Appendix C

Nuclear Regulatory Commission – Massachusetts Institute Of Technology
Collaborative Agreement

TASK 3

Air Ingress, Natural Convection, Graphite corrosion and correlations for improved safety analysis of reactors

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Progress Report

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I. Objective

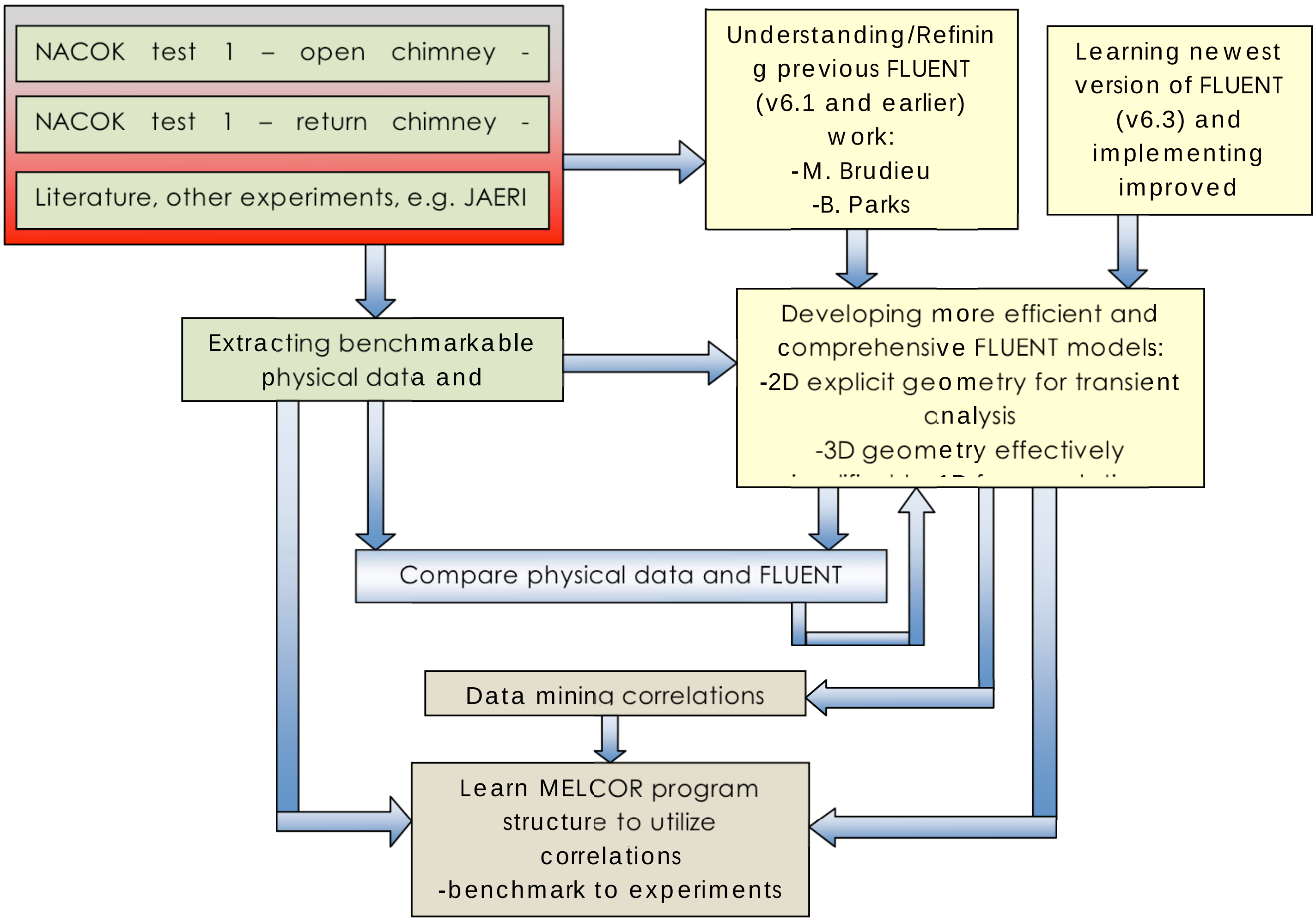
To build a full transient FLUENT model built upon previous work benchmarking its use for air ingress analysis, for complicated and more realistic natural convection behavior, and to take data from this and previous models, perform data mining and ultimately create an effective 1-D model and produce correlations applicable to heat transfer applications such as MELCOR and RELAP.

II. Scope of Work

This work has five main simultaneous lines of work:

- Understanding and refining previous work with FLUENT in explicit 3-D geometries for steady state and simplified, short period transient analysis,
- Working with the data received from two NACOK tests, research in literature, and possibly other benchmarking experiments to understand physical phenomena, driving parameters, and experimental limitations,
- Developing 2-D and effectively 1-D three-dimensional models in FLUENT in order to proceed with transient analysis without the prohibitively time-intensive calculations of the explicit 3-D geometries,
- Working with the data output of FLUENT and designing/refining models to optimize data mining, iterating this with learning data analysis software and other tools and their best inputs, and
- Acquiring and learning MELCOR or RELAP codes from other experts in the field and their structure, which helps guide the iterative work towards correlations from the steps above.

These can be thought of as two converging points of view: physical experiments and already published data or literature, which provide physical intuition and benchmarking, and the results from FLUENT, a sophisticated but complicated software to invoke artificial data in order to develop correlations, which is necessary to input into the data mining software. This is described pictorially below:



III. Relevance to the NRC

At the recent Next Generation Nuclear Power Conference held at the Idaho National Labotory, the topic of air ingress analysis, the difficulty of accurate analysis of the effects of air ingress on temperature, graphite corrosion, its effects on the structural integrity of any reactor using graphite as a reflector, and the lack of studies tying these aspects together quickly became central. High temperature Gas Reactors (HTGRs) especially require understanding of the effects of a Loss of Coolant Accident (LOCA), since the coolant used is helium, and may allow for much different air flow situations and accident scenarios. The NRC is addressing this by developing a modified version of MELCOR- the H2 version- but as yet, comprehensive modeling of these effects is not available, especially not in any industrially applicable or time un-intensive form. Outside of computation, there is little experimental work and data specific to this scenario to take into account the combined effects of a LOCA in HTGRs.

Even if information on the relationship of these important aspects for reactors were more available, the successful implementation of these factors in any finite-element, multi-physics simulation requires specialized knowledge and intricate model development of a system along with prohibitively high computational requirements.

The most advanced computational fluid dynamics/multiphysics code, FLUENT, requires transient analysis—as opposed to the simpler steady state analysis-- for any natural convection problems that involve large changes in temperature. Moreover, the maximum allowable time step is dictated by the geometrical constraints of the system and the initial parameters—in cases of reflectors and reactors with long and narrow geometries, combined with natural convection and complicated species transport and reactions with the graphite. This means a maximum time step on the order of 0.001 s, and requiring at least 5-10 iterations per time step. This makes any computation of air ingress in any reactor situation excessively long to be taken into account in safety analysis requiring many such simulations.

The potential development of correlations by benchmarked simulations for use in safety analysis software such as MELCOR presents a valuable and significantly more efficient method for reactor analysis, especially for HTGRs.

IV. Progress in the First Year

One of the major difficulties in this project since the last student (M.A. Brudieu 2006) completed her initial benchmarking work has been to reproduce the FLUENT calculations and the lack of clear data and test procedures used in the NACOK air ingress experiments used in the benchmark. Recall that Brudieu's work was a blind benchmark. This effort intends to improve the modeling using real data from the tests but this data is hard to obtain from the Juelich Research Institute. However, we have been able to make progress toward the goals of the project, and met a few milestones:

- Familiarizing with all acquired NACOK data, and experimental conditions of both the open chimney, experiment 1, and the return chimney, experiment 2. In absence of data, created spreadsheets from operators' log screen captures from the experiment, which allowed for a much better understanding of the open chimney experiment, where there was previously no internal temperature information. See below chart of temperatures by hour points in the return chimney experiment.

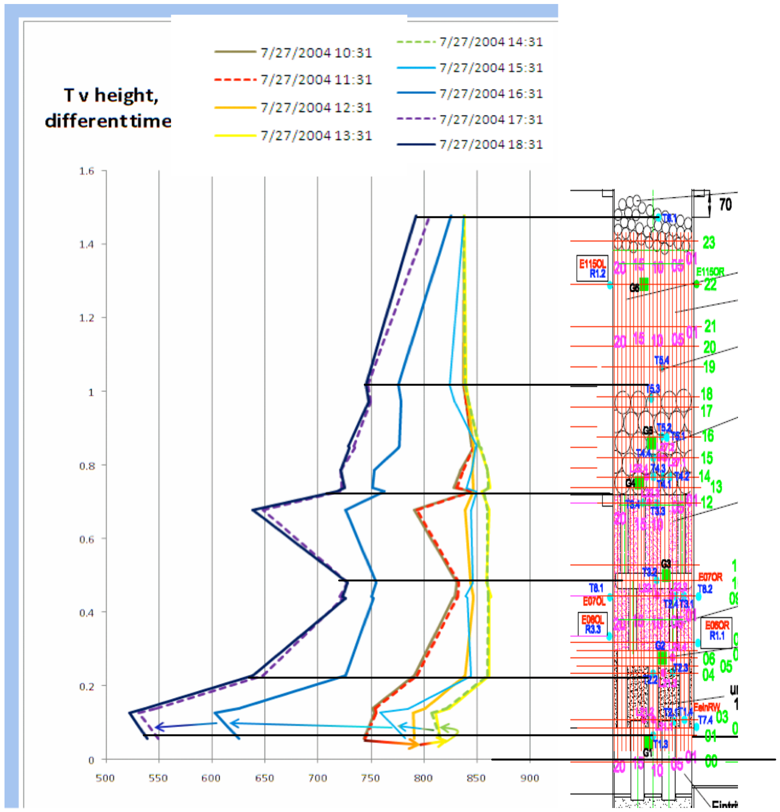


FIGURE 1: TEMPERATURE PLOTTED BY HEIGHT AND POINTS OF TIME IN THE RETURN CHIMNEY EXPERIMENT, PLOTTED AGAINST DRAWING OF RETURN CHIMNEY LAYOUT (NOTE: THIS IS ZOOMED IN PORTION OF HEIGHT)

Problems have ranged from having many model files done and redone by previous students without clear documentation of the hundreds of inputs and which files correlate to the results presented in Brudieu's thesis and other reports, to apparently not having certain important model files, to NACOK experiment and data problems mentioned in previous reports and simply not having important, but not critical, portions of data, or having reports or operator's logs only in abbreviated German. Further, technical difficulties with the FLUENT software beyond the department's control resulted in nearly a month with the program unavailable.

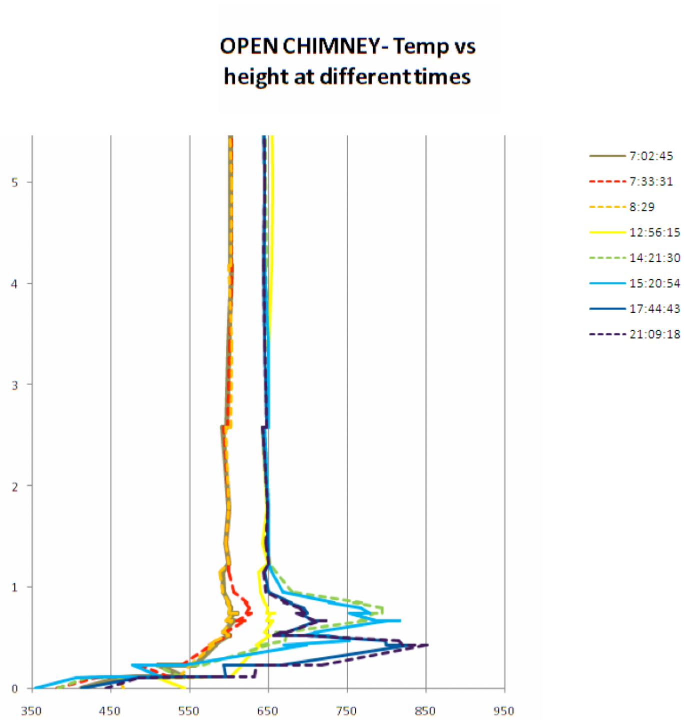


FIGURE 2: TEMPERATURE PLOTTED BY HEIGHT AND POINTS OF TIME IN THE OPEN CHIMNEY EXPERIMENT

- Learning FLUENT comprehensively. The software is extremely complex and natural convection with reactions in a high temperature and very long aspect ratio model presents challenges that require detailed knowledge.
- Interpreting the files of past work and learning the appropriate initial conditions and other inputs necessary to running previous FLUENT case files, e.g., material properties, operating conditions, heat transfer assumptions, inlet and outlet parameters, etc.,
- Running past steady-state files and comparing them to NACOK data,
- Isolating, through interactions with FLUENT email help involving many week-long delays, several possible improvements for the past models which will allow future models and correlations to match experimental results more reliably, including:
  - meshing issues,
  - turbulence settings, and
  - boundary condition inlet and outlet settings,

along with other tips found by reading both the manual for the older version of FLUENT and the new version of FLUENT, and other papers and advice. Other improvements or important factors found included:

- radiative heat transfer issues,
- porous media assumptions of thermal equilibrium between the solid and fluid media,
- limitations of past versions of FLUENT to the currently available versions, and
- limitations of steady state simulations when transient analysis is required for experimental conditions.

These are being taken into account for development of the refined transient models, which will translate into data for correlations.

- Correcting above issues and creating fully functioning transient FLUENT models and important analysis with respect to the experimental data and previous FLUENT benchmarking models,

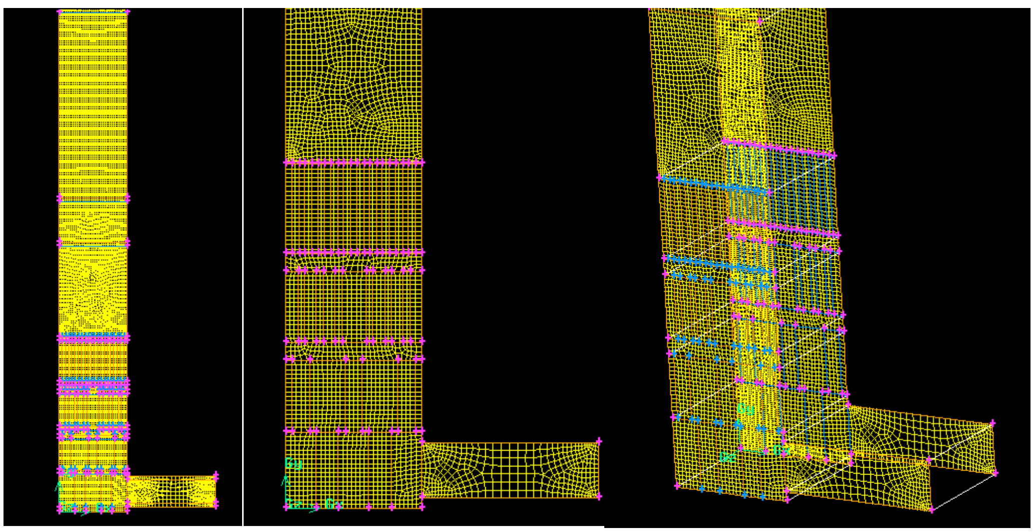


FIGURE 3: REFINED MESHES

- Attending the NGNP annual conference in May at the Idaho National Laboratory, and connecting with other experts in the field, such as Dr. Chang Oh and his student, who gave advice and offered potential collaboration through allowing the P.I. and his student to learn from his work in incorporating heat transfer correlations in RELAP.

- Through meetings with Harvard/MIT data consultants, decided on statistical analysis software best suited for data mining—SAS Enterprise Miner—and began tutorials, receiving first certificate for SAS Basics.

- Began examining the MELCOR structure via the user manual.

Specifically, the last quarter has brought the following results:

- Developed a meticulously meshed, 2-D model which has already allowed for ten times the experiment time run by the previous student with *double* precision, and has shown interesting results, such as that the arrival of a true steady state is not as quick as was shown previously using porous media assumptions. This is due to a few factors, one, is that although after about 1-2 minutes maximum velocity reaches a sort of steady state, this does not realistically represent the distribution of velocity in the channel. Below is a graph (Figure 4) of the FLUENT model maximum velocity, which very much resembles that of the previous work. However, in Figure 5 it can be seen this is the same time that oxygen is just reaching the reflectors, which will begin the reactions and, eventually, a steady state that includes reactions. *Diffusion alone, as assumed in previous analyses, is not sufficient to determine steady state points and conditions.* Also, in Figure 7 it can be seen that the velocity magnitude and especially direction are not uniform and further time points have shown they are not at a steady state.

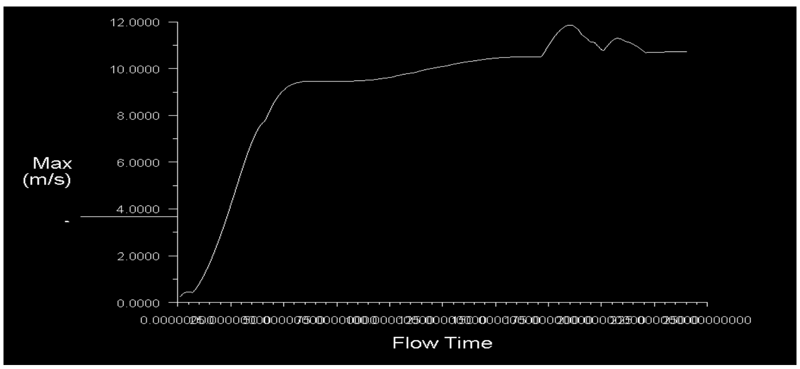


FIGURE 4: MAXIMUM FLOW VELOCITY AT INLET (NOTE MAX TIME HERE IS 4 MINUTES)

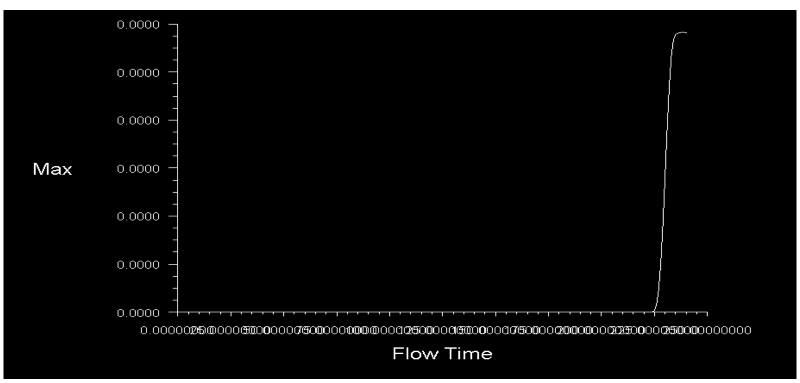


FIGURE 5: PERCENT MOLE FRACTION OF O2 AT THE FIRST REFLECTOR SAME TIME SCALE

Another reason for the difference in steady state estimates from previous work is that the heating of graphite to steady state temperatures takes longer than assumed by an effective conductivity and thermal inertia of a porous media. This also matches with NACOK data, as described below. Also shown below is an illustration of how much temperature varies within a channel even after 4 minutes.

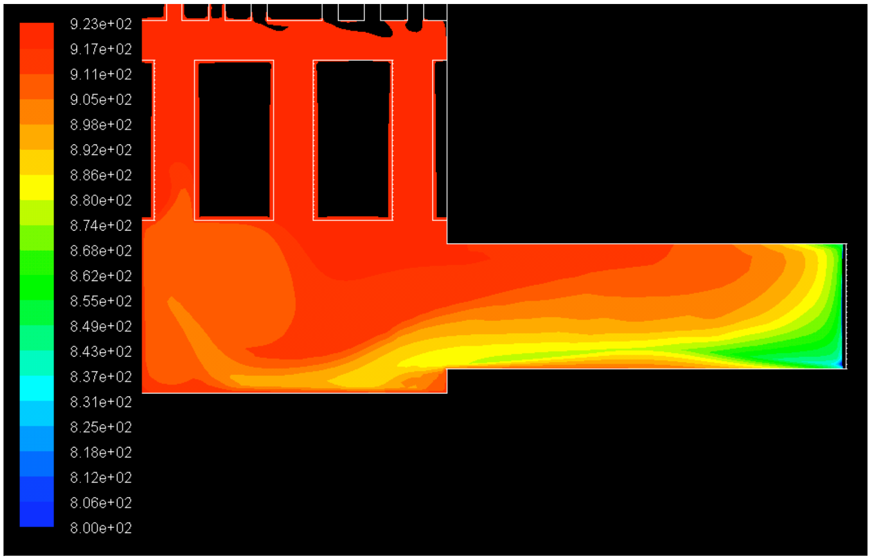


FIGURE 6: TEMPERATURE DISTRIBUTION OF FLUID AT 4 MINUTES

- The transient 2 dimensional model has also allowed for insight into fluid flow and velocity in the ingress experiment. For one, that fluid velocities may have high variations within certain points of the channel- from 0 to 10 m/s and that the velocity vectors are in different directions. The results of our model also aligned with the observations by Chang Oh at INL regarding stratified flow.

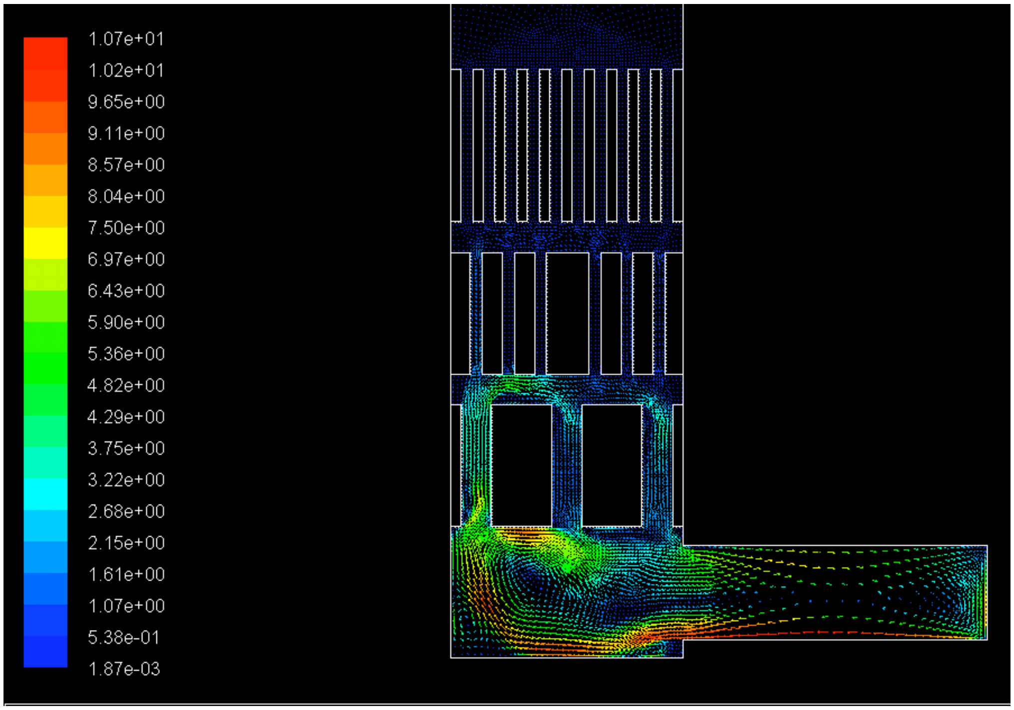


FIGURE 7: VECTORS OF VELOCITY MAGNITUDE (M/S) AT 4 MINUTES, ILLUSTRATING STRATIFIED FLOW AT INLET

- The transient model has shown more clearly at which points in time and what orders of magnitude species concentrations reach at different heights in the experiment assembly. This is important especially as it relates to when oxygen reaches the reflectors and if/when oxygen reaches the graphite coated pebble bed.

- Worked with the NACOK data and producing graphs which have illuminated some physical sense for benchmarking and correlations, but require some clarification from NACOK in order to be able to reliably use the data for benchmarking. One example of physical sense illuminated by examining the data was that reaching steady state did not require more than an hour as shown in the graph below for the open chimney experiment.

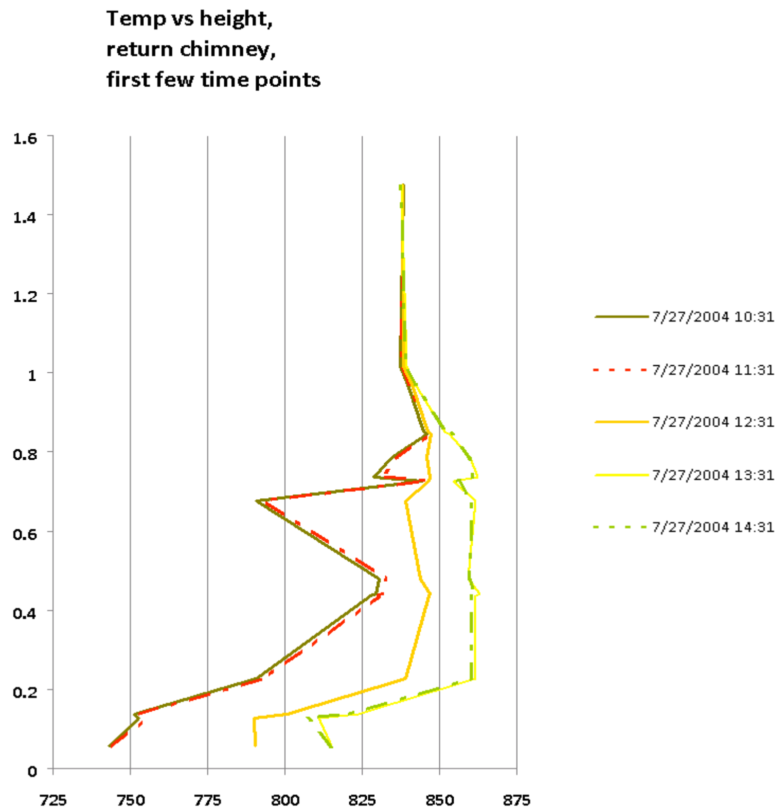


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FIGURE 8: TEMPERATURE AND HEIGHT AT FIRST TIME POINTS TO STEADY STATE.

Clearly sometime before 13:31 the system reaches what is more or less a steady value until cooling down. Note also it takes more than an hour for the reactions to cause significant heating

- Began work with FLUENT data output in both Tecplot and SAS programs and understanding the best way to create models, run the simulations, and export the data for use in these programs.
- Began work with the Harvard/MIT data consultants and the program SAS to learn how to automate data mining.

V. Plans for Future Work

Now that FLUENT and NACOK data are beginning to coincide, the next step is to focus in on key variables and their relationships, at steady state and with transient analysis. Especially critical is continuing correspondence with those from NACOK for clarification of discrepancies in data. We will continue to refine the transient analysis. By the end of fall, we will have fully benchmarked the 2D transient analysis with NACOK for the open chimney test, and will have developed a 2D model for the return chimney, and run the analysis to a sufficient amount of time, at least 1 hour.

We will work on a 3D model, made effectively into a nodal code like MELCOR via use of porous media approximations.

The correlations that we have suspected based on other research both done by previous students and the Jeulich Research Institute can be checked by these models, and iterated with use in SAS.

Simultaneously, we will utilize what data is produced and assess relationships with SAS. Now that competency in FLUENT has been reached, the next obstacle is competency in SAS and statistical data mining methods. Based on the review of the available data from the NACOK tests, it appears that test procedures were changed during the testing which is not fully reflected in the analysis since these changes were not disclosed to MIT.

The final large task will be to develop competency with pre-eminent safety and reactor modeling codes such as MELCOR and RELAP. The student expects that this will take place in the winter and spring.

A thesis will be produced through this fall and spring based on this work, and Ph.D. work will likely continue in order to fully vet the proposed correlations, to find error margins, to try test cases with the correlations vis-à-vis MELCOR and possibly RELAP, and to begin the process implementing these correlations as add-on applications into MELCOR.

The problems faced in this recent work has been caused by the time lapse since the last student completed her work not permitting a smooth transition from one researcher to another. Also the NACOK experiment was not well documented resulting in not having critical portions of data resulting in the use of operator's logs only in abbreviated German.

We would appreciate NRC staff engagement with this project with researchers following air ingress analysis to share knowledge and experience.