Contract No:

This document was prepared in conjunction with work accomplished under Contract No. DE-AC09-08SR22470 with the U.S. Department of Energy (DOE) Office of Environmental Management (EM).

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Benchmarking Results For Small Column Ion Exchange Model

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INTRODUCTION

A three dimensional computational model has been developed to simulate the thermal characteristics of Crystalline Silicotitanate (CST) ion exchange media fully loaded with radioactive cesium packed in a column configuration or distributed on the floor of a waste storage tank (Lee and King, 2011). The modeling was conducted to support the Small Column Ion Exchange (SCIX) program which is focused on processing dissolved, high-sodium salt waste for the removal of specific radionuclides such as Cs-137 through a column supported within a High Level Waste (HLW) storage tank at the Savannah River Site (SRS).

The primary objective of the current work was to benchmark the previously developed three dimensional model against literature data and theoretical results to demonstrate that the basic characteristics of the thermal dissipation through the system are properly captured. The benchmarking evaluations included cases involving both conduction and natural convection cooling behavior, since these cases were believed to be closely related to the passive heat transport mechanisms operative within the upper column plenum and the tank liquid space of the SCIX system. One case involved a transient conduction calculation through a steel plate, and the other involved natural convection calculations for enclosed and open channel systems. This paper will discuss the benchmarking modeling and analysis results.

DESCRIPTION OF THE WORK AND RESULTS

Benchmarking of the three dimensional model developed to support the Small Column Ion Exchange (SCIX) program was necessary to validate previously published thermal model predictions (Lee and King, 2011). These predictions were utilized for the development of the facility safety basis. The model was created using the body-fitted coordinate system and structured multi-block grids in the Computational Fluid Dynamics (CFD) preprocessing environment. The CFD computational model was developed to simulate the thermal characteristics of Crystalline Silicotitanate (CST) ion exchange media fully loaded with radioactive cesium packed in a column configuration or distributed on the floor of a waste storage tank. The column modeling domain included temperature distributions within the packed bed of ion exchange media as well as the upper column plenum region containing only fluid. Thermal modeling calculations were also performed for the entire waste storage tank domain for the case where spent and ground CST has been transferred to the waste tank.

Accident scenarios evaluated for the column modeling calculations included loss of salt solution flow through the bed and loss of active cooling. For the natural convective cooling calculations of the column region, the Boussinesq approximation was used for the gravitational term in the momentum equation to include buoyancy-induced natural convection. A two-part approximation was used which neglects all variable property effects in the governing equations and approximates the density difference term with a simplified equation of state. The primary objective of this work was to benchmark the model against literature data and theoretical results to demonstrate that the thermal behavior of the system was properly predicted.

For the benchmarking evaluations of conduction behavior in the SCIX system, a small stainless steel plate of thickness L shown in Fig. 1 was considered. The plate is sufficiently small that thermal equilibrium can be attained within a short time scale. Initially the plate was at a uniform temperature T_i, and at time zero the surfaces were suddenly lowered to $T = T_w$. Under transient conditions, the energy equation for the slab with an effective thermal conductivity $k_{b,eff}$ becomes

$$\frac{\partial T(x,t)}{\partial t} = \left(\frac{k_{b,eff}}{\rho C_p}\right)\left(\frac{\partial^2 T(x,t)}{\partial x^2}\right) = \alpha\left(\frac{\partial^2 T(x,t)}{\partial x^2}\right) \quad (1)$$

By using the separation of variable technique, a final series solution at position x and time t can be obtained from the initial and boundary conditions. That is,

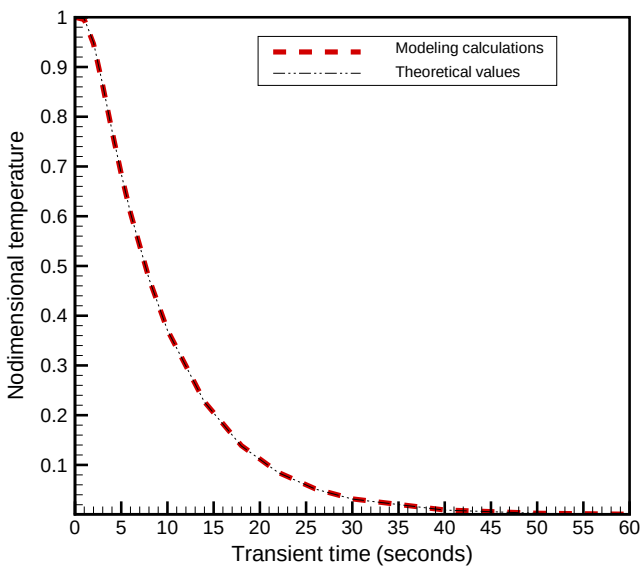
$$T(x,t) = T_w + (T_i - T_w)\left(\frac{4}{\pi}\right)\left[\sum_{n=1}^{\infty}\frac{1}{n}\exp\left\{-\alpha\left(\frac{n\pi}{L}\right)^2 t\right\}\sin\left(\frac{n\pi x}{L}\right)\right]_{n=1,3,5,--} \quad (2)$$

The material and thermal properties used for the benchmarking test are provided in Table 1. The transient temperature responses for the plate were calculated using the same basic approach used to model conduction heat transfer in the SCIX system when the initial plate temperature was 100°C and its wall surfaces were suddenly cooled to 20°C, The modeling results are quantitatively compared in Figure 1 to theoretical results calculated using Eq. (2). The modeling predictions are in agreement with theory within about 0.5%

relative error. Detailed spatial and transient distributions are also compared with the theoretical results, where the results are provided in non-dimensional units for temperature and distance. Close agreement between the model predictions and theoretical calculations was observed. This result indicates that the model accurately predicts conduction heat transfer through a simple system where no fluid movement is allowed, such as the SCIX modeling cases involving conduction controlled media with convective heat transfer.

Table 1. Material and thermal properties used for the benchmarking analysis

Parameters	Material and thermal properties		
	Density, ρ	Specific heat, C_p	Thermal conductivity, $k_{b,eff}$
Values	8000 kg/m^3	500 J/kg-K	20.0 W/m-K



Non-dimensional temperature, $\theta = \left\{ \frac{(T(x,t) - T_w)}{(T_i(x,t=0) - T_w)} \right\}$

Figure 1. Benchmarking results of the present model against the theoretical calculations for the transient thermal response

Experimental data was available for a natural convection heat transfer case within for a rectangular enclosure (aspect ratio (L/H) = 2.0) with given boundary temperatures as reported by Nansteel and Greif (1981). The basic geometry involved is shown in Figure 2, where the heat transfer across a water-filled, rectangular vessel is considered. For the modeling validation analysis of this experiment, a two-dimensional natural convection model was constructed using the following water properties:

L = 0.305m
H = 0.152m
k = 0.640 W/mK
Density (ρ) at test condition = 988.0 kg/m^3
Viscosity (μ) = 5.471 x 10^{-4} Pa-sec
Thermal expansion coeff. (β) = 4.33x10^{-4} T^{-1}
Pr = 3.7
T_H = 72 ^{o}C
T_C = 25 ^{o}C

$Gr_H = \left(\frac{g\rho^2\beta H^3 \Delta T}{\mu^2} \right)$ = 1.8x10^{10} < 1.0 x 10^{11} (assumed to be laminar flow regime for near-transition regime)

Based on the experimental conditions, the natural convection regime is near the laminar-turbulent flow transition, but is considered to be laminar in the present analysis.

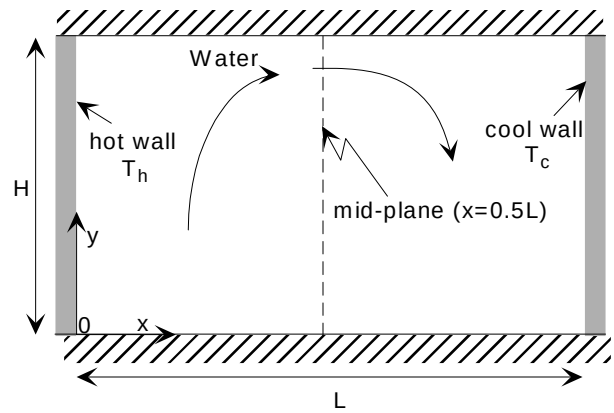


Figure 2. Natural convection experiment for the rectangular enclosure conducted by Nansteel and Greif (1981).

The benchmarking results are shown in Table 2. The results show that the predictions are in agreement with the test data within about 12% relative error. The non-dimensional temperature is defined by θ. Figure 3 shows a graphical comparison of the predictions with the test data is provided in terms of non-dimensional parameters, y/H and θ.

$$\theta = \left(\frac{T - T_c}{T_h - T_c} \right) \quad (3)$$

Table 2. Comparison of non-dimensional temperatures predicted by the model and the experimental data (1981) along the vessel midline at x = L/2.

Non-dimensional dist. (y/H)	Predictions, θ	Nansteel and Greif data (1981), θ	Relative error (%)
0.0	0.176	0.160	10.00
0.1	0.262	0.260	0.77
0.2	0.338	0.340	-0.59
0.3	0.396	0.403	-1.74
0.4	0.449	0.463	-3.02
0.51	0.505	0.520	-2.88
0.61	0.556	0.582	-4.47
0.70	0.604	0.644	-6.21
0.80	0.663	0.713	-7.01
0.90	0.738	0.794	-7.05
1.00	0.824	0.880	-6.36

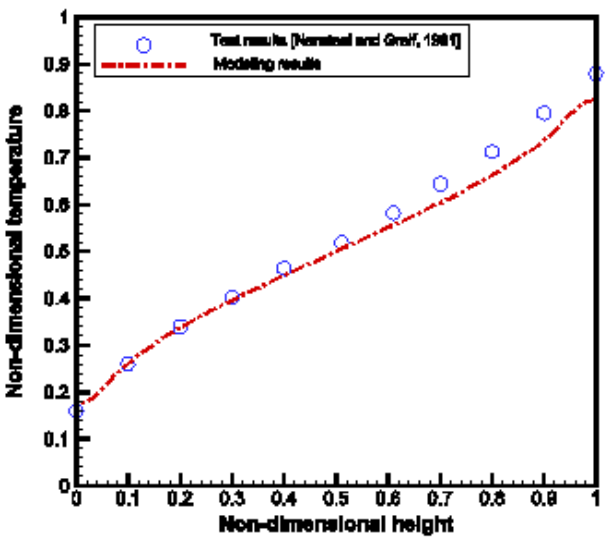


Figure 3. Comparison of the present modeling predictions with the literature experimental data (1981).

Experiments on chimney enhanced free convection were conducted by Fisher and Torrance (1999). These experiments involved a rectangularly-shaped vessel which was closed on the sides but open to the atmosphere on the top and bottom. A heating block with a set of fins was contained near the bottom and within the rectangular box. Heating the fins resulted in buoyancy-induced natural convection air flow up the vessel such that the upper portion of the vessel acted like a chimney. The temperature increase across the box was measured. Flow velocities at the exit of the chimney were also measured using a hot-wire anemometer. For the modeling validation and benchmarking analysis of these experiments, a three-dimensional model was constructed as shown in Fig. 4. These experimental results represent the best data identified thus far to date to evaluate the model performance for a system involving convective heat transfer with flow obstructions. This system is analogous to the SCIX modeling case involving loss of solution flow within a cesium-loaded ion exchange column (Lee and King, 2011). The chimney region is analogous to the SCIX column plenum and the thin slot flow channels provide flow obstructions just as the packed bed of ion exchange media in the SCIX column obstructs flow, although with markedly different flow characteristics.

Calculated temperature distributions driven by natural convection flow patterns at the middle plane of the apparatus are provided in Figure 5. A comparison of buoyancy-driven fluid flow velocities for the model predictions and the literature data along the centerline of the chimney exit plane is provided in Table 3. A comparison of the calculated and observed temperature rise is provided in Table 4. In all cases, the relative error was below 10%, indicating that the existing three-dimensional model accurately predicts convective heat transfer in this system.

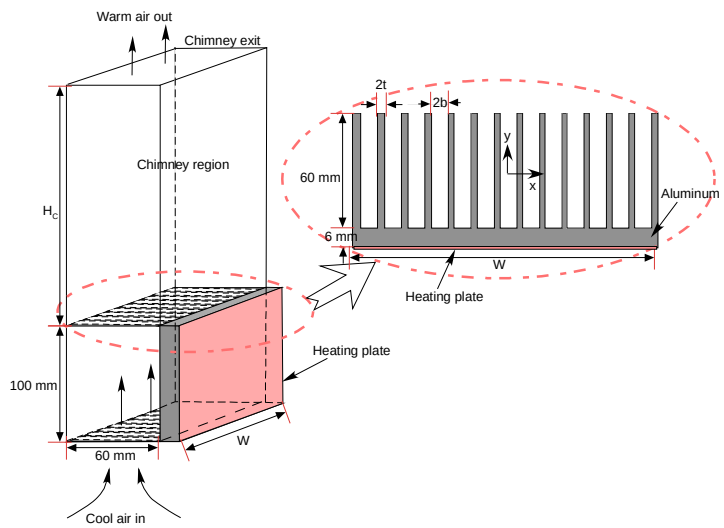


Figure 4. Test section geometry used for the natural convection experiments [Fisher and Torrance, 1999]

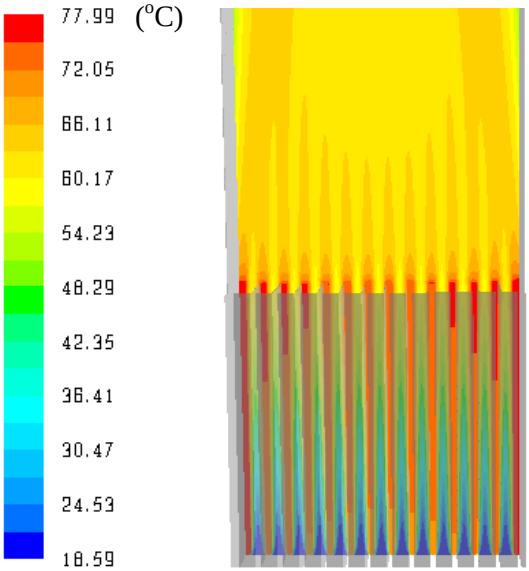


Figure 5. Temperature distributions at the middle plane of the test section with chimney (98.68 watts power and 18.59 °C ambient temperature).

Table 3. Comparison of buoyancy-driven velocities between the model predictions and the literature data [Fisher and Torrance,1999] along the centerline of the chimney exit plane.

Heat load (watts)	Ambient air temperature (°C)	Comparison of averaged natural convection velocities at chimney exit (m/sec)		% error
		Modeling predictions	Test results	
59.42	18.24	0.25	0.26	3.8
79.03	19.30	0.28	0.30	6.7
98.68	18.59	0.32	0.33	3.0

Table 4. Comparison of temperature rise between the model predictions and the literature data [Fisher and Torrance,1999].

Heat load (watts)	Ambient temperature (°C)	Comparison of temperature difference between the heated structure and ambient air (°C)		% error
		Modeling predictions	Test results	
59.42	18.24	38.88	41.57	6.5
79.03	19.30	47.61	51.80	8.1
98.68	18.59	56.93	61.13	6.9

DISCUSSIONS AND SUMMARY

The model used for the previous SCIX thermal analysis (Lee and King, 2011) has been benchmarked for a range of simple/classical and complex physical problems associated with conduction and natural convection cooling phenomena.

The benchmarked problems consisted of two main groups. The first group included well-defined and classical problems for which distinct analytical solutions existed. The other group involved complex and physical problems for which analytical solutions were difficult to obtain. For these test problems, CFD results were compared and validated through comparisons with experimental data. Both conduction and convection controlled CFD model predictions were benchmarked. The calculation results for the SCIX model showed that the code predictions are in reasonably good agreement (~10% relative error) with the analytical solutions or experimental test data. .

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