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Modeling Corrosion in Oxygen Controlled LBE Systems with Coupling of Chemical Kinetics and Hydrodynamics: Quarterly Progress Report August 16,2001- November 15, 2001

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Task 5. First Quarter Report

Modeling Corrosion in Oxygen Controlled LBE Systems with Coupling of Chemical Kinetics and Hydrodynamics

Quarterly Progress Report
8/16/01- 11/15/01

UNLV-AAA University Participation Program

Principle Investigator: Samir Moujaes
Co-Principle Investigator: Yitung Chen

Purpose and Problem Statement

The Lead-Bismuth eutectic (LBE) has been determined from previous experimental studies by the Russians and the European scientific community to be a potential material that can be used as a spallation target and coolant for the AAA proposed application.

Properly controlling the oxygen content in LBE can drastically reduce the LBE corrosion to structural steels. However, existing knowledge of material corrosion performance was obtained from point-wise testing with very limited density. The transport of oxygen and corrosion products, their interaction and variation of corrosion/precipitation along the flow are not well understood.

An experimental study monitored corrosion history of specimens in one test loop over several thousand hours and showed that corrosion would occur at higher temperatures i.e. 550 ^{0}C but precipitation occurs around 460 ^{0}C, which is at the intermediate temperature. This confirms that the temperature distribution in an LBE system is important for understanding the system corrosion performance.

The first subtask of this project involves using a CFD code (2-D simulation) such as STAR-CD to obtain averaged values of streamwise velocity, temperature, oxygen and corrosion product concentrations at a location deemed close to the walls of the LBE loop at more than one axial location along it. The oxygen and corrosion product inside the test loop will be simulated to participate in chemical reactions with the eutectic fluid as it diffuses through towards the walls. Details of the geometry of these loops will be obtained from scientists at LANL. These values will act as a set of starting boundary conditions to the second task.

The second subtask and the more important objective of this project is to use the information supplied by the first task as boundary conditions for the kinetic modeling of the corrosion process at the internal walls of the test loop. The outcome of the modeling will be fed back to the first subtask, and the steady state corrosion/precipitation in an oxygen controlled LBE system will be investigated through iterations. The information is hoped to shed some light on the likely locations for corrosion and precipitation along the axial length of parts of the test loop.

Personnel

Principle Investigator:

- Dr. Samir Moujaes (Mechanical Engineering)

Co-Principle Investigator:

- Dr. Yitung Chen (Mechanical Engineering)

Students:

- Mr. Chao Wu, M.S. Graduate Student, (Mechanical Engineering)
- Mr. Kanthi Dasika, M.S. Graduate Student, (Mechanical Engineering)

National Laboratory Collaborator:

- Dr. Ning Li, Project Leader, Lead-Bismuth Material Test Loop, LANL

Management Progress

Budget Issues:

- Two personal computers have been ordered in the beginning of the fall semester and those computers were received in the end of November.
- One Color laser jet printer has been misordered and we are waiting for the right one to arrive.
- One student was sent to the CD-Adapco at its Plymouth, Michigan training facility to get the fundamental training of how to run the commercial STAR-CD code.
- Salary expenditures need to be adjusted because the secretary of Mechanical Department has not revised the correct student's name (i.e. Mr. Chao Wu) according to the proper account number .
- A need for a wall chemistry module is being sought from ADAPCO, we are trying to negotiate with them to obtain a beta version of the module called CHEMKIN.

Management Problems

Mr. Chao Wu will be leaving for China for about three weeks to visit his family. He was just admitted to the department of mechanical engineering in the fall semester of this year. It was a decision that was made by the student and a ticket was bought before consulting with the PI.

Technical Progress

Hydrodynamics:

STAR-CD has been chosen as the CFD tool for analyzing the fluid flow in the test loop. The test loop geometry and the physical properties of LBE are expected very soon. Meanwhile, an effort to get well acquainted with the STAR-CD software is being made. Through some informal contacts like e-mails, we came to know that the test loop is cylindrical in geometry and the velocity of the LBE in the test loop is around 3-4m/s. With the suggestion of the Investigators, an intelligent approach is being made towards the basic problem by considering flow of water in a pipe with a velocity of 3.5 m/s with low K-E Reynolds number. Heat flux has been applied along the wall boundaries. A pollutant with a concentration other than the concentration of water has been introduced in the fluid and the concentration, velocity and temperature profiles have been plotted. The results of our model trials have been represented in the form of following figures.

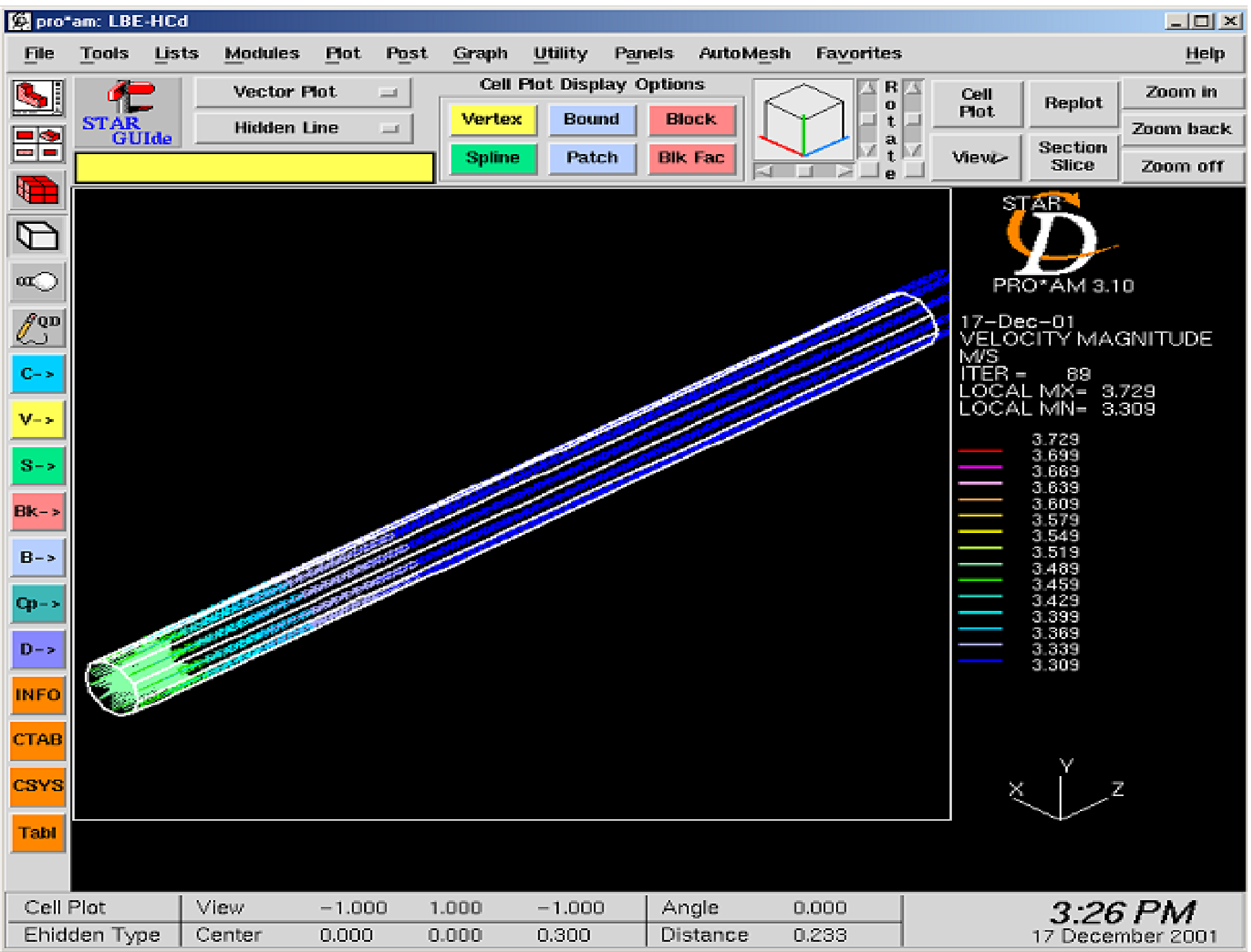

FIG-1: VECTORIAL REPRESENTATION OF THE VELOCITY OF THE FLUID IN THE PIPE

Figures 1,2 and 3 represent the velocity variation of the fluid flowing in the pipe. The inlet velocity is given to be 3.5m/s. As expected, the velocity in the center of the pipe is more than the inlet velocity and the flow profile along the diametrical section is parabolic in shape.

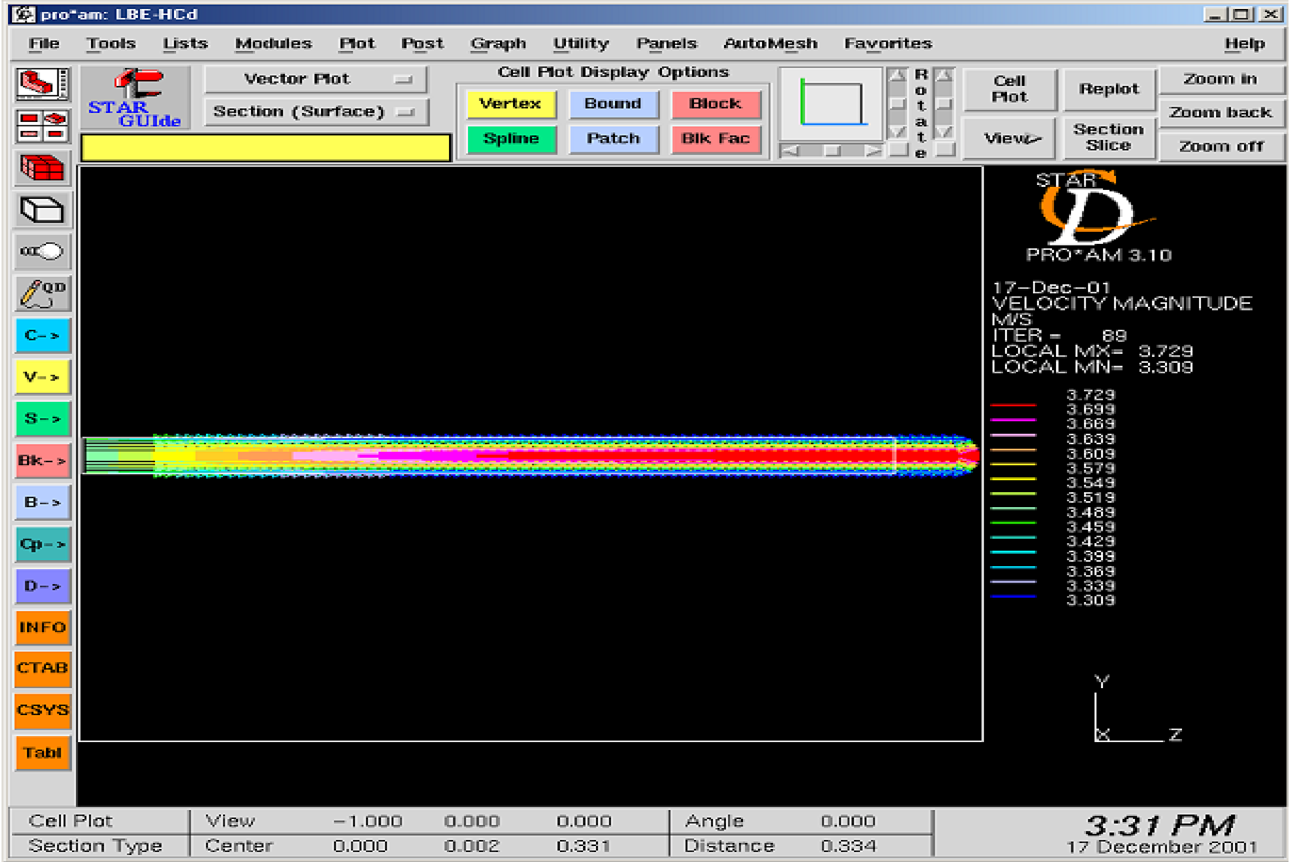

FIG-2: VELOCITY PROFILE ALONG AN AXIAL SECTION OF THE PIPE

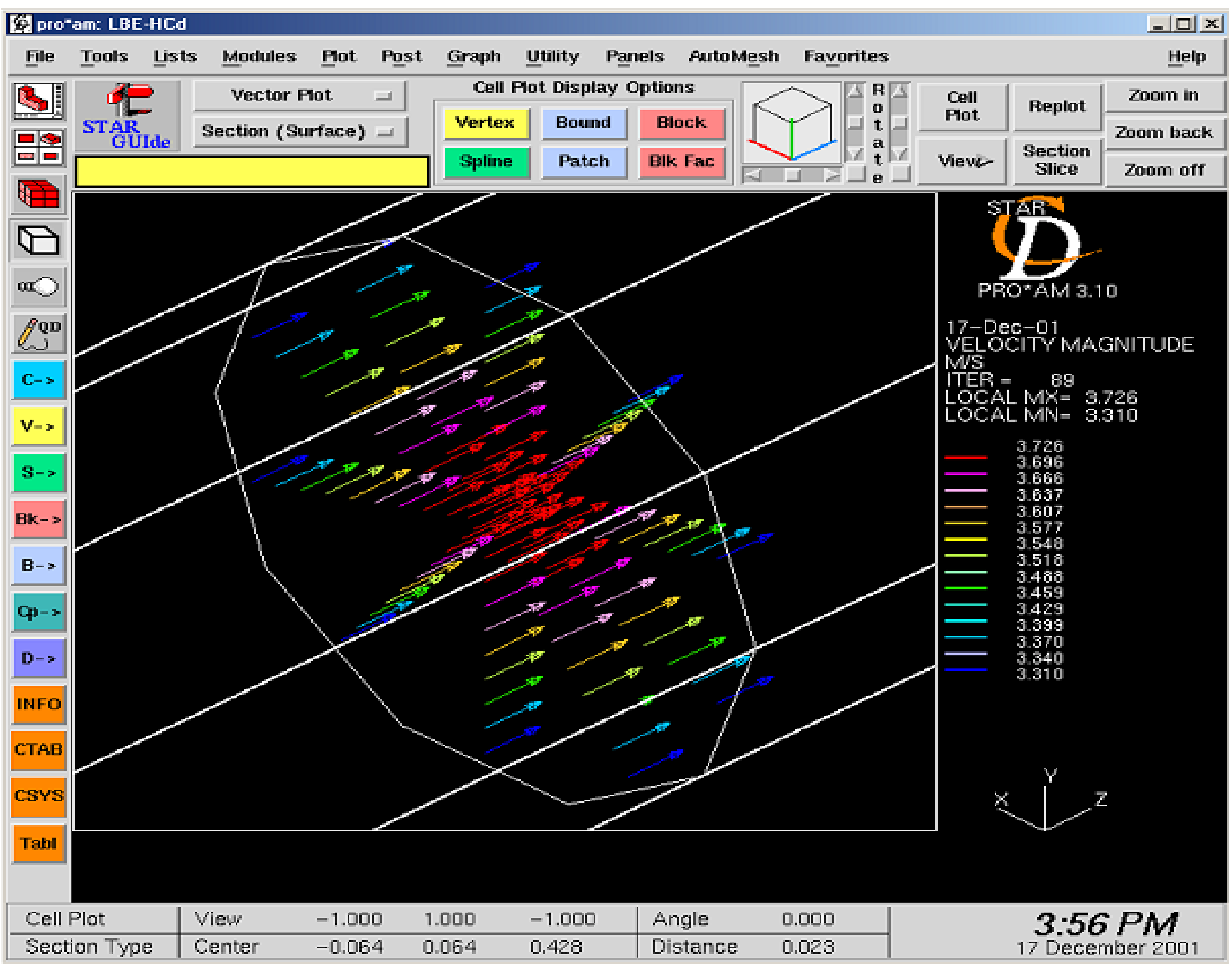

FIG-3: VELOCITY PROFILE ALONG THE DIAMETRICAL SECTION OF THE PIPE

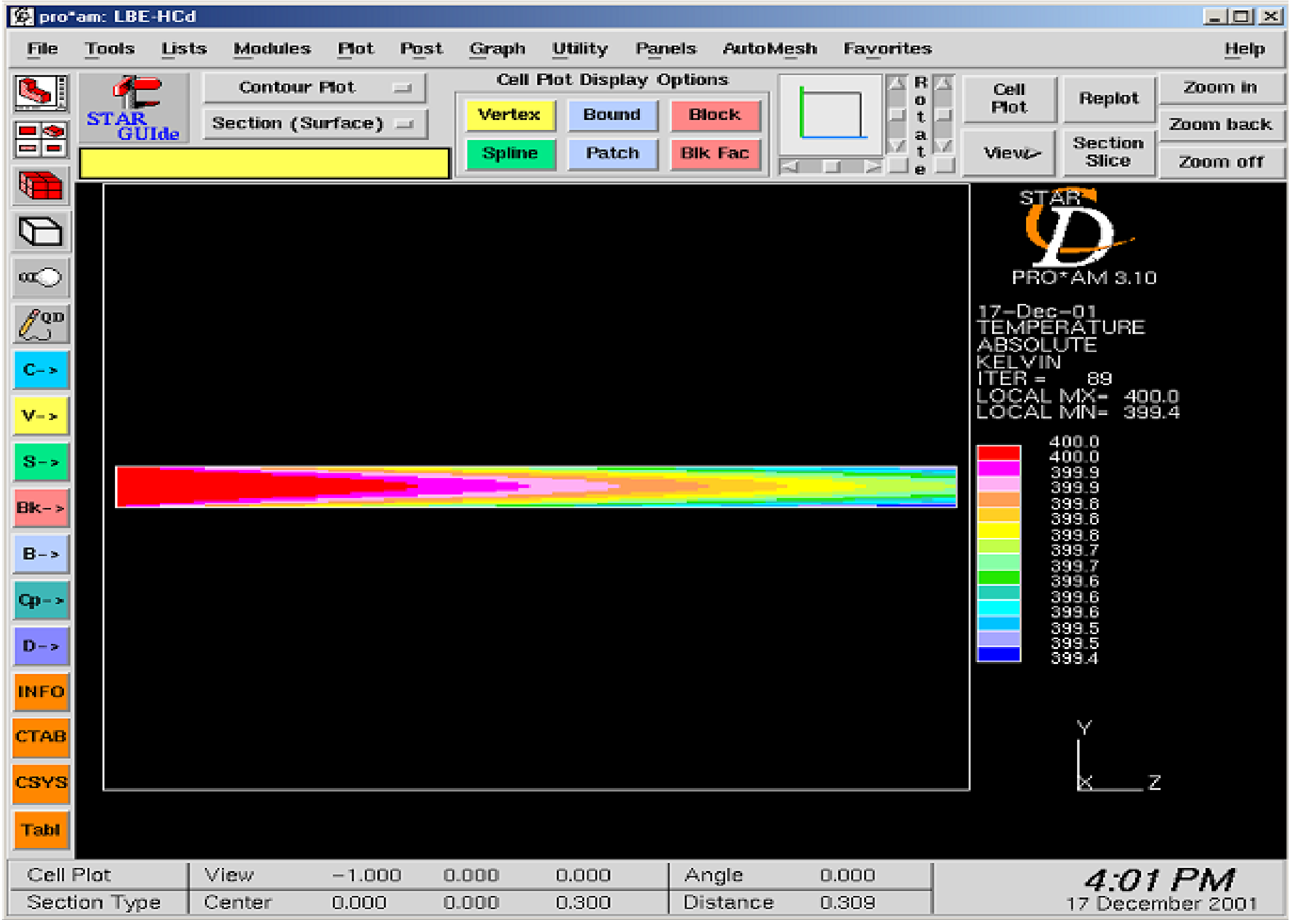

FIG-4: TEMPERATURE VARIATION ALONG THE AXIAL LENGTH OF THE PIPE

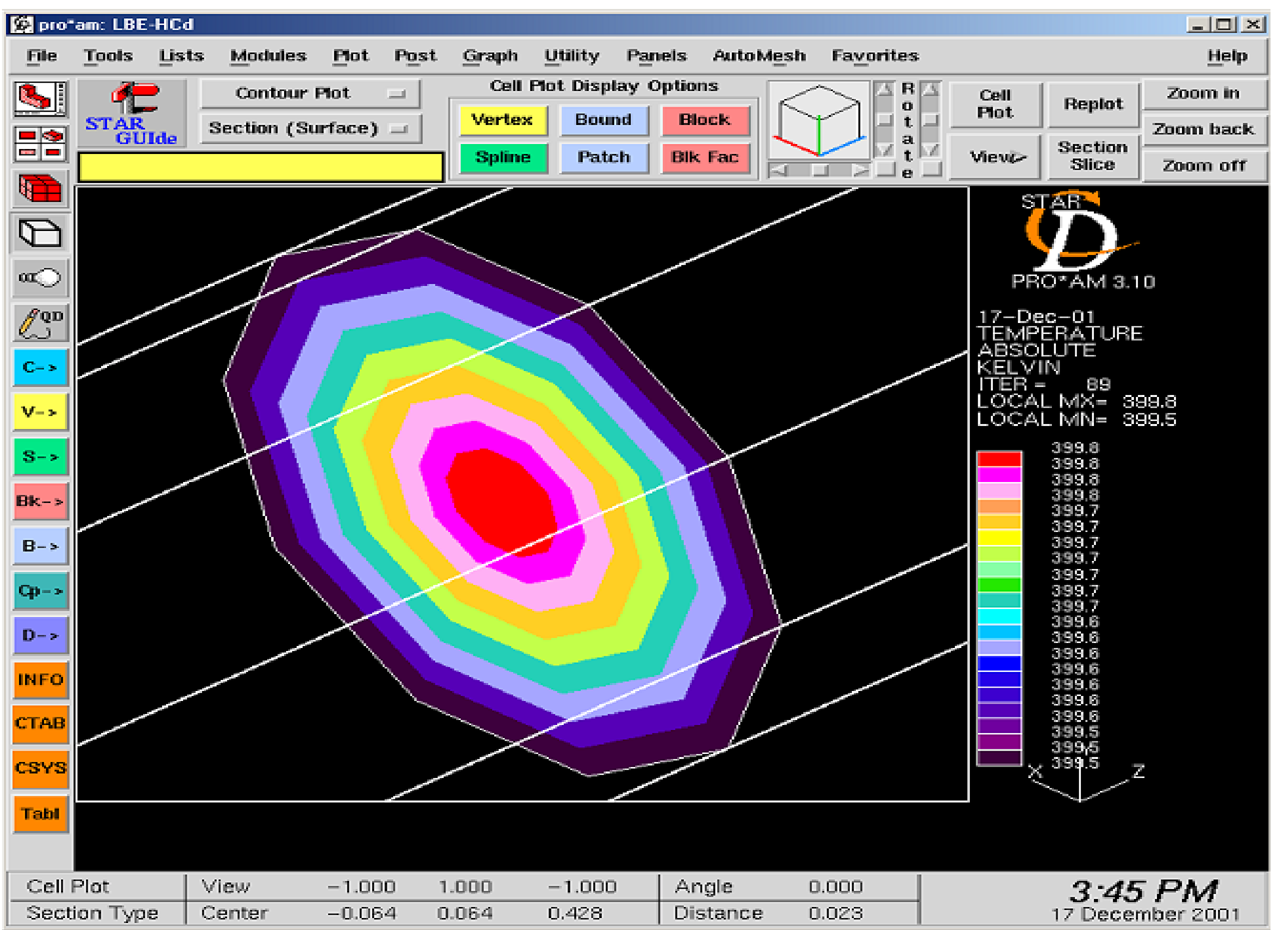

FIG-5: TEMPERATURE VARIATION ALONG A DIAMETRICAL SECTION OF THE PIPE

Figures 4 & 5 represent the variation of the temperature along the axial and diametrical section of the pipe respectively. A heat flux has been applied along the walls of the pipe and the inlet temperature is given as 400K. Fig 5 shows clearly the variation of the temperature along a diametrical section due to the introduction of the heat flux.

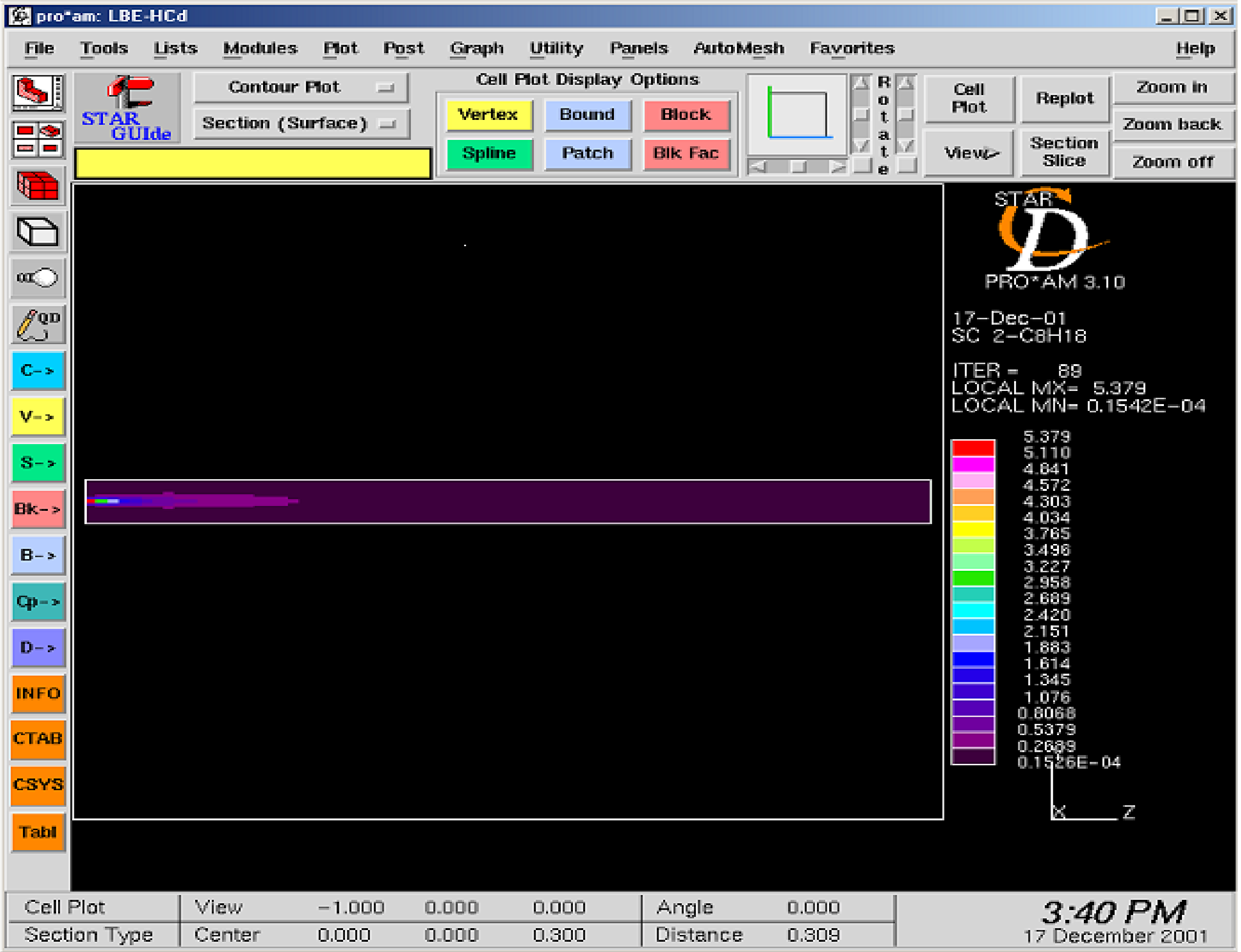

FIG-6: DIFFUSION OF THE POLLUTANT INTRODUCED IN THE TURBULENT FLUID FLOW

Figure 6 shows the affects of introduction of a pollutant in a flowing fluid. As has been mentioned earlier, the flow is turbulent and due to this, the pollutant, having a different concentration, mixes quite quickly with the fluid flowing in the pipe.

An attempt to construct an unstructured mesh is being made which helps in giving more accurate results at the critical points like the walls where the corrosion mainly takes place. A computational mesh will be setup and fluid flow analyzed as soon as we get the loop geometry and the physical properties of LBE from LANL.

Chemical kinetics of corrosions:

An intensive literature search has been done in recent months. More than ten journal papers and around five technical reports that are related with LBE coolant system have been found. The information about LBE system is very limited, especially on chemical kinetics and thermodynamic data. The corrosion mechanism on the material surface of whether it is kinetically controlled and/or diffusion control needs to be determined from the available data. If it is kinetic controlled, then the reaction rates and order and reaction mechanisms of the corrosion are needed. If there are many mechanisms, then we need to know what the most important bottleneck mechanisms are. If it is diffusion controlled, then the diffusion function or variation with oxygen concentrations and temperatures are needed. We also need to know whether or not the reverse reactions occur for lead and iron oxides, and under what kind of conditions etc. The deposition rates of iron and lead oxide variation with temperatures are also needed. A simple mechanism will be used at first. Then a set of parametric studies will be used to simulate the corrosion process with the lead-bismuth bulk flow that is expected to occur in the turbulent flow regime. Potential reactions between ferric oxide and lead are shown in Figure 7.

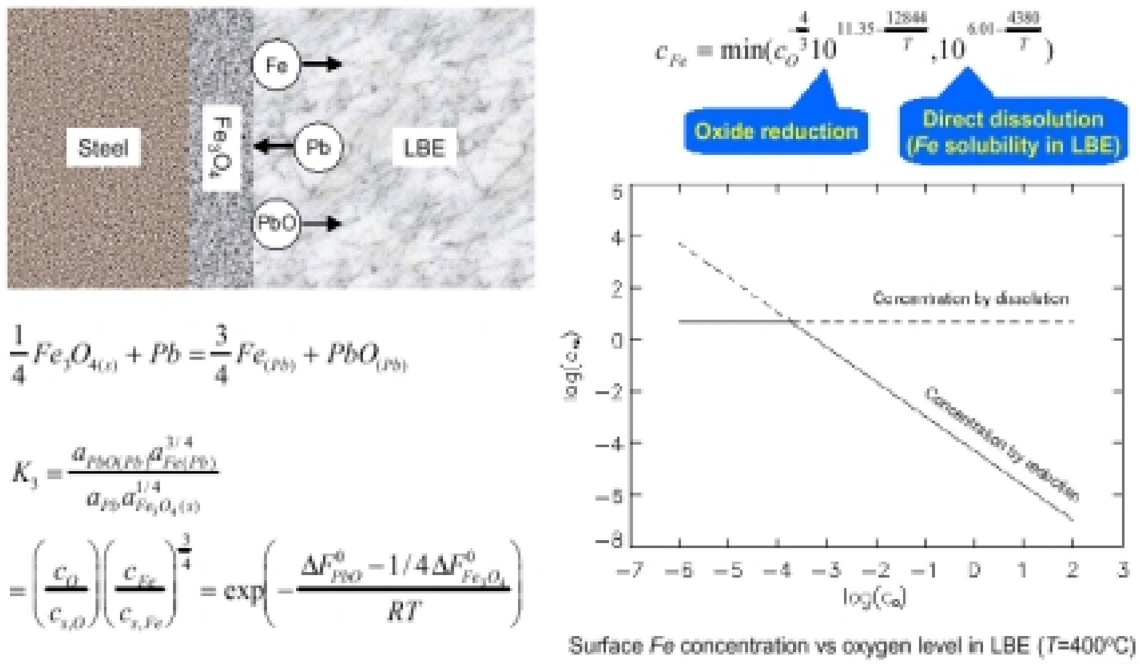

FIG-7: POSSIBLE REACTIONS BETWEEN IRON OXIDES AND LEAD AS PRESENTED IN A RECENT PAPER BY DR. NING LI et al. ANS CONFERENCE RENO 2001

The conceptual design of the LBE loop has been provided by LANL at the end of November. The computational mesh will be set up according to the provided physical dimensions.

A pipe flow with an injection point, from which the reactant gas of oxygen is added into pipe, has been studying in the first case. From this study, the concentration profiles of each species, temperature distributions, and velocity contours were calculated along the pipe flow. This study case is similar to the given research task that oxygen is injected into the LBE bulk flow and is reacted with both of Pb and Bi. The surface reactions will be included in the next case of study. Then the precipitation of iron and lead oxide can be calculated according to the concentration profiles of oxide and the temperature variations. Thus the precipitation downstream can be calculated in the bulk flow.

Future work:

1- To decide on how many locations to model for the corrosion effect along the loop length. We are in communication with the LANL for that.
2-The Star-CD with CHEMKIN software will be under evaluation for the surface corrosion reactions and diffusions. Other software such as STORM/CFD2000 developed by Adaptive Research of Simunet Corporation is also under evaluation.