

# Assessment of RELAP5-3D for Analysis of Very High Temperature Gas-Cooled Reactors

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Cliff B. Davis  
Larry J. Siefken  
Chang H. Oh

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## **ASSESSMENT OF RELAP5-3D FOR ANALYSIS OF VERY HIGH TEMPERATURE GAS- COOLED REACTORS**

Cliff B. Davis, Larry J. Siefken, and Chang H. Oh  
Idaho National Laboratory  
P.O. Box 1625, Idaho Falls, ID 83415-3890, USA,  
[cbd@inel.gov](mailto:cbd@inel.gov), [ljs@inel.gov](mailto:ljs@inel.gov), [chh@inel.gov](mailto:chh@inel.gov)

### **ABSTRACT**

The RELAP5-3D<sup>®</sup> computer code is being improved for the analysis of very high temperature gas-cooled reactors. Diffusion and natural circulation can be important phenomena in gas-cooled reactors following a loss-of-coolant accident. Recent improvements to the code include the addition of models that simulate pressure loss across a pebble bed and molecular diffusion. These models were assessed using experimental data. The diffusion model was assessed using data from inverted U-tube experiments. The code's capability to simulate natural circulation of air through a pebble bed was assessed using data from the NACOK facility. The calculated results were in reasonable agreement with the measured values.

### **KEYWORDS**

High temperature gas-cooled reactor, air ingress, chemical diffusion, natural circulation, RELAP5-3D.

### **1. INTRODUCTION**

The RELAP5-3D (RELAP5-3D Code Development Team 2003) computer code is being improved for the analysis of very high temperature gas-cooled reactors. Recent code improvements include the addition of models that simulate pressure loss across a pebble bed and molecular diffusion. These models affect the simulation of natural circulation following a loss-of-coolant accident and can be particularly important for the analysis of gas-cooled reactors.

Flow through the reactor vessel may stagnate following a loss-of-coolant accident due to a non-uniform concentration of helium and air. However, molecular diffusion will eventually result in a uniform concentration of air and helium. The difference in fluid temperatures within the reactor vessel may then establish natural circulation that can supply significant amounts of air to the reactor core. The heat released by the resulting oxidation of graphite in the core has the potential to increase the peak cladding temperature. In order to analyze the effects of oxidation on the response of the reactor during accidents, a molecular diffusion model was added to an experimental version of RELAP5-3D. The diffusion model was assessed using isothermal and non-isothermal data from inverted U-tube experiments (Hishida and Takeda 1991). These experiments have been used previously by other researchers, including Hishida and Takeda (1991) and Lim and No (2003), to assess other computer codes, but the work described here is the first assessment of the diffusion model in RELAP5-3D. This paper describes the diffusion model, the inverted U-tube experiments, and the results of the assessment calculations.

Some of the design options being considered for very high temperature gas-cooled reactors utilize pebble bed cores. A pebble bed differs substantially from the types of cores traditionally simulated

with RELAP5-3D. Consequently, models were recently added to the code to simulate the pressure loss and heat transfer characteristics of a pebble bed. The pressure loss across a pebble bed affects the flow rate during natural circulation. Consequently, the model was assessed using natural circulation experiments from the NACOK facility (Kuhlmann 2002). This paper describes the code's model for pressure loss across a pebble bed, the NACOK facility and experiments, and the results of the assessment calculations.

Although RELAP5-3D has models that allow it to simulate multi-dimensional problems, the assessments described here utilized one-dimensional models. Consequently, the results that are obtained are relevant to the one-dimensional capability of the code.

## 2. ASSESSMENT OF THE MOLECULAR DIFFUSION MODEL

The molecular diffusion model used in RELAP5-3D is based on Fick's Second Law for spatially uniform pressure and temperature. The binary diffusion coefficient,  $D_{AB}$ , is obtained from the correlation of Fuller et al. given in Reid et al. (1987) as

$$D_{AB} = \frac{0.00143 \left( \frac{1}{M_A} + \frac{1}{M_B} \right)^{0.5} T^{1.75}}{\sqrt{2P} \left[ (\Sigma_A)^{1/3} + (\Sigma_B)^{1/3} \right]^2} \quad (1)$$

where  $M$  is the molecular weight in g/mol,  $T$  is the temperature in K,  $P$  is the pressure in bar,  $\Sigma$  is the atomic diffusion volume, and the subscripts A and B refer to species A and B, respectively. The model currently simulates only binary diffusion. At least one of the species must be simulated using the code's noncondensable model, which employs ideal gas assumptions, while the other species may be simulated either as a working fluid, which incorporates real gas properties, or as a noncondensable gas. The gaseous phase is treated using Gibbs-Dalton mixture relationships. The diffusion model is described further by Oh (2005).

The experimental apparatus of Hishida and Takeda (1991) is shown in Figure 1. The apparatus consisted of an inverted U-tube, ball valves, and a tank. The inner diameters of the U-tube and the tank were 0.0527 and 1.0 m, respectively. The heights of the U-tube and tank were 1.45 and 0.5 m, respectively.

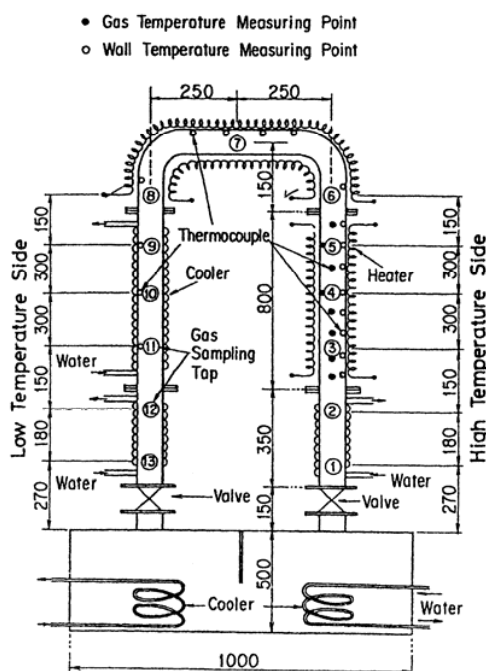


Figure 1. Inverted U-tube experimental apparatus (from Hishida and Takeda (1991)).

The ball valves that separated the inverted U-tube from the tank were closed before the start of the test. The tank and the inverted U-tube were then evacuated and filled with nitrogen and helium, respectively. Electrical heaters controlled the fluid temperatures of one vertical leg and the horizontal leg at the top of the inverted U-tube. The temperature of the other vertical leg was controlled by external cooling with water. After the temperatures had stabilized, the pressures in the tank and inverted U-tube were adjusted to match atmospheric pressure. The test was initiated by opening the ball valves, which allowed nitrogen to diffuse from the tank upwards through the U-tube. The mole fraction of nitrogen was measured at several locations in both legs of the inverted U-tube. The uncertainty in the mole fraction measurement was 5%. Two tests were conducted; one utilized isothermal conditions at room temperature, while the other utilized a non-isothermal profile with values varying between 18 and 256°C.

A RELAP5-3D model of the inverted U-tube was developed as illustrated in Figure 2. The model represented the inverted U-tube, ball valves, and tank components. The tank was divided into two halves, with a connecting junction at the bottom, because the experimental version of the diffusion model does not currently allow more than one junction to be connected at each face of a control volume. Heat structures were used to simulate the walls of the inverted U-tube and the tank. The temperatures of the outer surface of the heat structures were set at the measured values. The RELAP5-3D model shown in Figure 2 is much more detailed than typical reactor models and consists of 144 control volumes, most of which are 2.45 cm long. The nodalization is similar to that used previously by Hishida and Takeda (1991) and Lim and No (2003).

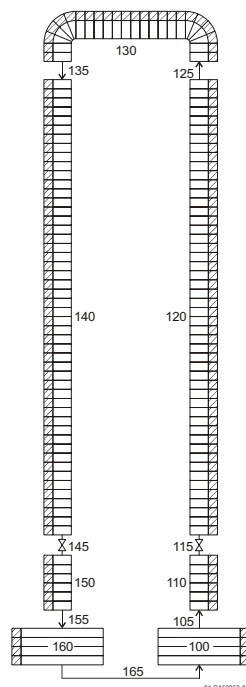


Figure 2. RELAP5-3D model of the inverted U-tube experiment.

RELAP5-3D calculations were performed for both the isothermal and non-isothermal experiments. Results for the isothermal experiment are presented in Figure 3. The figure shows measured and calculated mole fractions of nitrogen versus time at four elevations, ranging from 0.6 to 1.35 m above the top of the tank. The measured results are represented with symbols, while the calculated results are represented with solid lines containing symbols.

The calculation reasonably represented the trends observed in the isothermal experiment. First, the mole fraction of nitrogen initially increased more rapidly at the lowest elevation, due to the shorter distance from the tank, which was initially full of nitrogen, and more slowly at the higher elevations. Second, because there were no buoyancy differences between the two vertical legs of the U-tube in this experiment, the mole fractions in both legs increased symmetrically. The calculated results were also generally in reasonable quantitative agreement with the measured values. The calculated results were slightly outside the uncertainty of the measurements at the elevation of 0.6 m, but within the uncertainty at the higher elevations. The cause of the larger discrepancy at the 0.6-m elevation is not known, but could be related to the location of the ball valve, which was assumed to be near the center of the lower 270-mm section shown in Figure 1. Improved results would have been obtained if the valve had been modeled higher in the 270-mm section. Similar results were obtained by Lim and No (2003), which indicates that possible errors in the RELAP5-3D code or input model are not the likely causes of the discrepancy at the 0.6-m elevation.

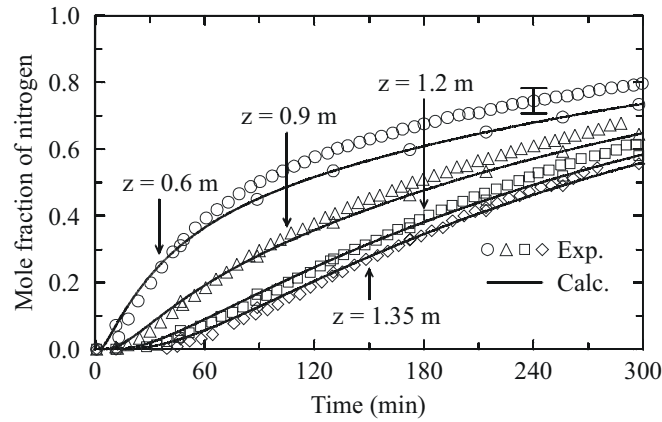


Figure 3. Measured and calculated results for the isothermal test.

A sensitivity calculation was performed in which the number of control volumes was doubled from that shown in Figure 2. As shown in Figure 4, the calculated results were slightly better with the more detailed nodalization. Slightly more than twice the computer time was required to simulate the experiment with the more detailed nodalization. The calculated results are not expected to be as accurate using a coarser nodalization that is typical of most reactor system models, where the core is generally modeled with about 10 control volumes. However, the more coarsely nodalized system models are expected to show correct trends.

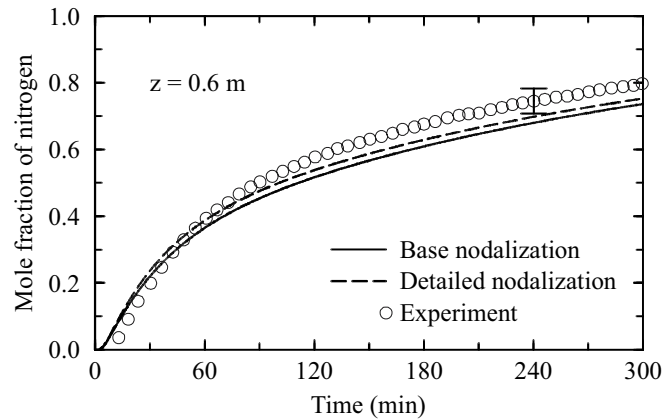


Figure 4. The effect of nodalization on calculated results for the isothermal experiment.

Calculated and measured results for the non-isothermal experiment are shown in Figures 5, 6, and 7, which correspond to elevations 0.6, 0.9, and 1.35 m above the top of the tank, respectively. Each figure shows results for both the hot and cold legs of the inverted U-tube. In both the calculation and the test, the mole fraction of nitrogen increased more rapidly on the hot side of the U-tube than on the cold side due to a larger diffusion coefficient, which increases with temperature, and buoyancy effects, which aided the movement of nitrogen on the hot side of the U-tube and opposed it on the cold side. The rapid increase in mole fraction near 220 min was caused by the onset of natural circulation.

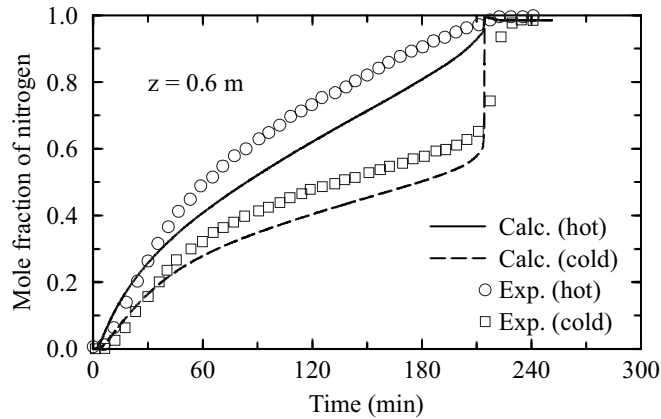


Figure 5. Measured and calculated results for the non-isothermal experiment at 0.6 m.

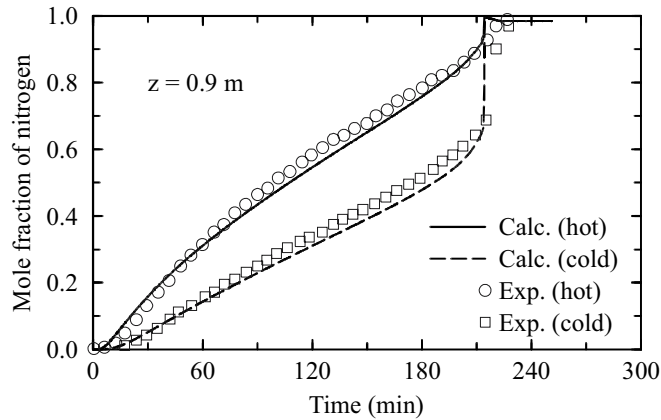


Figure 6. Measured and calculated results for the non-isothermal experiment at 0.9 m.

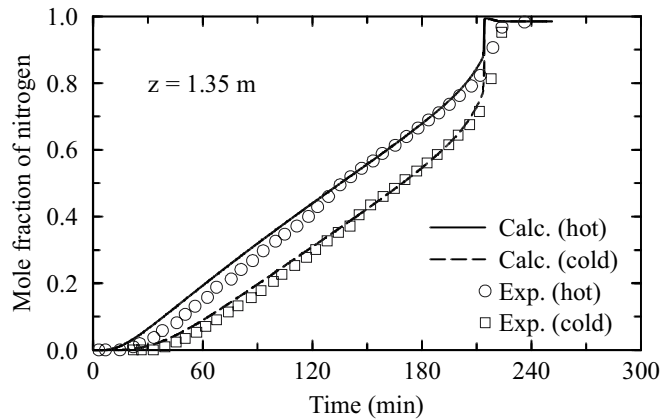


Figure 7. Measured and calculated results for the non-isothermal experiment at 1.35 m.

The calculated results were in reasonable quantitative agreement with the measured values. The differences between the calculated and measured results were generally within the reported uncertainty at all measurement locations except for the lowest one. The calculated results at the lowest locations are similar to those obtained by Lim and No (2003). The timing of the onset of natural circulation, which introduces relatively large amounts of air into the core and therefore could initiate significant graphite oxidation in a reactor, was calculated to within a few minutes.

### 3. ASSESSMENT OF NATURAL CIRCULATION THROUGH A PEBBLE BED

The RELAP5-3D computer code was assessed using natural circulation data generated in the NACOK experimental apparatus (Kuhlmann 2002). The NACOK experiments were designed to investigate the effects of air ingress into the core of a high-temperature reactor following a loss-of-coolant accident. The experiments investigated the effects of molecular diffusion, natural circulation, and oxidation. The natural circulation experiments were used for this assessment.

The NACOK experiments simulated natural circulation of air through a scaled model of a high-temperature reactor containing a pebble bed core as shown in Figure 8. The experimental apparatus consisted of an experimental channel, a coaxial duct, supply and return tubes, and heating elements. The experimental channel had a square 300x300 mm cross-section and a total height of 7.3 m. The experimental channel consisted of three axial sections including a bottom reflector, a 5.0-m long section containing packed spheres, and an empty 1.7-m long section hereafter called the top reflector. The 60-mm diameter spheres were packed in a regular arrangement of 25 spheres per layer. Every other layer used half spheres along two of the four channel walls. The resulting porosity of the packing was 0.395. The inner diameter of the supply and return tubes was 125 mm. The coaxial duct was a horizontal annulus with both the inner and outer tubes connected to the atmosphere.

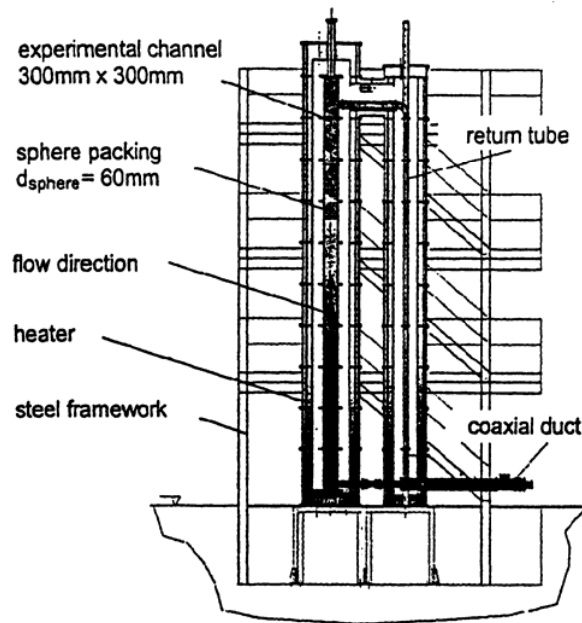


Figure 8. Schematic of the NACOK experimental apparatus (from Schaaf et al. 1998).

Heating elements were used to control the temperature of the walls in the experimental channel and the return tube during the experiments. The wall temperature of the return tube was set at 200, 400, 600 or 800°C. The temperature of the experimental channel was controlled between a minimum value that was 50°C higher than the temperature of the return tube and a maximum value of 1000°C. The difference in temperature between the experimental channel and the return tube induced air to naturally circulate through the supply tube, up through the experimental channel, down through the return tube to the outer tube in the coaxial duct, and back to the atmosphere. The packed spheres in the pebble bed represented the dominant hydraulic resistance in the flow circuit. Thus, the experiments were used to indirectly test the calculation of friction factors in a pebble bed through comparisons with the measured flow rates.

The RELAP5-3D model of the NACOK facility is shown in Figure 9. The model represented all the hydraulic components of the experimental apparatus, including the coaxial duct, supply tube, bottom reflector, packed spheres, top reflector, and return tube. Boundary conditions of atmospheric pressure and 20°C were applied in Components 100 and 170. The thickness of the supply and return tubes was



taken as 4 mm based on Schaaf et al. (1997). The inner diameter of the outer tube in the coaxial duct was then calculated from the area of 0.0080 m<sup>2</sup> reported by Kuhlmann (2002).

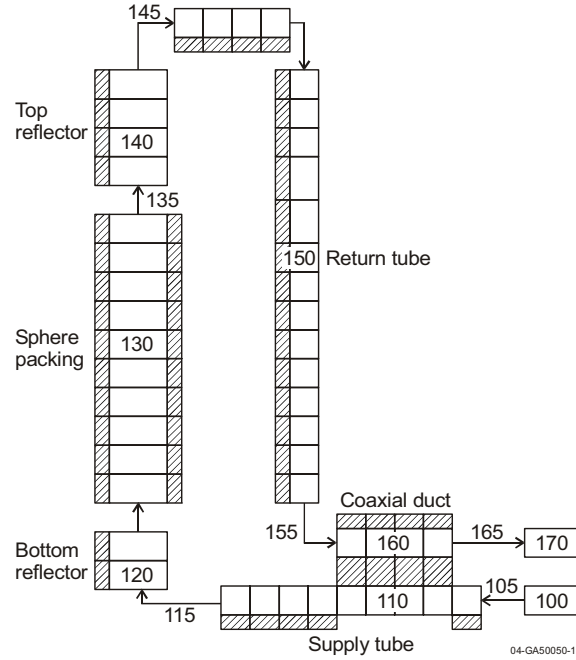


Figure 9. RELAP5-3D model of the NACOK natural circulation experiment.

Heat structures were used to represent the walls of the coaxial duct, the supply and return tubes, and the experimental channel. The packed spheres were also modeled with a heat structure. The wall temperature of the bottom reflector, spheres, top reflector, and the horizontal portion of the return tube were set at the measured value of the experimental channel. The wall temperature of the vertical portion of the return tube was set at the measured value of the return tube. The code calculated the temperature drop due to conduction across each heat structure and the heat flux to the fluid in the adjacent control volume. Because of the small mass flow rates involved, the heat transfer coefficients were generally calculated using the code's natural convection or laminar correlations (RELAP5-3D Code Development Team 2003).

The inner wall of the coaxial duct was modeled to preheat the air entering the experimental channel. The surface temperature of the first heat structure in the supply tube downstream of the coaxial duct was set at the measured temperature of the return tube to represent the portion of the tube within the heating vessel of the return tube. Similarly, the surface temperature of the last heat structure in the supply tube was set at the temperature of the experimental channel. The remaining heat structures in the supply tube were set at the ambient temperature. As described later, the calculated air flow rates were relatively sensitive to the preheating of the air entering the experimental channel.

The pressure loss across the packed spheres was calculated using the model from SCDAP/RELAP5-3D (SCDAP/RELAP5-3D Code Development Team 2003). For single-phase flow, the model reduces to the Ergun equation given by Bird et al. (1960). The Ergun equation is

$$\Delta P = \rho V_o^2 \left( \frac{150(1-\varepsilon)^2}{Re_o \varepsilon^3} + \frac{1.75(1-\varepsilon)}{\varepsilon^3} \right) \frac{L}{D_p} \quad (2)$$

where

$\Delta P$  = pressure drop due to friction

$\rho$  = fluid density

$V_o = \varepsilon V$  = superficial velocity, where  $V$  is the actual fluid velocity

$\varepsilon$  = porosity or void fraction

$$Re_o = \frac{\rho V_o D_p}{\mu} = \text{Reynolds number based on superficial velocity}$$

$\mu$  = fluid dynamic viscosity

$L$  = length of the pebble bed

$D_p$  = diameter of a pebble.

The RELAP5-3D model shown in Figure 9 was used to perform a series of calculations in which the wall temperatures were held constant at the measured values until a steady state was achieved. The results of the calculations are illustrated in Figure 10, which shows mass flow rate of air as a function of the temperature in the experimental channel for temperatures of the return tube,  $T_R$ , that varied between 200 and 800°C. The calculated results were in reasonable agreement with the measured values. The important trends observed in the experiments were predicted by the code. In particular, the shape of the curve at  $T_R = 200^\circ\text{C}$  was similar in the calculations and the experiment. The mass flow rate initially increased sharply with increasing experimental channel temperature, reached a maximum value near 550°C, and then gradually decreased. The volumetric flow increased monotonically with experimental channel temperature because the increased temperature difference between the channel and the supply tube caused an increased driving head for natural circulation. However, the mass flow decreased at higher temperatures because the density decreased at a faster rate than the volumetric flow increased, and, to a lesser extent, because the Reynolds number was decreasing, which caused increased hydraulic resistance as indicated by Equation 2. The code also correctly predicted the trend of decreasing mass flow as  $T_R$  increased at a given experimental channel temperature. This trend was primarily caused by the decreased temperature difference between the experimental channel and the return tube, which decreased the driving head for natural circulation. The RELAP5-3D model was used to simulate all 40 data points reported by Kuhlmann (2002). The root-mean-square error in the calculated flow rate was 0.21 g/s, which corresponds to about 5% of the maximum measured value. The value of  $Re_o/(1-\varepsilon)$  varied between 9 and 120 in the calculated results shown in Figure 10.

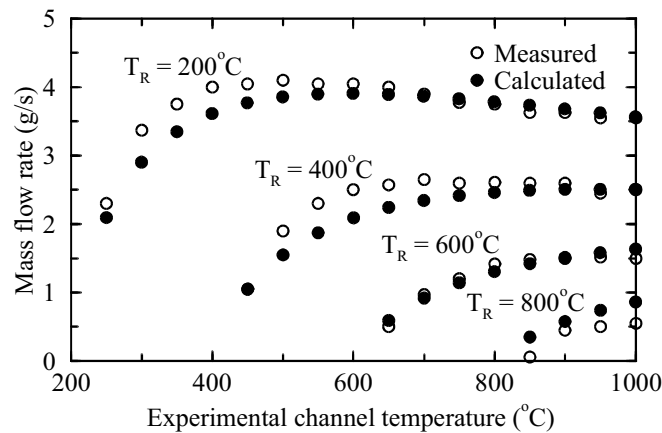


Figure 10. Measured and calculated air flow rates for the NACOK natural circulation experiments.

The average calculated fluid temperature in the experimental channel was less than the reported wall temperature because a certain distance was required to heat the fluid in the experimental channel up to the temperature of the wall. Similarly, the average calculated fluid temperature in the return tube was less than the imposed wall temperature of the return tube. As a result, the actual driving head for natural circulation was less than that obtained from the difference in fluid densities corresponding to the difference in wall temperatures between the experimental channel and the return tube. The calculated driving head for natural circulation varied between 60 and 90% of the value calculated from the difference in wall temperatures.

The calculated mass flow rates were sensitive to the temperature boundary conditions applied to the walls of the heat structures, which affected the relative fluid temperatures and densities in the experimental channel and the return tube and thus affected the driving head for natural circulation. For example, a sensitivity calculation was performed in which the boundary condition in the horizontal leg at the top of the return tube was changed from the temperature of the experimental channel to the temperature of the return tube. Although Kuhlmann (2002) did not report the average wall temperature in this portion of the return tube, the actual temperature is expected to be between the reported values for the experimental channel and the return tube, and probably nearer to that of the experimental channel as assumed in the original calculation. Applying a lower wall temperature in this relatively short region resulted in a lower average fluid temperature in the return tube, which increased the driving head for natural circulation and resulted in an increase in the calculated mass flow rate of 0.26 g/s averaged over all 40 data points. A second sensitivity calculation was performed in which the wall temperatures of the last heat structure in the supply pipe and of the two heat structures in the bottom reflector were changed from the reported temperature of the experimental channel to a value halfway between the ambient and experimental channel temperatures. Applying a lower wall temperature in this portion of the experimental channel decreased the average fluid temperature in the channel, which decreased the driving head for natural circulation and resulted in an average decrease in the calculated mass flow rate of 0.23 g/s. The average change in the flow rate for each sensitivity calculation is significant compared to the root-mean-square error of 0.21 g/s reported earlier.

#### 4. CONCLUSIONS

The RELAP5-3D code was used to simulate isothermal and heated experiments in an inverted U-tube. Molecular diffusion was the dominant transport mechanism in the isothermal experiment, while diffusion and buoyancy were both important mechanisms in the heated experiment. The calculated results were in reasonable quantitative agreement with the measured values for both experiments. The differences between the calculated and measured results were generally within the reported uncertainty at all measurement locations except for the lowest one, where the calculated results were similar to those obtained by other researchers. The timing of the onset of natural circulation, which introduces relatively large amounts of air into the core and therefore could initiate significant graphite oxidation in a reactor, was calculated to within a few minutes.

The RELAP5-3D code was used to simulate natural circulation experiments conducted in the NACOK facility. These simulations tested the code's model for pressure loss across a pebble bed core. The calculated mass flow rates of air were in reasonable agreement with the measured values. Thus, the pressure loss predicted by the Ergun equation is also in reasonable agreement with data from the NACOK natural circulation experiments.

#### ACKNOWLEDGEMENTS

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