6-15-2002

Modeling Corrosion in Oxygen Controlled LBE Systems with Coupling of Chemical Kinetics and Hydrodynamics: Quarterly Progress Report 03/16/02- 06/15/02

Samir Moujaes  
*University of Nevada, Las Vegas, samir@me.unlv.edu*

Yitung Chen  
*University of Nevada, Las Vegas, yitung.chen@unlv.edu*

Follow this and additional works at: [https://digitalscholarship.unlv.edu/hrc_trp_sciences_materials](https://digitalscholarship.unlv.edu/hrc_trp_sciences_materials)  
🔗 Part of the [Materials Chemistry Commons](https://digitalscholarship.unlv.edu/hrc_trp_sciences_materials), [Metallurgy Commons](https://digitalscholarship.unlv.edu/hrc_trp_sciences_materials), [Nuclear Engineering Commons](https://digitalscholarship.unlv.edu/hrc_trp_sciences_materials), and the [Oil, Gas, and Energy Commons](https://digitalscholarship.unlv.edu/hrc_trp_sciences_materials)

Repository Citation  
**Available at:** [https://digitalscholarship.unlv.edu/hrc_trp_sciences_materials/60](https://digitalscholarship.unlv.edu/hrc_trp_sciences_materials/60)

This Report is brought to you for free and open access by the Transmutation Research Program Projects at Digital Scholarship@UNLV. It has been accepted for inclusion in Transmutation Sciences Materials (TRP) by an authorized administrator of Digital Scholarship@UNLV. For more information, please contact [digitalscholarship@unlv.edu](mailto:digitalscholarship@unlv.edu).
Modeling Corrosion in Oxygen Controlled LBE Systems with Coupling of Chemical Kinetics and Hydrodynamics

Quarterly Progress Report
03/16/02-06/15/02

UNLV-AAA University Participation Program

Principal Investigator: Samir Moujaes
Co-Principal 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. Scientists have noticed that the concentration of oxygen dissolved in the liquid alloy could control the corrosion rate of steels exposed to Pb or Pb-Bi. At high oxygen concentration, an oxide layer could be formed on the steel surface (lead oxides are less stable than iron oxide), which protects it from corrosion. At low oxygen concentration, there is no oxidation and corrosion occurs by dissolution of the steel components in the liquid metal. The surface of oxide layer in contact with the bulk flow of liquid metal may also be eroded under a high fluid velocity. Then the metal of surface will no longer be under protection because a porous oxide layer will be formed.

The first subtask of this project involves using a CFD code (2-D simulation) such as STAR-CD to obtain averaged values of stream wise 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. Kanthi Dasika, M.S. Graduate Student, (Mechanical Engineering)
- Mr. Chao Wu, M.S. Graduate Student, (Mechanical Engineering)

National Laboratory Collaborator:
- Dr. Ning Li, Project Leader, Lead-Bismuth Material Test Loop, LANL

Management Progress

Technical Progress

Hydrodynamics:

Combined codes of STAR-CD and CHEMKIN are being used for analyzing the fluid flow and the reactions taking place both in the bulk flow and the on the surface. Two sections from the MTL have been chosen for the analysis. The first one is cylindrical section with 1” diameter and 20” length. Another section is an elbow model with 2” diameter. Lead and Oxygen are allowed to flow through the inlet. The liquid lead reacts with oxygen in both the cases. The walls are defined as made of stainless steel and the surface reactions between iron and oxygen have been considered. An adiabatic condition has been applied on the walls and the fluids are allowed to flow at 950K. The inlet velocity is assumed to be 0.95m/s. The results from the runs of the straight cylindrical pipe model are shown in the following figures and each of them is discussed in detail.

Figure – 1 shows the velocity profile along a section from the center of the pipe. A K – E low Reynolds number turbulent model has been considered, due to which a flat profile at the exit of the pipe has resulted.

Figure – 2 shows the variation of oxygen concentration along the section of the pipe. The initial concentration of oxygen is 1E-06 weight percentage. The concentration reduces to 9.912E-07 as the flow reaches the exit of the pipe.

The variation of Lead Oxide concentration has been shown in the figure – 3, which has a similar pattern as of the variation of the oxygen concentration. The initial concentration of PbO is zero and the concentration increases to 1.292E-08.

Thermal data for the species have been obtained from the LANL. Thermal constants of lead, required for running the CHEMKIN code have been calculated and the input data for calculating these constants have been obtained from the NASA, GLENN EQUILIBRIUM PROGRAM. Effort is being made to calculate the transport data for each of the species involved in the reactions.
Fig – 1: Velocity flow at a section cut through the center of the pipe.

Fig – 2: Variation of concentration of Oxygen at a section cut along the center of the pipe.
Due to some problems with the post processing of the codes, the surface reactions could not be shown. But research is being done and the support personnel from the code developers are being contacted to overcome this problem. We are also in the pursuit of obtaining the thermal and transport data for Bismuth and Lead Bismuth Eutectic which are needed for the simulation of the actual flow in the MTL. The properties of Bi and LBE could not be obtained from the NASA, GLENN EQUILIBRIUM PROGRAM.

Once the above tasks are completed, a parametric study would be carried out, by varying the velocities and temperatures of the fluids. The analysis is hoped to help us decipher the most appropriate temperatures, velocities and concentrations of each of the species in the MTL for the minimization of corrosion.

Chemical kinetics of corrosions:

Corrosion is one of the major concerns with using of LBE. Liquid metal corrosion can proceed via various processes: dissolution, formation of inter-metallic compounds at the interface, penetration of liquid metal along grain boundaries, which depend on experimental factors such as: temperature, thermal gradients, solid and liquid compositions, velocity of the liquid metal. Research indicates that the corrosion rate of martens tic steels, at 475°C (hot leg temperature) and for a temperature gradient of 60°C (cold leg temperature is 415°C), increases from 21 to 93 µm per year when the alloy of lead-lithium velocity increases from 0.019 to 0.18 meter per second. In the MTL, velocity of liquid lead-bismuth could reach values up from 3 to 5 meters per second in the spallation module.
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 °C but precipitation occurs around 460 °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.
Future work:

1- To figure out how to obtain the concentration diagrams for the reactions on the surface and try to estimate the boundary layer thickness.
2- To run the parametric studies for both the geometries and try to decipher the velocity and temperature range for which the corrosion is minimum.