve drops below that pressure for temperatures lower than 300°C. For the bulk density values from 300°C to 0°C, a program developed by D. Archer was used, based upon the framework presented in Archer [1992]. Specific enthalpies between 300° and 600°C were compiled using the framework of *Tanger and Pitzer* [1989]. Enthalpies below 300°C were compiled by integrating specific heats derived from Archer’s program (mentioned above) from 300°C downward, and using the enthalpies at 300°C to solve for the first constants of integration. Enthalpies between 600° and 800°C were compiled by integrating the specific heats at 600°C (from *Tanger and Pitzer* [1989]) upward, using the enthalpies at 600°C to solve for the first constants of integration. Enthalpies on the upper boundary of the two-phase region are calculated from the bulk enthalpies at the  $T$ - $P$ - $X$  values on that surface. Finally, the salinities on the salt saturated vapor surface were obtained using the correlation equation from *Palliser and Mckibbin* [1998], and the other quantities on that surface are obtained from the bulk quantities at the  $P$ - $T$ - $X$  values on that surface. Additional information and plots of density and salinity along the two-phase surface are given in *Lewis* [2007].

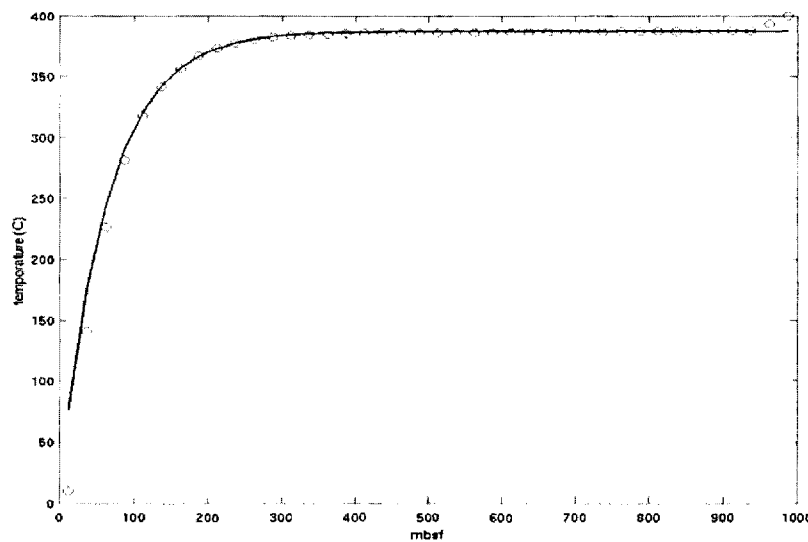
### (2) *Development of numerical modelling code*

FISHERS uses the finite volume method, as developed in *Patankar* [1980], with upstream weighting applied to the coefficients of the temperature equation to solve the coupled non-linear partial differential equations describing conservation of mass, momentum, energy, and solute. For the time marching, the fully implicit method was used for all the equations, so that the newest available values of  $T$ ,  $P$ , and  $X$  dominate over each time step. Iteration loops with relative convergence criteria can be turned on or off in the input files. Additionally, to avoid having to use an impractically small time step size for

some simulations, under-relaxation is used. The FISHES code is written in FORTRAN 90 with extensive internal documentation, intuitively named variables, and with the new equation of state incorporated into it from the start. A user's guide to FISHES is an Appendix to the doctoral dissertation of *Lewis* [2007]. When it is finalized the user's guide and the program will be placed on the PI's website, where it can be downloaded for use by the scientific community.

### (3) Testing the FISHES code

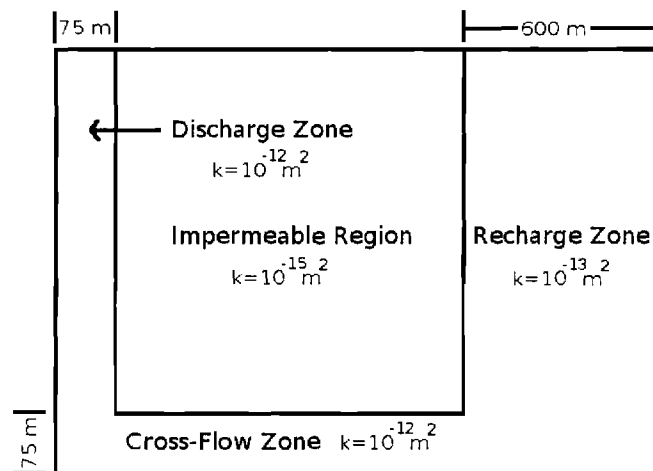
FISHES has been tested by running a number of sample problems that have been investigated using other codes. In particular, FISHES was tested against three different problems. To test how FISHES handled phase separation, the results of a submarine geothermal heat pipe simulation were compared with previously published results from the code GTHSW [*Bai et al.*, 2003]. To test the coupling between the salinity and pressure equations, the code was tested against published numerical solutions to the Elder problem [*Geiger et al.*, 2006; *Ackerer et al.*, 1999; *Simpson and Clement*, 2003]. Finally, the code was applied to a single pass system, where it was able to reproduce the well-known solution to the thermal convection-diffusion equation in the discharge zone. Details are given in *Lewis* [2007]. As an example, the comparison of FISHES with a one-dimensional advection-diffusion solution is shown here.



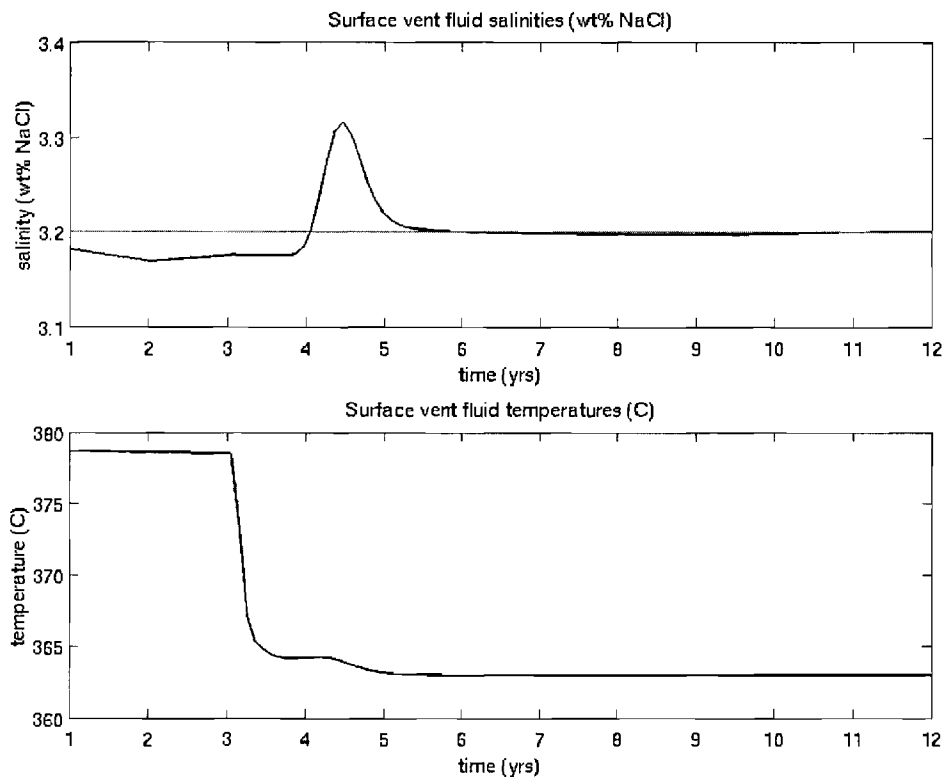
**Figure 1** Output temperatures as a function of depth at steady state (circles) plotted against the exact solution to the steady one-dimensional convection-diffusion equation (solid curve).

### (4) Single-Pass Models and the Main Endeavour Vent Field

FISHES was then used to simulate two-phase flow and phase separation in a single-pass hydrothermal model shown schematically in Figure 2. The main emphasis of this study is to first investigate how a two-phase region near evolves near the base of a hydrothermal system and how vent salinity and temperature evolve with time. To do this we first run the model to steady state in a configuration in which two-phase flow is absent. We then raise the temperature in the lower left-hand corner of the model so that a two-phase zone is developed there. We find that saline brine collects in that corner and that a lower-than-seawater vapor phase ascends to the surface. After some time we return the base of the model to the single phase regime and investigate how the sequestered brine phase is gradually transported to the seafloor. Figure 3 shows a typical result. *Lewis* [2007] has explored the effects of (1) varying the permeability of the discharge zone, (2) increasing the temperature at the base of the system (to increase the intensity of phase separation) and (3) increasing the width of the two-phase zone.



**Figure 2. Basic geometry and permeability structure for the single pass model.**



**Figure 1. Vent fluid temperatures and salinities corresponding to an initial two-phase simulation (first 3 yrs) followed by purely single-phase flow in which brine is flushed from deep within the system. The system geometry is shown in Figure 2.**

The most interesting result of these simulations is that extending the width of the two-phase zone at the base of the system result is lower vent salinities, even if the maximum temperature at the bottom is not changed.

The Main Endeavour Vent Field (MEF) is characterized by gradients in vent fluid salinity and temperature; salinity tends to decrease from N-S, whereas temperature tends to increase [Kelley *et al.*, 2002]. We are developing single-pass simulations to determine whether we can match both salinity and temperature distributions along the MEF. Based on the single-pass modeling discussed above, we suspect that salinity gradient fluids exhibited by structures at the MEF indicate that each structure is tapping a two-phase region of different lateral extent, and perhaps of slightly different basal temperature. If we are able to successfully match the gradients at the MEF in this fashion, our simulations will shed some light on the differences in subsurface plumbing between northern and southern end of the MEF, and perhaps the relationship between fluid flow and the magmatic heat source.

## References

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