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


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**Project Title:**

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

**August 10, 2001**

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**Investigators (UNLV):** Two Graduate Students to be determined

**AAA Project Collaborator:** Dr. Ning Li, Los Alamos National Laboratory  
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**AAA Research Area:** **Transmuter**

**Requested Funds:** \$109,010 (Year One)

**Abstract**

The proposed work will combine 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, and provide guidance for optimization in LBE system designs. The task includes of two subtasks. The first subtask is to try to develop the necessary predictive tools to be able to predict the levels of oxygen and corrosion products close to the boundary layer through the use of Computational Fluid Dynamics (CFD) modeling. The second subtask is to study the kinetics in the corrosion process between the LBE and structural materials by incorporating pertinent information from the first subtask.

**Work Proposed for Academic Year 2001-2002**

The first subtask 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. The oxygen and corrosion products inside the test loop will be simulated to participate in chemical reactions with the eutectic fluid as it diffuses 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 subtask as the 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 expected to help predict the likely locations for corrosion and precipitation along the axial length of parts of the test loop.

## **1. Background and Rationale**

Lead bismuth eutectic (LBE) has been determined from previous experimental studies by the Russian and the European scientific communities to be a potential material that can be used as a spallation target and coolant for AAA-proposed applications.

Properly controlling the oxygen content in LBE can drastically reduce the LBE corrosion of 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, and their interaction and variation of corrosion/precipitation along the flow are not well understood. This has been illustrated by the work of Xiaoyi and Li and was recently presented at seminars and meetings at UNLV by Dr. Ning Li of Los Alamos National Laboratory.

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 level. This confirms that the temperature distribution in an LBE system is important for understanding system corrosion performance.

The proposed research is divided into three phases. Each phase will be carried out over a one-year period.

- Phase I will simulate the corrosion process and history at the tube walls for a number of loop conditions.
- Phase II will simulate numerically the effect of corrosion on other components placed in the loop at predetermined ports that will be available for this purpose.
- Phase III will involve the experimental testing of placing these components inside the loop and obtaining experimental data on corrosion effects for comparison with results of Phase II.

## **2. Research Objectives**

The following are the three research objectives for Year One of this project:

1. Predict the distributions of LBE streamwise velocity, temperature and oxygen and corrosion product concentrations in the test loop in the interior of the LBE flow.
2. Predict locally the corrosion rates of the steel pipe surfaces using the information from objective 1 in iterations.
3. Compare with data available from previous experimental studies and improve the modeling.

The simulation in the bulk region of the test loop can use STAR-CD in a basic 2-D mode along the axial direction and the radial direction. The results of values of oxygen and corrosion concentrations, axial velocity and temperature will be obtained at a location close to the wall.

Appropriate models for the flow regime will be incorporated for this bulk flow such as two-equation models for turbulent flow when the need arises.

STAR-CD will accept thermophysical properties that are functions of temperature to be used as inputs into the conservation equations.

The second objective requires that we will look more closely at the reaction rates close to the wall where structural metals react with oxygen. Since the reaction kinetics of oxygen and substrate in the LBE loop is not well understood, a parametric study of chemical kinetics is needed to understand the corrosion process in the LBE loop design.

This parametric study will be coupled with CFD from the first subtask. The velocity of the LBE in the loop along with the temperature, oxygen, and corrosion product concentrations will be predicted close to the substrate to support the calculation of corrosion and precipitation rates in the entire system.

Finally the results of the second subtask will be compared with existing experimental data to ascertain the validity of the model and will look to see how improvements and tweaking can be made to both models of subtasks 1 and 2.

All of the above work will be performed with close communication with LANL scientists to ensure that the objectives of the research are appropriately focused on AAA Project needs.

## **Technical Impact**

**Corrosion effects on U.S. steels:** The AAA Project requires a more thorough understanding of the effect and rates of corrosion inside LBE systems. Direct testing, although absolutely essential, can be relatively expensive, time consuming and inadequate to predict system corrosion performance beyond test conditions.

**Results of previous experimental studies:** Several U.S. steels [316 (tube), 316L (rod), T-410 (rod), HT-9 (tube), and D-9 (tube)] in an oxygen controlled LBE flow loop have been tested at the Institute of Physics and Power Engineering (IPPE) in Obninsk, Russia. These tests were contracted by LANL. In the tests, the Russia steel EP823 (rod) was also included for

comparison. These samples were inserted in IPPE's CU-1M non-isothermal loop for time intervals of 1000, 2000 and 3000 hours at two temperatures of 460 C and 550 C. The oxygen level in LBE is controlled at 30-50 ppb by weight. The velocity in the test section is around 1.9 m/s, typical of coolant flow in LBE-cooled reactor cores. Local metal corrosion, typically on T410 and 316L have been observed in these tests. The proposed research will should help explain these observations.

**Long term effects:** There also exists an initial oxidization stage lasting about 2000 hours in which the formation of oxide films are observed at both corrosion and precipitation sites. The corrosion rate beyond this initial stage is quite different from that in the initial stage. Corrosion occurs at a site at 550 C, but precipitation appears to occur at a site at 460 C. This implies the results from a site at 460 C cannot be used to predict performance of materials at the same temperature but in a different location in a system.

**Asymptotic corrosion rates prediction:** Using CFD with chemical kinetics can assist the experimental design to get reliable data for the asymptotic corrosion rate and the thickness of the oxide films that is non-uniform along the flow direction. In addition, a predictive capability needs to be established in the U.S. through the use of CFD codes coupled with knowledge about the reaction chemistry and kinetics of these potential corrosion rates so that if new components need to be investigated as far as their behavior when exposed to LBE and oxygen one can use the code with reasonable confidence after its proper validation.

**Primary Hurdles:** One of the technical hurdles to overcome is to develop an efficient numerical model that has the right chemistry reaction rates for use in different components of a typical LBE flow loop.

## **Research Approach for Phase I**

The proposed project has been broken into seven tasks for the Phase I (first year of funding). Two graduate students will be involved in this effort.

1. Literature search: A detailed literature search and documentation will be made in the open literature and especially the European and Russian (English language publication) literature to find more completely what has been done in this research topic. Dr. Li has indicated that this area of modeling is still in its infancy and hence the interest in the proposed research.
2. Development of the numerical model through the use of one of the available commercial codes such as STAR-CD. This code has already been used for simulations in the general area of the AAA by other European researchers. Average values of the needed variables will be obtained from the code as the starting point for the more important task of describing corrosion chemical kinetics (item 4).
3. Testing and shakedown of developed model to make sure reasonable thermal-hydraulic values of the variables are obtained. This step includes the injection of the appropriate reaction rates in the bulk region of the loop/system for reactions between the LBE and oxygen.

4. Development of appropriate chemical kinetics modeling for the corrosion process near the wall of the LBE loop that will use in part information (as boundary conditions) from the simulation completed in item 3.
5. Presentation of the results of the simulation in item 3
6. Presentation of the results in item 4
7. Reporting requirements: weekly updates may be reported to the Intercollegiate Programs Coordinator, monthly updates will be provided to the UNLV AAA Program Director, quarterly progress reports will be delivered to the UNLV AAA Program office and LANL researchers overseeing the project. A final report will also be published as well as papers in conferences and journals at the end of the project.

### **Research Approach for Phase II**

Expanded modeling effort: Using the two codes developed in Phase I, one can simulate other objects placed in the loop/system for the purpose of predicting their corrosion rate histories.

### **Research Approach for Phase III**

Experimental effort: The LANL Materials Test Loop (MTL) offers an excellent platform to perform testing for validation and improvement of the model. There is also a possibility that a LBE test loop will be built at UNLV. This would offer an opportunity to validate some of the simulation results performed in Phase I and Phase II by performing the necessary long-term corrosion experiments for these objects.

### **Capabilities at UNLV and LANL**

UNLV has a 2000 ORIGIN parallel processor with several other mainframes for the purpose of this computational task. The university is consistently trying to increase the number of processors available on this machine to speed up the processing time needed for large-scale problems.

**Prof. Samir Moujaes** is an Associate Professor of Mechanical Engineering at the University of Nevada, Las Vegas and will serve as Principal Investigator for this project. Prof. Moujaes has worked for five years on computational aspects of cooling of canisters for the Yucca Mountain Project for DOE. Two emplacement configurations of high level waste containers were investigated and the temperature profiles and air velocity profiles under natural convection conditions were calculated. Other computational work involved developing two- and three-dimensional models for the description of heat transfer processes in residential gabled attics under the influence of the three modes of heat transfer. Currently a model is also being developed to describe the interaction of this heat transfer on the heat pickup of the supply air through a typical attic placed supply duct. Other experimental work has involved two-phase flow hydrodynamics and the determination of profiles of localized values of void fraction and dispersed phase axial velocity through the use of locally developed dual-tipped fiber optics

probes. Prof. Moujaes has also been involved with R&D on the testing for three-phase hydrodynamics and heat transfer of slurry derived from coal for a Solvent Refined Coal (SRC-I) process. He has published several papers in ASME, ASHRAE, and the Journal of Energy Engineering and is a reviewer for these organizations. He is an Associate Editor for the JEE and has also organized and chaired sessions in some of their conferences.

**Prof. Yi-Tung Chen** is Research Associate Professor of the Department of Mechanical Engineering and Assistant Director of the NCACM at the University of Nevada, Las Vegas. He received his B.S. degree in Chemical Engineering in 1983, and his M.S. and Ph.D. degrees in Mechanical Engineering in 1988 and 1991, respectively, from the University of Utah. He has a minor degree in Nuclear Engineering. Prof. Chen is an expert in experimental and computational aspects of momentum, heat, and mass transfer. His research interests include chemical kinetics modeling, high level radioactive waste repository design, atmospheric sciences, magnetohydrodynamics modeling, ground water transport, energy conservation, and biomedical engineering. He also has a strong background in organic chemistry, biochemistry, polymer chemistry, and physical chemistry. His research experience includes being PI and co-PI on projects involving the study of flow and heat transfer and species transport in unsaturated porous media funded by DOE, the burning of rocket motors under the Joint Demilitarization Technology (JDT) program funded by DoD, and atmospheric modeling funded by the NOAA Cooperative Institute for Atmospheric Sciences and Terrestrial Applications. He is also co-PI on an EPA project dealing with environmental monitoring for public access and a groundwater modeling project funded by DOE.

**Dr. Ning Li**, staff scientist from LANL will be the AAA Project collaborator of this project as he is one of the original participants and designers of the model target geometry that was devised and tested at IPPE. Hence, he has an interest in exploring what some of the CFD results show and how they compare with experiments for predictive purposes. Dr. Li does not require funding from UNLV to participate in this project.

### **Project Timetable and Deliverables**

Two meetings are scheduled for the first year of the project. The first to discuss preliminary results of code simulations and the second towards the end of Year One to present final results and obtain feedback from collaborators.

### Time Schedule and Major Milestones

Tasks	Qtr 1			Qtr 2			Qtr3			Qtr 4		
	Sept	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May	June	July	Aug
1. Literature search												
2. Development of model												
3. Testing and shakedown for items 2&4												
4. Development of chemical kinetics model at wall												
5. Running and presentation of results for item 2												
6. Running and presentation of results for item 4												
7. Reporting Requirements			○			○			○			○
Travel for LANL for meetings							★					★
<b>TRIP EXPLANATION</b>												
Trip 1	To discuss with LANL scientists progress so far on modeling effort											
Trip 2	To discuss and obtain feedback from LANL on preliminary final results											

(Work is assumed to begin September 1, 2001).





From: Ning Li, Ph.D.  
AAA, Los Alamos National Laboratory

Date: July 12, 2001

To Whom It May Concern:

Corrosion and materials compatibility in LBE systems present one of the critical challenges in the R&D areas of AAA, especially for deploying high-powered LBE spallation targets. Testing experience exists in Russia for specially developed alloys, but it is sorely lacking for US materials. Limited preliminary testing showed promise of some candidate steels. In any case, test results cannot be applied to systems with conditions different from the test loops used without better understanding of the influence of flow and temperature distributions on corrosion in LBE systems. This is demonstrated in the modeling effort we undertook at LANL ("A Kinetic Model for Corrosion and Precipitation in Non-isothermal LBE Flow Loop", Journal of Nuclear Materials (2001)).

I have had several technical discussions with Drs. Moujaes and Chen on modeling the system corrosion performance in oxygen-controlled LBE systems, and interacted with them throughout the preparation of the proposal. I think some very unique and valuable results will emerge from this work, and will help the AAA Program establish international leadership in this particular area. I strongly support the proposal "Modeling Corrosion in Oxygen Controlled LBE Systems with Coupling of Chemical Kinetics and Hydrodynamics" by Drs. Moujaes and Chen.

Yours truly,

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(Ning Li)