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Task 21

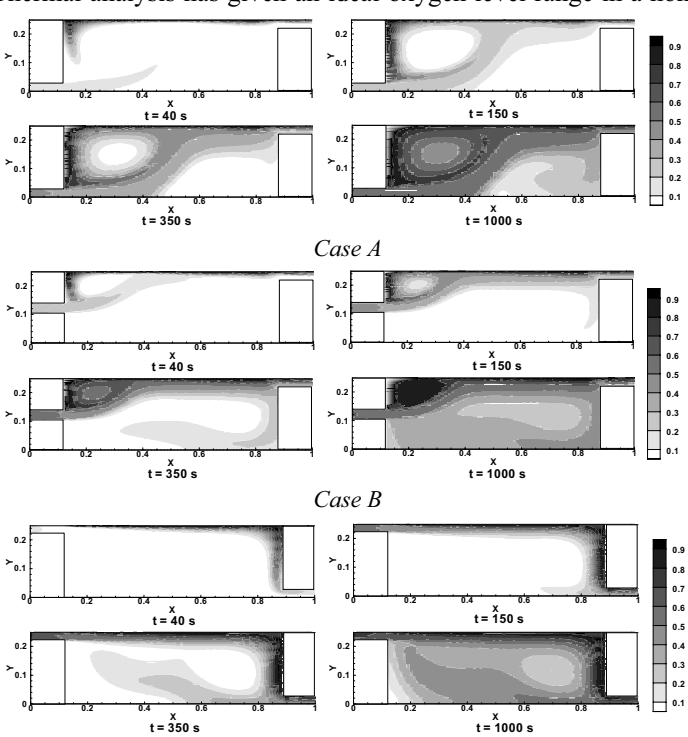
Theoretical Modeling of Protective Oxide Layer Growth in Non-isothermal Lead Alloy Coolant Systems

Y. Chen, J Zhang, H. Chen, J. Li

BACKGROUND

In advanced nuclear energy systems, lead-alloys (e.g., lead, lead-bismuth eutectic) emerge as strong candidates for transmutation and advanced reactor systems as nuclear coolants and high-power spallation neutron targets. However, it is widely recognized that corrosion of materials caused by lead-alloys presents a critical barrier to their industrial use. A few experimental research and development projects have been set up by different groups such as LANL to study the corrosion phenomena in their test facilities and to develop mitigation techniques and materials. One of the central or main techniques in lead-alloys coolant technology under development is to use active control of oxygen thermodynamic activity (OTA) to provide protective oxide layers.

Setting OTA in flowing lead-alloys makes corrosion highly dependent upon the oxygen concentration and the oxidation processes at materials surfaces. The active oxygen control technique exploits the fact that lead and bismuth are chemically less active than the major components of steels, such as Fe, Ni, and Cr. By carefully controlling the oxygen concentration in LBE, it is possible to maintain an iron and chrome based oxide film on the surfaces of structural steels, while keeping lead and bismuth from excessive oxidization that can lead to precipitation contamination. Thermal analysis has given an ideal oxygen level range in a non-isothermal lead-alloys coolant system. However, in a practical coolant loop, the proper oxygen level depends not only on thermal factors but also on hydraulic factors (system operating temperature, temperature profile, flow velocity, etc.). In addition, the oxygen distribution in a non-isothermal leadalloys coolant system is still unclear. The optimal oxygen levels still need to be investigated.



Oxygen concentration contours at different times (t = 40, 150, 350 and 1000 s) for different convection mode. Re = 1143 and Sc = 5 for all cases.

The goal of this research project is to provide a basic understanding of the protective oxide layer behaviors and to develop oxide layer growth models of steels in non-isothermal leadalloys (lead or lead-bismuth eutectic) coolant systems. Precise studies and simulations of all hydrodynamics with thermal conditions encountered in practical coolant loop systems by use of different flowing conditions in the laboratory are difficult and expensive, if not impossible. Therefore it is important and necessary to develop theoretical models to predict the protective oxide layer behaviors at the design stage of a practical lead-alloy coolant system, to properly interpret and apply experimental results from test loops, and to provide guidance for optimization in leadalloys nuclear coolant systems. The research project, therefore, is aimed at filling the gaps of protective oxide layer growth and the oxygen concentration level before lead-alloys nuclear coolant is ready for programmatic implementations and industrial applications.

RESEARCH OBJECTIVES AND METHODS

The research objectives are:

- To elucidate the mechanism of the protective oxide layer growth of steels in static, non-isothermal flowing lead-alloys coolant systems with oxygen concentration level control.
- To elucidate the mechanism of mass transport of oxygen, corrosion products in the multi-phase system.
- To develop oxidation growth models of steels in lead alloy coolant systems.
- To clarify the dependence of oxidation process on the hydraulic factors (system operating temperature, temperature profile, flow velocity, etc) and the oxygen concentration distribution and level.
- To clarify the optimal oxygen concentration levels in practical coolant system scales.
- To interpret the experimental results from test loops and to apply them to the design of practical nuclear coolant systems.

RESEARCH ACCOMPLISHMENTS

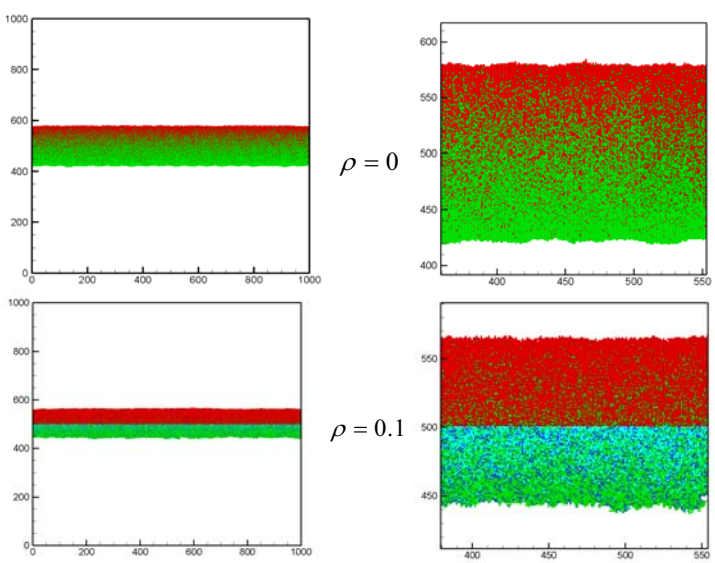
<u>Numerical analysis on oxygen transport in LBE system</u>

The Lattice Boltzmann simulations of oxygen transfer in the liquid lead alloy system were performed to investigate the enhancement of the oxygen transport by force convection. To mix the oxygen uniformly and quickly, the forced convection is proposed to enhance the oxygen transport with a cover gas scheme. The

oxygen control technique with cover gas scheme is formulated. To optimize efficient mixing of the oxygen, three different forced convection flow patterns on the oxygen transport are investigated.

Stochastic modeling on morphology of oxide layer growth.
A cellular automaton model, which combines the surface growth and internal oxidation, was created to explain the oxidation mechanism of steels in liquid lead-alloys. Based on Rebertson's theory, the morphology of steel under the mechanism of corrosion and oxidation under lead-alloy environment is modeled by a cellular automaton method, which uses the simple mathematical model to investigate self-organization in statistical mechanics, and especially suitable for complex systems. A global random walk method is included to characterize the diffusion process of iron. Working on the mesoscopic level, three main processes, which include the corrosion of the substrate, the diffusion of iron species across the oxide layer and precipitation of iron on the oxide layer, are included. In contact with liquid lead alloy, a piece of steel (mainly Fe and Cr) is corroded. The oxide layer is formed by one part of the corroded steel at the local place where corrosion occurs. Meanwhile, the remaining part of iron starts to diffuse across the oxide layer till they reach the layer boundary where they precipitate as new oxide product.

Numerical modeling on the oxygen-diffusion controlled oxide layer growth model
The numerical modeling of the oxygen-diffusion controlled oxide layer growth model was developed. This moving boundary problem was solved by finite difference method with transformation



Snapshots of the simulated layer in the presence of corrosion and surface growth. They correspond to 2.5×10^4 time step.

ACADEMIC YEAR HIGHLIGHTS

- "Modeling corrosion and precipitation in non-isothermal LBE Pipe/Loop Systems," was published in *Journal of Nuclear Science and Technology*, 2005, 42(11): 970-978.
- "Oxygen Control Technique in Molten Lead and Lead Bismuth Eutectic Systems" was submitted to Nuclear Science and Engineering, 2006, in press.
- "Numerical analysis of corrosion behavior and oxygen transport in the nature convection Lead-Bismuth flow" was present in 2005 ASME International Mechanical Engineering Congress, November 5-11, 2005, Orlando, FL.
- "Theoretical modeling and numerical simulation of the corrosion/precipitation process in non-isothermal pipe system" was present in 2005 ASME International Mechanical Engineering Congress, November 5-11, 2005, Orlando, FL.
- "Modeling one oxygen transfer in the forced convection lead-bismuth eutectic flow" and "Corrosion and precipitation Process in non-isothermal LBE pipe/loop system" were present in ICAPP'06, Reno, NV, June 4-8, 2006.

of the dependent variables and the coordinates. Also, the numerical code was benchmarked with available publication results.

Theoretical modeling on oxidation with scale removal in LBE system
An oxidation model with scale removal in LBE system was developed. The common kinetics of the oxide layer thickness and weight change per unit area depend on the pre-oxide thickness and the critical spallation thickness of the oxide. The steady state thickness was found to be a function of the operation conditions, such the materials, oxygen concentration, the flow velocity and the temperature.

FUTURE WORK

The next phase of the project involves accomplishing the following tasks:

- Illustration of the erosion-corrosion process mechanisms in oxygen control lead-alloys systems.
- Identification of the protective oxide layer growth under corrosion and oxidation mechanism with using stochastic methods.
- Optimal operation conditions for oxygen control lead alloys systems.
- Analytical models for various limiting process regimes.
- Development of correlations and tools for calculation of the oxidation rate, oxygen concentration level and distribution, and oxygen consumption.

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