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


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## Task 5

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

S. Moujaes and Y. Chen

## BACKGROUND

The corrosion of structural materials is a major concern for the use of lead-bismuth eutectic (LBE) systems for nuclear applications such as in transmuter targets or fast reactors. Corrosion in liquid metal systems can occur through various processes, including, for example, dissolution, formation of inter-metallic compounds at the interface, and penetration of liquid metal along grain boundaries. Predicting the rate of these processes depends on numerous system operational factors: temperature, system geometry, thermal gradients, solid and liquid compositions, and velocity of the liquid metal, to name a few. Corrosion, along with mechanical and/or hydraulic factors, often contributes to component failure.

The goal of this project is to develop a corrosion model that combines the chemical kinetics and hydrodynamics in the system to predict corrosion rates. In this effort, these models will be developed for the Delta test loop at Los Alamos National Laboratory (LANL) and a theoretical LBE accelerator target system. The resulting models will be predictive tools that can be validated with corrosion test data and used to systematically design tests, interpret the results, and provide guidance for optimization in LBE system designs.

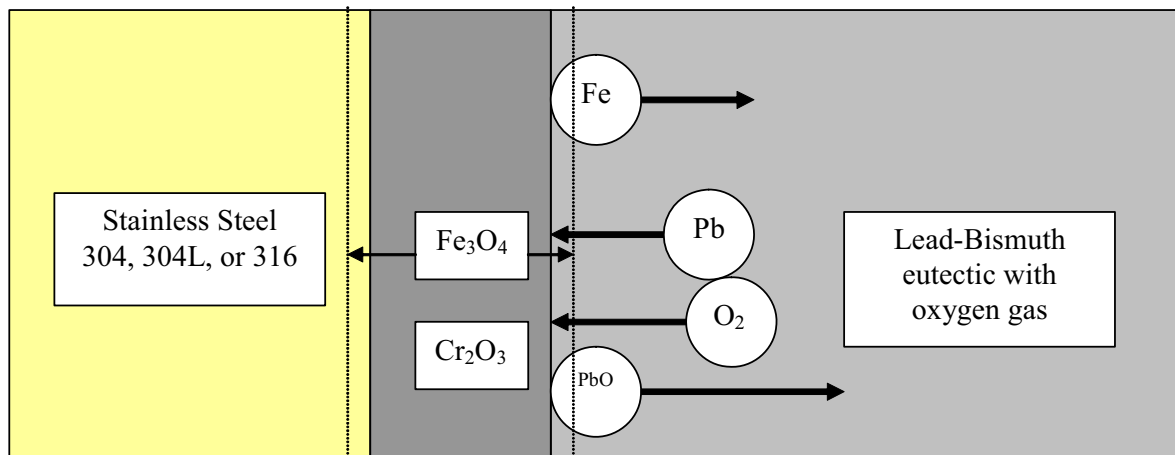
## RESEARCH OBJECTIVES AND METHODS

There are two subtasks to this research. The first subtask develops the necessary tools to predict the levels of oxygen and corrosion products close to the boundary layer using Computational Fluid Dynamics (CFD) modeling. The second subtask predicts the corrosion process kinetics between the LBE and structural materials by incorporating pertinent information from the first subtask.

STAR-CD software was used to model the corrosion and precipitation rates in the LBE loop. This allowed researchers to compare the theoretical analysis with available experimental results. The surface corrosion analysis is being developed as a user supplied subroutine to STAR-CD. The information obtained from this analysis theoretically predicts likely locations for corrosion and precipitation along the axial lengths of the test loop.

The first subtask involved performing a series of parametric runs. Models prepared from the previous year were used as guides for the parametric studies. Variables investigated included the average eutectic flow velocity, average mean bulk eutectic flow, inlet temperatures, and average inlet oxygen concentrations in the three geometries: a straight flow section, an elbow bend, and a tee section. The thermal-hydraulics study involved using a 3-D CFD code simulation to obtain averaged values of stream-wise velocity, temperatures, and oxygen and corrosion product concentrations at various axial locations close to the walls of several partial loop sections within the LBE loop. The oxygen and corrosion products inside the test loop were simulated to participate in chemical reactions with the eutectic fluid as it diffused towards the walls. Details of the geometry of these loops will be obtained from scientists at LANL. These values acted as a set of starting boundary conditions for the second task.

The second subtask focused on the kinetics of the dissolution/deposition process as a function of temperature, flow velocities, dissolved metal concentrations, oxygen potentials of the system, the kinetics of film formations in the presence of oxygen, and the kinetics of metal transport through the oxidized surface film.



*Schematic of corrosion processes between the metal surface and the liquid metal.*

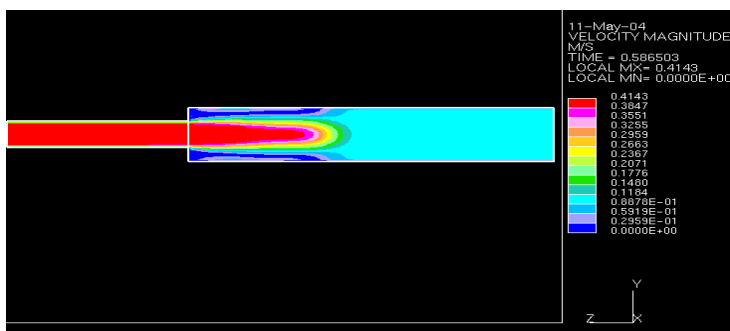
## RESEARCH ACCOMPLISHMENTS

Geometries and flow conditions similar to experimental results in the literature were set up and used to benchmark the models assembled using the STAR-CD software. Test case studies indicated that the outcome from STAR-CD was correct and that numerical modeling is applicable to the research in this problem.

Using these models, concentration flux profiles were obtained for both laminar and turbulent profiles in a straight pipe. This information was then used for the chemical kinetics analysis for corrosion on the inside walls of the LBE loop.

A 3-D model problem was simulated under the premise that the expected corrosion rate along the pipe's length may vary as a result of local flow condition differences and concentration profiles normal to the wall. Different pipe fittings are being simulated to shed some light on the effects of thermal-hydraulics on the corrosion chemical-kinetics inside these fittings. Location of extreme cases of corrosion/precipitation locations inside these fittings will be noted.

An additional set of simulations was executed on a closed loop using a straight pipe. These runs compared previously obtained results representing a diffusion-controlled reaction with conditions similar to the Delta loop at LANL. A "momentum source" within STAR-CD simulated the effect of a pump. This provided constant flow without the need for a detailed description of the pump flow. Analytical and numerical simulations show several similarities. However, the numerical results showed some peculiarities and differences from the straight loop concentration flux distribution. These happen to coincide with the location of the elbows around the loop. This may suggest that a secondary phenomenon occurs that does not take place in the straight loop.



*Profile of Oxygen Concentration along the Pipe Axis*

## HIGHLIGHTS

- ◆ Chao Wu completed his M.S. in Mechanical Engineering (July 2003), thesis entitled "Study of Geometry Effects on Local Corrosion Rates for LBE Loop."
- ◆ Kanthi K. Dasika completed his M.S. in Mechanical Engineering (November, 2003), thesis entitled "Modeling Corrosion in Oxygen-Controlled LBE Systems with Coupling of Chemical Kinetics and Hydrogen Transport."
- ◆ "Study of the Geometry Effects on Local Corrosion Rates for LBE Loop" presented at the ANS Annual Meeting, San Diego, CA, June 1-5, 2003.
- ◆ "Simulation Considerations in Lead-Bismuth Transmutation Loops: Corrosion Concentration, velocity and Temperature Profiles of LBE Loops", S. Moujaes, Y. Chen, K. Dasika, C. Wu, N. Li, J. Zhang, NURETH-10, South Korea, October 5-9, 2003.
- ◆ "3-D Thermal hydraulic Flow Effects and Chemical Kinetics on Wall Concentration Gradient Profiles of Corrosion/Precipitation Phenomena in LBE Loops", S. Moujaes, N. Armbya, G. Li, Y. Chen, ANS Student conference, Madison, WI, April 1-3, 2004.

## FUTURE WORK

Research to simulate the results of diffusion-controlled reactions and reaction-controlled kinetics on the three predefined geometries will continue. Comparisons will be made with previously obtained experimental values and other analytical studies to compare and validate the code. Attempts will be made to compare some of the simulation results with any experimental data available in the literature.

The STAR-CD models will be used to simulate the 3-D hydrodynamics of the LBE loop. The concentrations and mass fluxes of species that diffuse into the surface will be calculated. Programming scripts for the species transport equations will be written using the STAR-CD subroutine. Fluxes of iron and lead oxide from the surface will be calculated based on the product concentrations from the reactions. Corrosion and precipitation for the entire loop will also be calculated. Finally, 3-D corrosion kinetic finite difference models will be developed to study the corrosion rates for sudden expansion and contraction geometries, as well as for multi-branch outlets at junctions placed in a 5.0 m loop.

### Research Staff

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### Students

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### Collaborators

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