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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

### GOAL AND BACKGROUND

Many of the international efforts to develop transmutation technology, including the U.S., Russian, and European scientific communities, have determined that lead bismuth eutectic (LBE) is a potential material for use as both a spallation target and a coolant. To exploit this potential, a more thorough understanding of the effect and rates of corrosion on steels, particularly non-Russian alloys, inside the LBE systems is required. Properly controlling the oxygen content in LBE systems has been observed to drastically reduce the corrosion of structural steels in LBE. However, the transport of oxygen and formation of corrosion products is not well understood; thus, their interaction, variation, corrosion, and precipitation along the flow path requires further characterization.

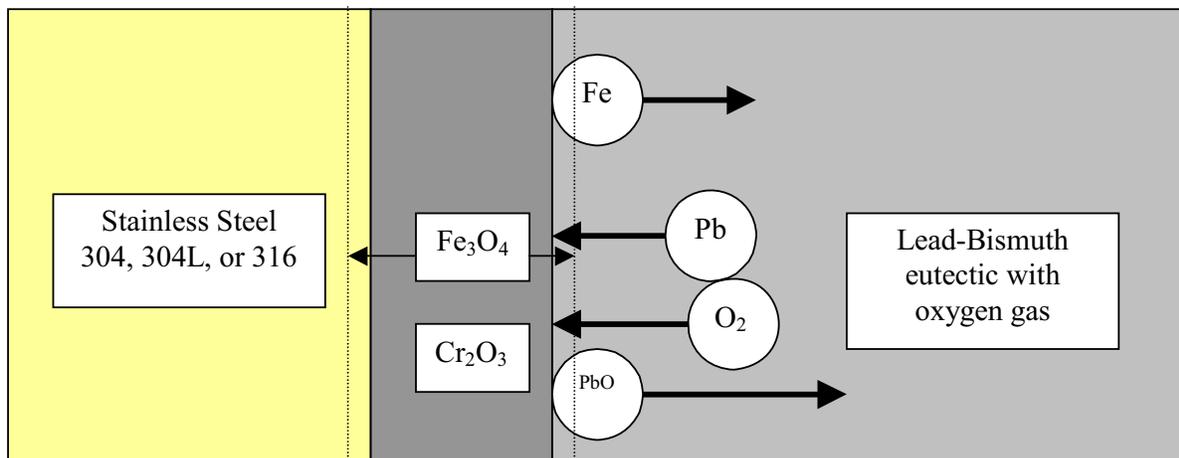
Direct testing, although absolutely essential, can be relatively expensive, time consuming, and inadequate to predict system corrosion performance beyond test conditions. The proposed work combines chemical kinetics and hydrodynamics in target and test-loop lead bismuth eutectic (LBE) systems to model system corrosion effects. This approach will result in a predictive tool that can be validated with corrosion test data used to systematically design tests and interpret the results. It also provides guidance for optimizing LBE system designs. Initial steps include developing predictive tools necessary to determine oxygen levels and corrosion products through computational fluid dynamics (CFD) modeling. Finally, invaluable information will be acquired by incorporating results from CFD modeling with kinetic information highlighting the corrosion process between LBE and structural materials.

### OBJECTIVES AND RESEARCH METHODS

The UNLV researchers have broken down their effort into three phases. Phase I simulates the corrosion process and phenomena occurring at the tube walls for a number of loop conditions. Phase II numerically simulates the effect of corrosion on components placed in the loop at predetermined ports. Phase III involves experimental testing of Phase II objectives. The experimental data acquired regarding corrosion effects will be compared with numerical simulations and used to benchmark the models. Variables to be analyzed include the distribution of LBE stream velocity, temperature, oxygen, and corrosion product concentrations close to the substrate. This will support the calculation of corrosion and precipitation rates in the entire system.

Using CFD coupled with chemical kinetics assists the researchers in obtaining reliable data for the experimental design. This will also serve to establish a predictive capability in the United States. Coupled with knowledge regarding the reaction chemistry and kinetics of potential corrosion rates, these codes can be used with reasonable confidence after proper validation, to investigate the behavior of new components exposed to LBE and oxygen.

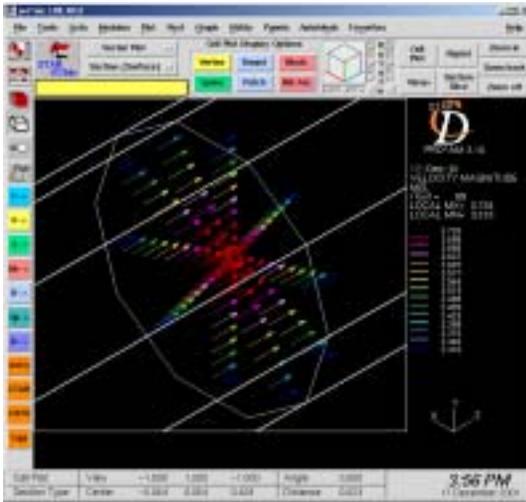
The most difficult challenge facing this work involves overcoming and developing an efficient numerical model with the correct chemistry reaction rates for use in different components of a typical LBE flow loop. Anticipated obstacles, progress, and research methods require intimate communications with Los Alamos National Laboratory scientists. This ensures that the research objectives are appropriately focused on the Transmutation Research Program needs.



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

## RESEARCH ACCOMPLISHMENTS

An intensive and ongoing literature search has provided limited information about the LBE system, especially with regards to chemical kinetic and thermodynamic data. However, researchers have been able to glean some insight regarding the corrosion mechanism on the material surface from the open literature. With this insight, researchers are attempting to determine what mechanisms foster the corrosion process. Potential scenarios include differentiating whether they are a function of kinetics, diffusion, or multiple mechanisms.



*Velocity profile along a cross section of the pipe.*

The transport of oxygen and corrosion products as well as their interaction and variation of corrosion and/or precipitation along the flow path are not well understood. Past experimental studies monitored corrosion history of specimens in one test loop over several thousand hours. This showed that corrosion occurs at higher temperatures but precipitation occurs at intermediate temperature. The model developed by the UNLV research team has confirmed that the temperature distribution in an LBE system is important for understanding the corrosion process in the system.

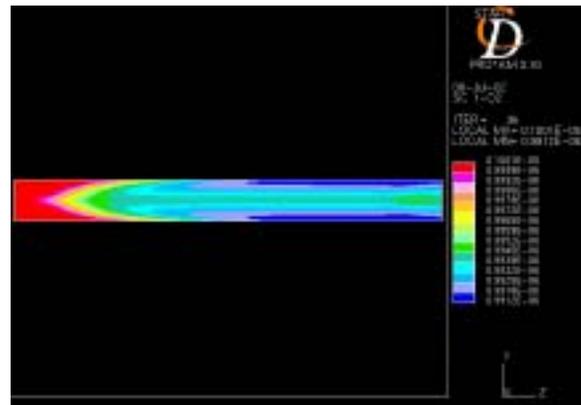
Thermal data for the species have been obtained from LANL. Thermal constants of lead, required for running the code, have been calculated and the input data for calculating these constants have been obtained. Effort is being made to calculate the transport data for each of the species involved in the reactions.

Finally, various codes are analyzing the fluid flow and the reactions taking place in the flow and on the surface. Two sections from the test loop have been chosen for the analysis. Lead and oxygen are allowed to flow through the

## HIGHLIGHTS

- A student was sent to the CD-Adapco at its Plymouth, Michigan training facility to receive the fundamental training on how to run the commercial code (STAR-CD)
- Presentation of “Modeling Corrosion in Oxygen Controlled LBE Systems with Coupling of Chemical Kinetics and Hydrodynamics” by Kanthi Dasika at the International Youth Nuclear Congress 2002 in Daejeon, Korea April 16-20, 2001
- Presentation by C. Wu and K. Dasika at the ANS Student Mini-Conference in Reno, Nevada, November 2001 “Modeling Corrosion in Oxygen Controlled LBE Systems with Coupling of Chemical Kinetics and Hydrodynamics”
- Presentation of a paper “Numerical Modeling of Lead Oxidation in Controlled Lead Bismuth Eutectic Systems: Chemical Kinetics and Hydrodynamic Effects” by Chao Wu at the ICAPP/ANS Conference in Hollywood, Florida, June 2002

system and the liquid lead reacts with oxygen. The walls are defined as made of stainless steel and the surface reactions between iron and oxygen have been considered.



*Variation of concentration of oxygen along the pipe.*

## CONTINUED PROGRESS AND FUTURE GOALS

The next step in the modeling process is to perform a parametric study examining the impacts of velocities and temperatures of the fluids on the corrosion rates. From this analysis, researchers hope to help decipher the most appropriate temperatures, velocities and concentrations of each of the species in the test loop for the minimization of corrosion.

### Research Staff

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### Students

Chao Wu and Kanthi Dasika, Graduate Students

### Collaborators

Ning Li, LBE Project Leader, Los Alamos National Laboratory