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Modeling Corrosion in Oxygen Controlled LBE Systems with Coupling of Chemical Kinetics and Hydrodynamics - Phase Three

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Project Title:

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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 predicative 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 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 predict the kinetics in the corrosion process between the LBE and structural materials by incorporating pertinent information from the first subtask. In many cases a component fails because of the combined effect of mechanical or hydraulic factors and corrosion. Such cases are of three types: stress corrosion, corrosion fatigue, and liquid-velocity effects (corrosion, erosion and cavitations). The compatibility issues arising from the interaction of liquid metals, corrosion/dissolution, with structural materials at temperatures of interest are important while lead alloy as a coolant for a fast breeder type nuclear reactor is used. The third year of the second subtask will focus on the kinetics of the dissolution/deposition process as a function of temperatures, flow velocities, dissolved metal concentrations and the oxygen potentials of the system, the kinetics of film formations in the presence of oxygen, and the

kinetics of transports of metal through the oxidized surface film. Both mass transfer controlled and reaction controlled of dissolved species will be parametrically studied for the corrosion process.

Work Proposed for Academic Year

The first subtask of phase III is similar to that of Phase II but more expanded where a series of parametric runs will be performed over a realistic range of values of the average eutectic flow velocity, average mean bulk eutectic flow inlet temperatures and average inlet oxygen concentrations in three defined geometries already agreed on by our group and after discussions with our collaborators Dr. Ning Li and Dr. Jinsuo Zhang from LANL. These are three-dimensional flow objects of interest to the corrosion study i.e. (1) 3-D sudden pipe expansion and contraction, (2) 3-D multiple branches component, and (3) 3-D simulation of the DELTA loop. The thermal-hydraulics study involves using a CFD code (3-D simulation) such as STAR-CD to obtain averaged values of streamwise velocity, temperature, oxygen and corrosion product concentrations at location deemed close to the walls of the LBE loop at more than one axial location to determine the maximum and minimum locations of corrosion and precipitation. 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 the loop will be obtained from scientists at LANL.

In the first subtask the numerical simulations of the diffusion-controlled reaction will continue for these three geometries. A serious attempt will be started and maintained that will perform simulations of the reaction controlled mechanism type. This will be a more involved endeavor as it will require the development of a user supplied subroutine to STAR-CD and needs the more involved help of STAR-CD chemical engineering staff. Currently we are negotiating this possibility with the company and should hopefully have a favorable decision soon as our group will be the first one to develop this capability for that code.

It is proposed for this effort to:

(1) Keep using STAR-CD to simulate the 3-D hydrodynamics of Pb-Bi loop.

(2) Calculate the quantities of species that diffuse into surface based upon the diffusion rates. Reasonable values of species diffusion coefficients will be calculated by using the mole or volume fractions of each species that appears in the bulk flow.

(3) Use the user subroutine of STAR-CD to write the programming scripts of the species transport equations (partial differential equations) with reaction terms which can be the ordinary differential equations. The reaction rate constants can be theoretical equations or the empirical or semi-empirical equations. The diffusion-controlled or reaction-controlled will be studied at and near surface. The diffusion-controlled is the overall reaction is controlled by the rate at which the reactants encounter one another. The reaction-controlled is related to the potential energy surface that controlled the reaction. The input variables and data structures of main programs and user subroutines need to be studied in order to combine with functions that provide access and output to the data. The data is accessible only through the functions, that is, the functions provide an

interface to the data. The simple reaction kinetics of iron oxide and lead oxide will be expressed and coupled to the user subroutines. Mole balances, rate law, stoichiometry, overall material balance, definition of conversion, definition of production rates of iron oxide and lead oxide, temperature, pressure, boundary condition for exposed surface, velocity, mass diffusion coefficient, initial conditions, etc. will be needed for the user subroutine. The more detail information about how to use the user subroutine will be provided by the STAR-CD. We will learn what kind of input variables we need to provide in order to simulate the simple reactions at surface. And we will follow what kind of parameters or variables are needed associated with our mass transfer equations, reaction equations, and reaction rate law etc.

(4) Calculate the fluxes of iron and lead oxide from surface based on the product concentrations from the reactions. The concentration fluxes from surface can be calculated from the following equation:

$$J = -D\frac{\partial C}{\partial n}$$

For mass transfer-controlled cases, the surface reaction is sufficiently fast that the component concentrations are always at their saturated or equilibrium levels and functions of temperature. While for the reaction-controlled, the mass transfer rates are fast enough to take the reaction products, then the species fluxes are functions of the reaction rate constant K(T) and the component concentrations at the surface are functions of temporal and spatial and they need to be calculated from the species transport equations with reaction terms.

(5) Calculate the corrosion and precipitation for the entire loop.

(6) Develop a simple 2-D and 3-D corrosion kinetic finite difference code to study the corrosion rates of sudden expansion/contraction, and multi-branch outlet at junctions.

Oxygen is added into LBE to form iron oxide on the stainless steel pipe surface. The reaction is very fast at first. Later O_2 will diffuse into the oxide layer and make the layer expand in both directions. In this way, the dissolution of many metal elements in steel can be greatly decreased. At the present, research on LBE corrosion problem with high O_2 concentration has not yielded any validated data yet. But there are some models that have been published for low O_2 concentration. We will compare our results with those models and loop test.

As the quick formation of oxide film on the surface continues, the dissolution of metal elements is down to a negligible level. The concentration of iron in bulk flow is decided by following reaction:

$$\frac{1}{4}Fe_3O_4 + Pb = \frac{3}{4}Fe + PbO$$

It is of great significance to track the concentration of iron, so that we can prevent the clogging in loop. By focusing on this, we are able to provide valuable data for loop design.

Lead Bismuth Corrosion Perspective

Corrosion is a major concern when using of Pb-Bi eutectic and with its compatibility with the containment structure. Liquid metal corrosion can proceed via various processes: dissolution, formation of intermetallic 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. [Georgi Ilincev, *Nuclear and engineering and Design* 217(2002) 167].Sannier, Flament, and Terlain have shown that the corrosion rate of martensitic steels, at 475^0C (hot leg temperature) and for a temperature gradient of 60^0C (cold leg temperature is 415^0C, 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 1999, Pointevin, Bergerson, Deffain, Enderlehave, Lenain, and Raballand have also shown that the velocity of liquid lead-bismuth could reach values up from 3 to 5 meters per second in the spallation module. Balbaud, Barbier, and Konys [J. Knoys, "Development of Oxygen Meters for the Use in Lead-Bismuth," Journal of Nuclear Materials 296 (2001) pp. 289-294] have developed an experiment device which consists in a rotating cylinder operating under controlled hydrodynamic conditions in order to evaluate the Pb-Bi velocity effect on the corrosion of steels.

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 [Li, *J. Nuclear Materials* 300(2002) 73]. 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. [Balbaud-Celerier and Barbier, Journal of Nuclear Materials, Vol. 289, pp 227-242, 2001]. 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.

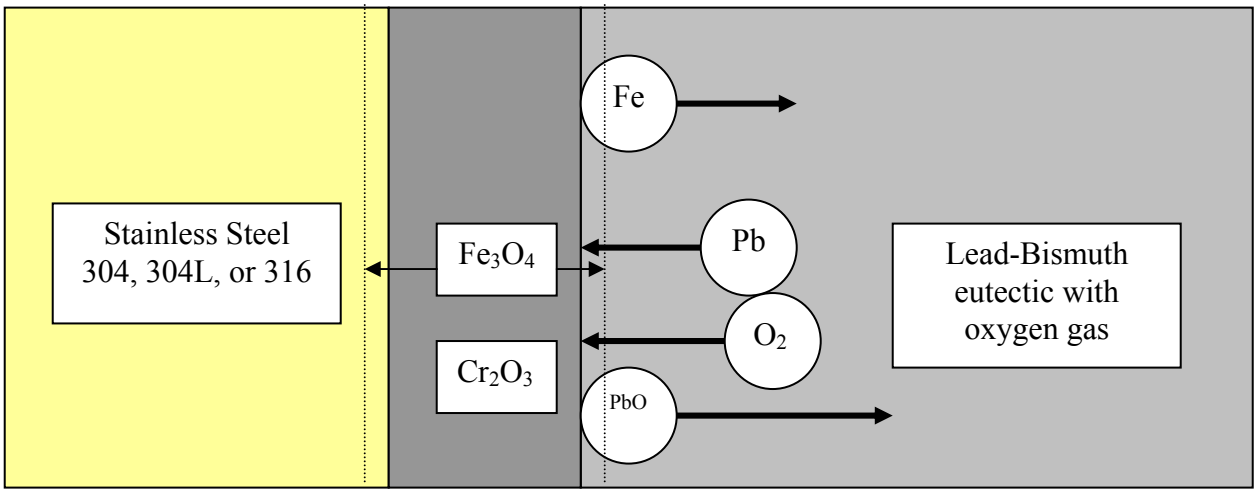

Figure 1. Schematics of corrosion processes between the metal surface and the liquid metal

Balbaud-Celerier and Barbier have indicated that the different mechanisms of combined action of flow and corrosion lead to basically four types of flow-induced corrosion: mass transported-controlled corrosion, phase transport-controlled corrosion, erosion-corrosion and cavitation-corrosion. The main interactions between a flowing fluid and a solid surface are dependent on momentum transport and mass and heat transfer such as convective diffusion-controlled and kinetics-controlled. A justification of the need of this parametric approaches is the fact that some of the kinetics and mass transfer coefficients are not well-known and defined yet. Also previous published studies indicate the importance of the thermal-hydraulics on the corrosion and core flow reactions. (i.e.. Ballinger and Lim report 2000) Oxygen is added into LBE to form iron oxide on the stainless steel pipe surface. The reaction is very fast at first stage. Later O_2 will diffuse into the oxide layer and make the layer expand in both directions. In this way, the dissolution of many metal elements in steel can be greatly decreased. From present research status, researches on LBE corrosion problem with high O_2 concentration have not yielded any validated data yet. But there are some models been published for low O_2 concentration.

Chemical kinetics may be described as the study of chemical systems whose composition changes with time. These changes may take place in the gas, liquid, or solid phase of a substance. A reaction occurring in a single phase is usually referred to as a homogeneous reaction, while a reaction which takes place at an interface between two phases is known as a heterogeneous reaction. An example of the latter is the reaction of a gas adsorbed on the surface of a solid.

The chemical change that takes place in any reaction may be represented by a stoichiometric equation such as

$$aA + bB \rightarrow cC + dD$$

where a and b denote the number of moles of reactants A and B that react to yield c and d moles of products C and D. For example, the formation of lead oxide from iron oxide and lead may be written as the balanced, irreversible chemical reaction. After quick formation of oxide film on the surface, the dissolution of metal elements is down to a negligible level. The concentration of iron in bulk flow is decided by following reaction:

$$\frac{1}{4}Fe_3O_4 + Pb = \frac{3}{4}Fe + PbO$$

It is of great significance to track the concentration of iron, so that we can prevent the clogging in loop. By focusing on this, we are able to provide valuable data for loop design.

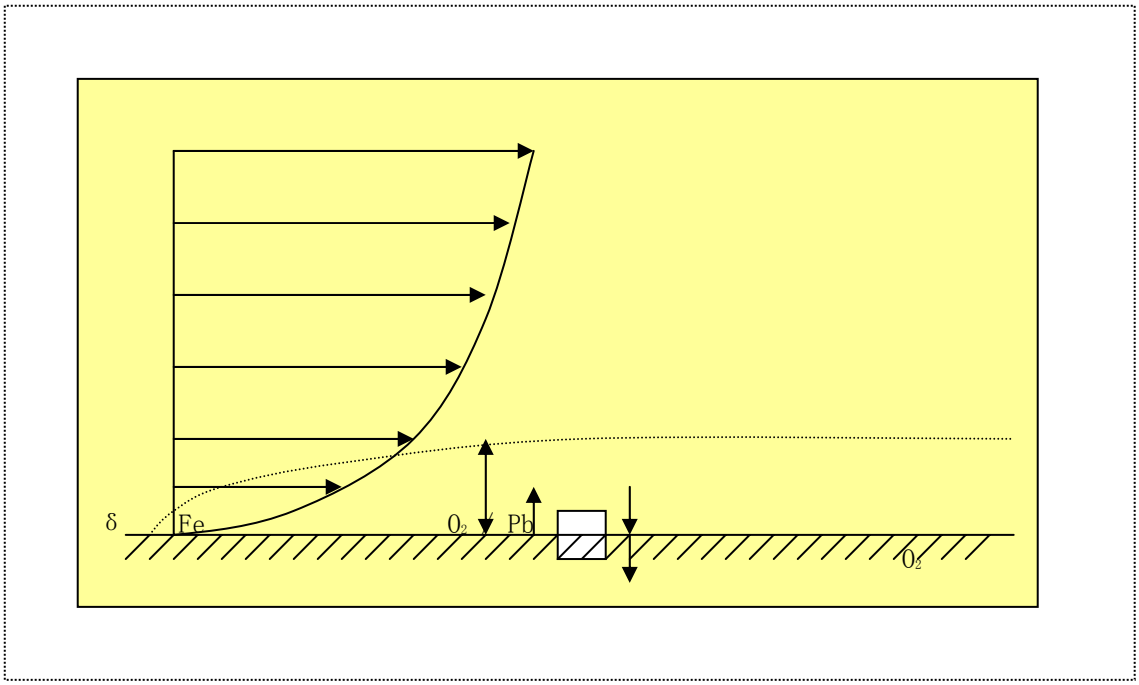

Figure 2. The diffusion process of species through the hydrodynamics boundary layer

The change in composition of the reaction mixture with time is the rate of reaction, R. The rate of consumption of reactants A and B and the rate of formation of products C and D can be written as

$$R = -\frac{1}{a}\frac{d[A]}{dt} = -\frac{1}{b}\frac{d[B]}{dt} = +\frac{1}{c}\frac{d[C]}{dt} = +\frac{1}{d}\frac{d[d]}{dt}$$

In virtually all chemical reactions that have been studied experimentally, the reaction rate depends on the concentration of one or more of the reactants. In general, the rate may be expressed as a function of these concentrations,

$$R = f\left([A],[B]\right)$$

In some cases the reaction rate also depends on the concentration of one or more intermediate species, e.g. in enzymatic reactions. In other cases the rate expression may involve the concentration of some species which do not appear in the stoichiometric equation; such species are known as catalysts. The most frequently encountered functional dependence given by above

equation is the rate's being proportional to a product of algebraic power of the individual concentrations, i.e.

$$R \propto [A]^m [B]^n$$

The exponent m and n may be integer, fractional, or negative. This proportionality can be converted to an equation by inserting a proportionality constant k, thus;

$$R = k[A]^m [B]^n$$

This equation is called a rate equation or rate expression. The exponent m is the order of the reaction with respect to reactant A, and n is the order with respect to reactant B. The proportionality constant k is called the rate coefficient. The overall order of the reaction is simply p=m+n. Since the mechanisms of reactions are not well defined, the reaction rates will also be studied parametrically.

The second subtask and important objective of this project is to simulate a reaction controlled situation at the inner wall of the different geometries listed above.

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 Advanced Fuel Cycle Initiative (AFCI)-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 He 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 application and validity of a commercially available thermal-hydraulics and used empirically supplied surface reaction corrosion kinetics for a diffusion controlled reaction on the surface to predict the corrosion/precipitation fluxes on a 10 m long loop in steady state.

- Phase II is simulating numerically the effects of diffusion reactions in 2-D sudden expansion geometries and 3-D short loops where by a momentum source has been used to bypass the need for simulating a pump placed in that loop. Also grid independence and the effects of various Schmidt numbers on the actual distribution of the corrosion/precipitation flux along that loop.
- Phase III is intended to pursue the simulation results of the diffusion controlled reactions and reaction controlled kinetics on the three geometries mentioned above. Comparisons with previously obtained experimental values T.Y. Risk et al.[10] and other analytic studies will be made (Ning Li et al. 2002) for comparison and validation of code.

2. Research Objectives

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

1. Simulate 3-D sudden expansion and contraction pipe geometry in laminar and then turbulent flow conditions similar to the conditions in the Delta loop in the range of Re~$2x10^5$ by considering both chemical reaction kinetics models i.e. diffusion controlled and reaction controlled at the surface.
2. Simulate 3-D multiple branch geometry in laminar and then turbulent flow conditions similar to the conditions in the Delta loop in the range of Re~$2x10^5$ by considering both chemical reaction kinetics models i.e. diffusion controlled and reaction controlled at the surface.
3. Simulated 3-D Delta loop as provided by LANL scientists in laminar and then turbulent flow conditions similar to the conditions in the Delta loop in the range of Re~$2x10^5$ by considering both chemical reaction kinetics models i.e. diffusion controlled and reaction controlled at the surface.

In all the above simulated runs a transient option will be invoked as it was found from Phase II studies that the flow is unsteady and fluctuates periodically in some of these geometries.

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

STAR-CD will accept thermophysical properties that are functions of temperature to be used as inputs into the conservation equations which will be also useful when natural thermosiphon flows will be simulated later on.

A Sample of Work in Progress This Year 2002-2003: Work on 2-D Sudden Expansion Simulation

Geometry effects on the LBE loop have a great influence on the local corrosion rates. The Delta Loop designed by Los Alamos National Lab (LANL) has different sections that differ in diameter from one to another. The sudden expansion, sudden contraction and multi-branch outlet at junctions are expected to show great differences in the local corrosion rate. According to the suggestions from LANL, an intensive study on the geometry effects is hence necessary and valuable. One of the important tasks of this project is to use the STAR-CD software to model the

corrosion and precipitation rates in the LBE loop and to show a reasonable good comparison to the theoretical analysis and experimental results from the journal articles and LANL.

It is necessary to benchmark STAR-CD software before we can use it to simulate the Delta loop. A few published papers regarding the experimental results on geometry effects to the fluid flow and species distribution were found in the literature research [1-6]. Similar geometries and flow conditions to those experiments have been set up and used to benchmark the data from STAR-CD.

First, a 2-D model problem was used. Two parallel flat plates are 6 meters long each, and the distance between them is 0.5 meter. Temperature along the length of the plate is assumed constant. A uniformly generated mesh is used, which means the length and height are divided into equally spaced grids. The Reynolds Number of the flow is given as 1,000 and 10,000. Initially, the inlet concentration is set as 0 which means the flow does not contain any species at inlet. A constant concentration of species on the surface of walls is used. In this way the species on the plates will diffuse into the bulk flow, and the expected corrosion rate along the length may vary due to the difference of local flow condition and concentration profiles normal to the wall. LANL data points out that the analytical solution to this problem shoes the corrosion rate q is inversely proportional to $x^{1/3}$, where x is the coordinate in the flow direction. By definition, $q = -D\frac{\partial C}{\partial x} \approx -D\frac{\Delta C}{\Delta x}$. Obviously, q is proportional to ΔC in this expression because of uniform meshing normal to the surface. As a result, we can expect that ΔC is inversely proportional to $x^{1/3}$. Figure 3 shows the curves of concentration gradient (between the wall and the layer of nodes which is next to wall) versus x coordinate which are obtained from STAR-CD. For the consideration of scale, the function of one tenth of $x^{1/3}$ is included (the pink line) as a comparison. In the plot, the dash line is the curve obtained when Reynolds Number is equal to 10,000, and solid line stands for the Reynolds Number of 1,000. From the curves, the results show a good agreement with the analytical solutions. The value of concentration difference shows an exponential decrease as expected.

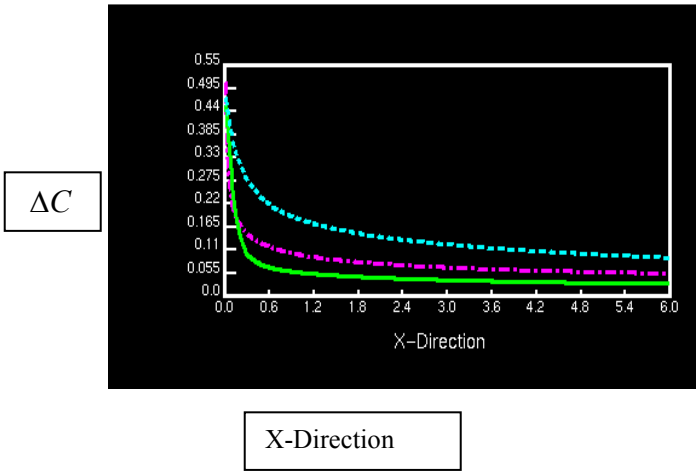

Figure 3. Profile of Concentration along Flow Direction

Another 2-D test case was set up with sudden expansion geometry as shown in Figure 4. The same temperature and concentration boundary conditions were used. Similar to the previous model, the inlet height, d, is 0.5 m, while the expanded area is 1.0 m high and 10.0 m long.

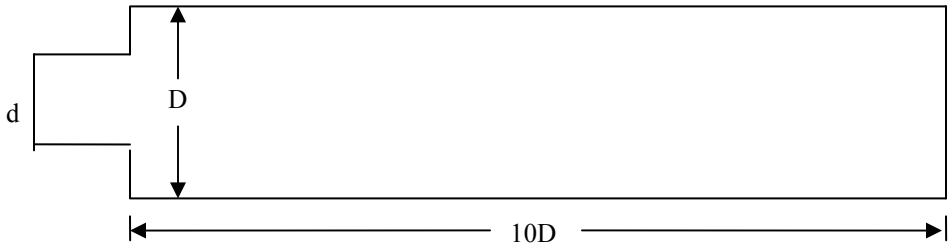

Figure 4. The schematic of sudden expansion pipes

Two Reynolds numbers were chosen for the benchmark test. One is 40, and the other is 1,000. A symmetric result is found in Reynolds number of 40. The concentration profile is shown in Figure 5.

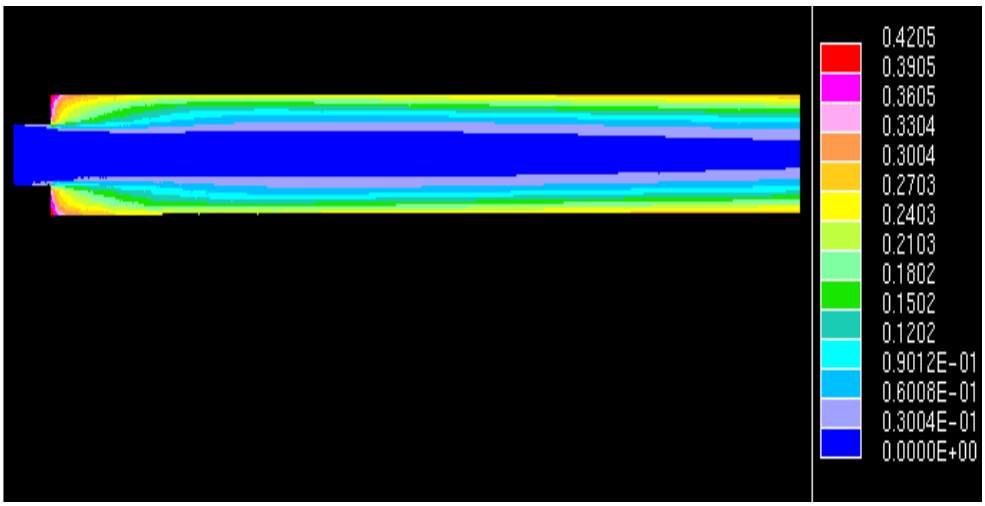

Figure 5. Concentration contours for Re=40

An interesting phenomenon is observed, when Re is equal to 1,000. The concentration difference is shown in Figure 7. Each peak value of concentration on the curve occurs at the location where the separation point exists. Contour of axial velocity component (Z component) is presented in Figure 6. From the contour, fluctuation of flow velocity in the bulk region can be seen. This fluctuation gives rise to the production, propagation and disappearance of vortexes in near-wall region. The extent of the vortex in the flow is an important factor which affects the corrosion rate greatly. According to the data provided by T. Y. Rizk *et. al.*[10] the curve shows a good

consistency with experimental results. Because flow is constantly changing and is periodic, concentration near the wall should be averaged over several discrete iterations in order to get reasonable results over a reasonable time period. The profile of concentration and its variation indicates that the effect of geometry is important, because of the complicated flow conditions that result from the sudden expansion geometry.

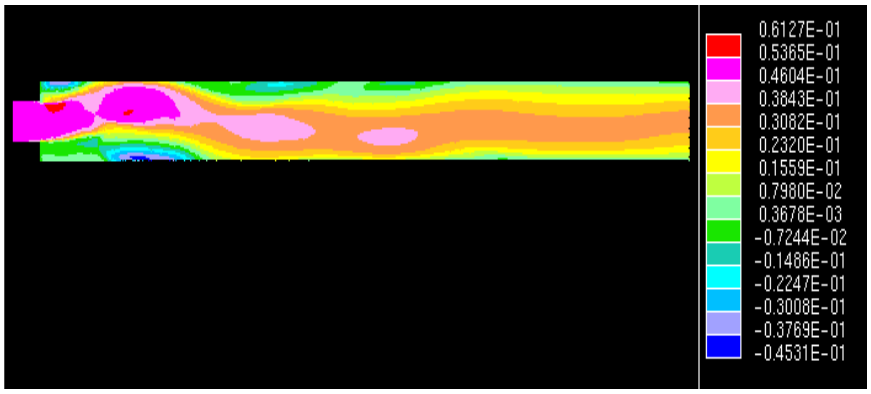

Figure 6. Contour of Axial Component of Velocity for Re=1,000

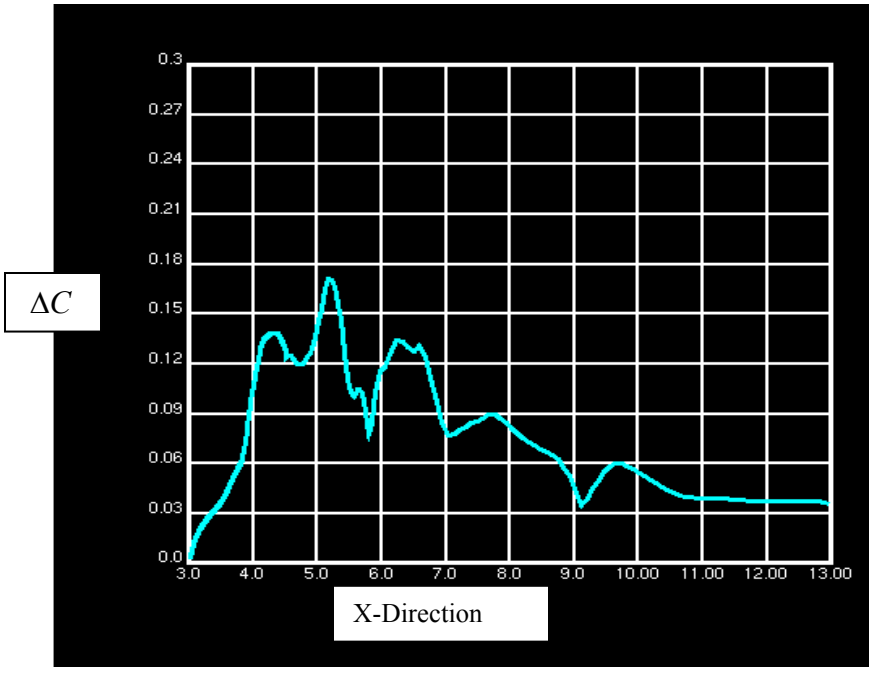

Figure 7. Concentration gradient of expanded area for Re=1000

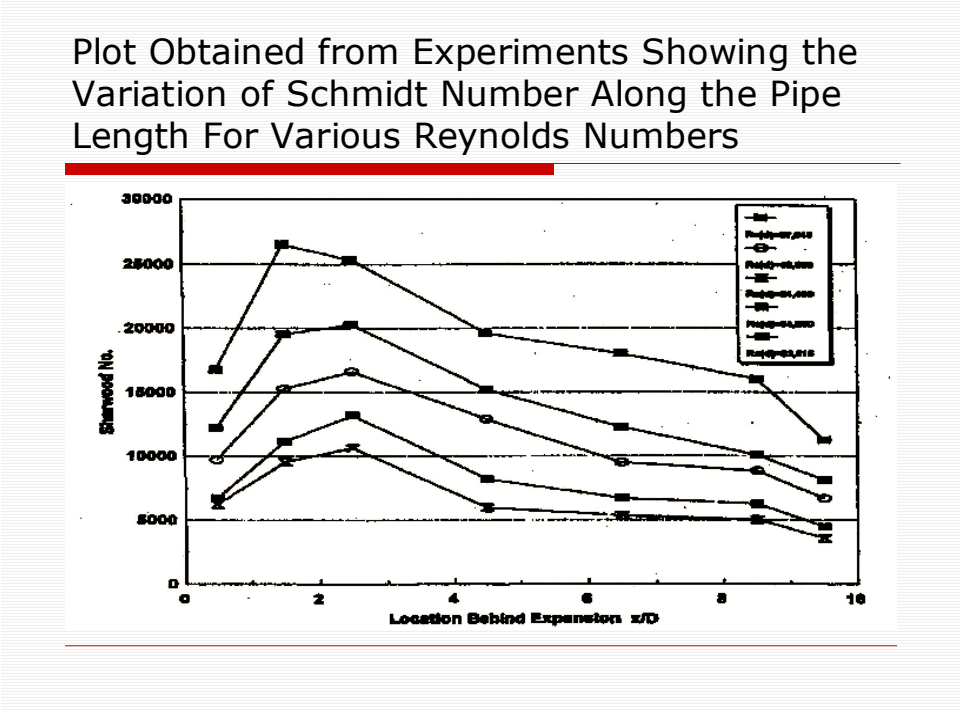

Figure 8. Calculated Sherwood Number From Experiments along the DownstreamWall of a Pipe Sudden Expansion Geometry

Additionally, a 3-D gradually expanding pipe model has been built i.e. conical shape. The diameters of inlet and outlet are 0.025cm and 0.05cm, respectively . The length of this divergent geometry is 34.34cm. It should be noted that, unlike the previous two cases, the distance between the wall and the first layer of cells which are next to the wall is not uniform along the axial direction, namely Z-direction because the pipe cross-sectional area increases and the same number of nodes are used in the transverse direction. As a result, the corrosion rate is proportional to $\frac{\Delta C}{\Delta x}$, where x is the direction along the radius, instead of ΔC only as in the previous case. A run was performed at Reynolds Number equal to 10,000. Figure 9 shows a decrease of $\frac{\Delta C}{\Delta x}$ along the Z-direction. Compared to the sudden expansion the gradual expansion shows a less complicated corrosion profile and shows that the corrosion rate is closely related to the flow condition.

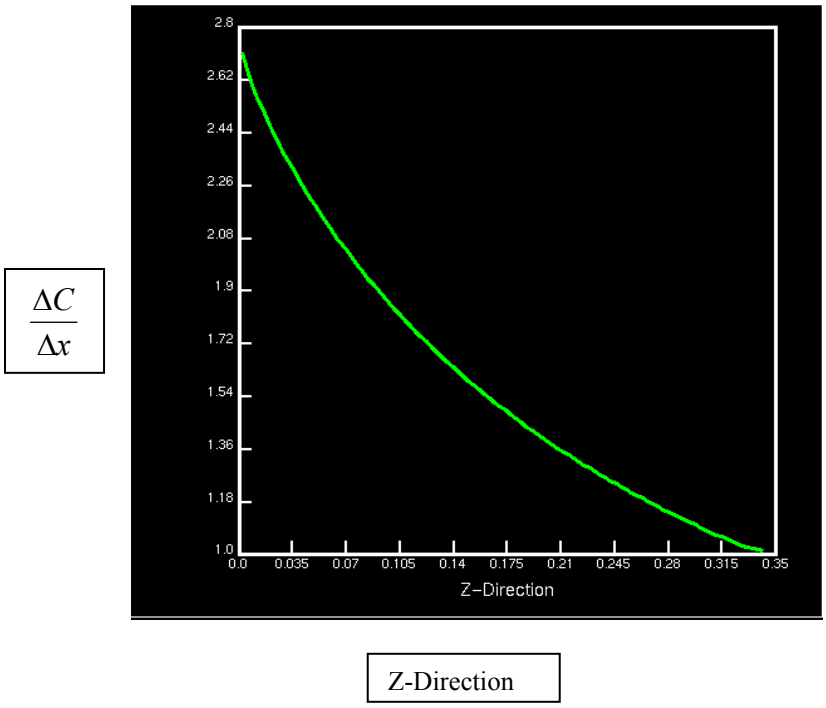

Figure 9. Concentration gradient for the linear expanding geometry

From these test cases, it proves that the outcome from STAR-CD is correct and that numerical modeling can help shed some light on this research problem..

Simulations on a Closed Loop and a Straight Pipe

Also based on several discussions with Drs. Li and Jinsuo Zhang from LANL it was decided to carry another set of simulations on a closed loop simulating flow of a lead-bismuth eutectic of 5 m long and a straight pipe. The importance of these runs is to compare with some previously obtained results from work of Dr. Li and Zhang that represent a diffusion controlled reaction described by a prescribed wall concentration as a function of temperature on the wall and a prescribed axial temperature profile similar to the Delta loop at LANL. Only a brief comparison of the trends of the simulation results vs. the analytical studies is given. Figure 10 shows the profile of imposed wall temperature and wall concentration flux. A new option was used in STAR-CD and this is the use of a "momentum source" that would simulate the effect of a pump which provides constant flow without the need for a detailed description of the simulation of the pump flow. Figure 11 shows results of the analytical calculations of the loop concentration wall flux versus the simulated numerical results from a 3-D simulation of the 5.0m loop. Laminar and turbulent results are shown here as well. Although the analytical and numerical simulations show several similarities the numerical results show some peculiarities and differences from the straight loop concentration flux distribution. These additional dips and sharp rises happen to coincide with the location of the elbows around the loop which initially suggests that there is some secondary phenomena that is taking place not captured in the straight loop.

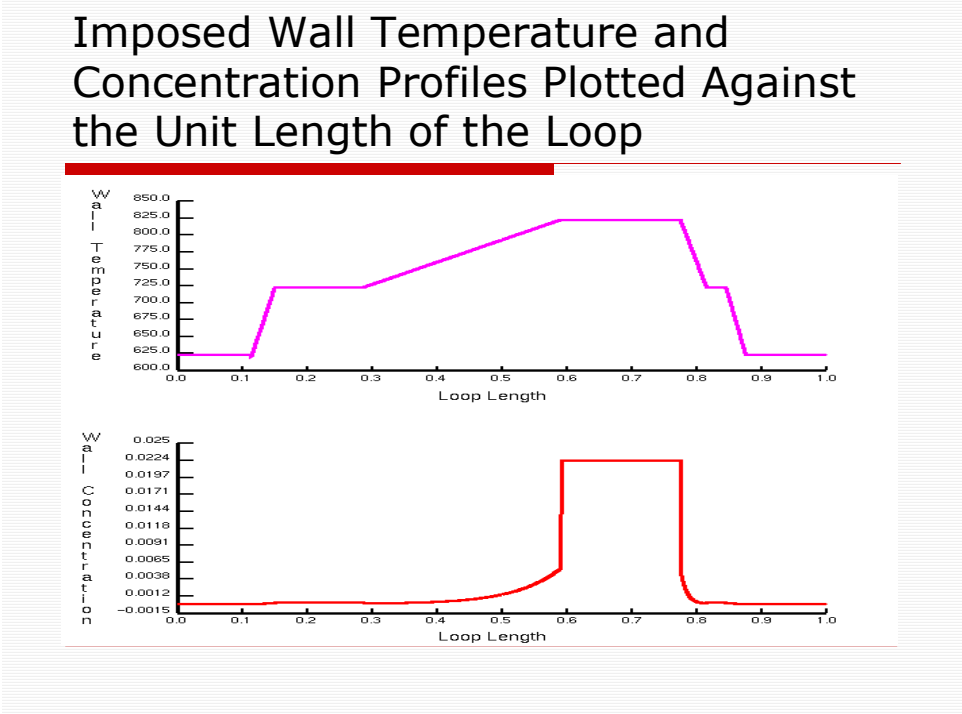

Figure 10. Wall Temperature and Concentration Profiles

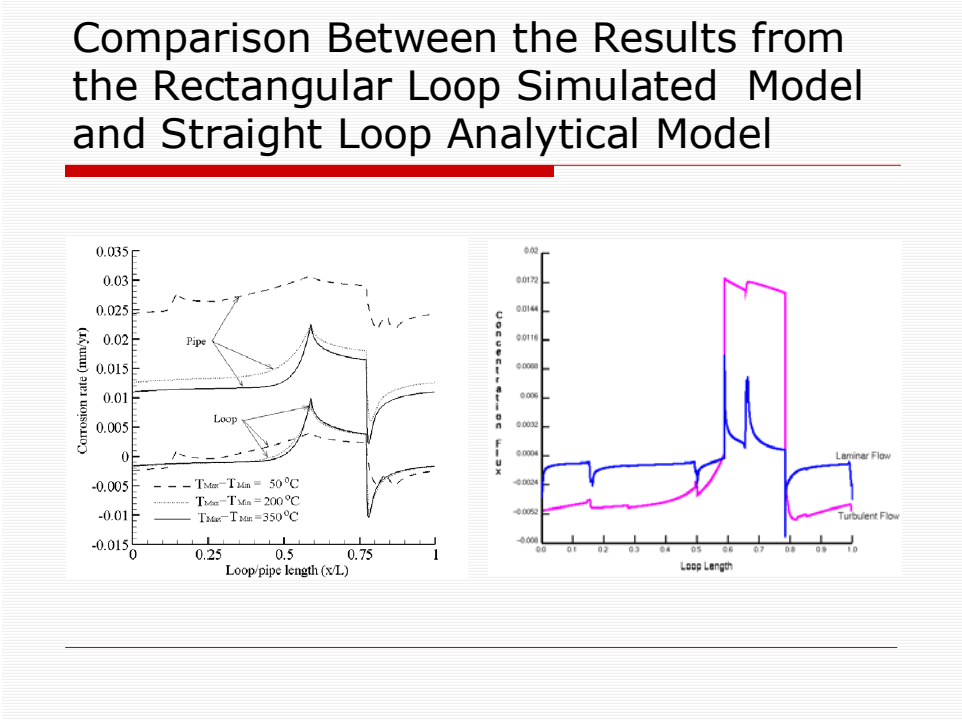

Figure 11 Comparison of The Wall Concentration Gradients Between Analytical and Numerically simulated Loop Results

Technical Impact

Corrosion effects on U.S. steels: The AFCI 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 that can have a realistic turn around time and has reasonable accuracy.

Research Approach for Phase III

The proposed project has been broken into five generic tasks for the Phase III (third year of funding) and will be applicable for the four general research goals of Phase III listed above. Two graduate students will be involved in this effort (Mr. Mojtaba Eshragi (Ph.D. candidate), Mr. N. Armbya (MS candidate)).

1. Literature search: A detailed literature search and documentation will continue to 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. The literature search has of course been started since Phase I work was started and is still continuing.

2. New nodal models have to be prepared (i.e. 3-D) which are an extension of work from Phase II study (i.e. 2-D models) will be used to perform the parametric study and investigate the effect of several parameters on the corrosion simulated rates. This part of the study should point out to the importance of the thermal-hydraulic conditions close to the wall on the corrosion/precipitation dynamics on that wall surface. This fact is highlighted by a recent report written by Ballinger and Lim (2000) emphasizing the first effect on the second one. These parameters are:
   a-average inlet eutectic axial bulk velocity would determine the velocity profiles close to the wall.
   b-average eutectic inlet temperature will determine average simulated temperature values and to a certain if heat flux conditions are known the temperature profiles close to the wall and reaction kinetic boundary conditions needed for the simulation.
3. Testing and shakedown of developed models with their related corrosion models will be used to run some limiting cases of the parameters to make sure reasonable thermal-hydraulic/corrosion kinetic values of the variables are obtained.
4. Presentation of the results of the simulation in item 3 and for all the other intermediate parametric values chosen so that as complete a picture as possible is obtained of the variation of corrosion kinetics as a function of these parameters.
5. Reporting requirements: weekly updates may be reported to the Intercollegiate Programs Coordinator, monthly updates will be provided to the TRP/UNLV Program Director, quarterly progress reports will be delivered to the TRP/UNLV 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 Phase III project period. Already the research team along with our collaborators have published about five conference papers since the start of the project in various conferences such as ANS, ICONE and ASME.

Research Approach for Phase IV and Beyond

The experimental effort is on the agenda except this is closely dependent on when a functioning loop at UNLV would be available. Two other simulation works are worth looking into though and these are thermosiphon flow in the loop and a detailed flow simulation in the area of the target plate where some very interesting and complicated flow dynamics are taking place especially downstream from the flow holes. Some of the interest there lies in the potential flow maldistribution of the Lead-Bismuth flow has been shown to exist from some previous Russian experimental studies. Also interesting and not very well understood phenomena are exhibited in regards to temperature fluctuations in the downstream region of the flow plate/flow holes area.

Capabilities at UNLV and LANL

UNLV has a new parallel processor (named ELKO) 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 impending projects have to do with the newly established National center for Energy Management and Building Technologies (NCEMBT) established at UNLV whose funding is going to be around $2.4M for 03-04 of which Dr. Moujaes will be involved in about $600K expenditure of that funding. A new project that is coming on line is the investigation of the potential of high temperature thermochemical production of hydrogen by solar means. UNLV is involved in an overall effort for 03-4 of over $2.0M out of which UNLV will obtain about $670K and out of which Dr. Moujaes will obtain a funding of approximately $75K. 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 Interim 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 AFCI 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.

Dr. Jinsuo Zhang, visiting post-doctoral scientist who is in his second year at LANL at the Center of Non-Linear Studies. Dr. Zhang has published several related papers on the lead bismuth flow and basic reaction kinetics. He has visited our campus several times and is working very closely with researchers and students from UNLV on this project. Dr. Zhang does not require funding either, to work with our group.

Project Timetable and Deliverables

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

Time Schedule and Major Milestones For Phase III Project
Task V

	Qtr 1			Qtr 2			Qtr3			Qtr 4		
Tasks	Sept	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May	June	July	Aug
1. Literature search												
2. Development of 3-Dmodels												
3. 3-D Sudden expansion model												
4. 3-D sudden contraction												
5. 3-D DELTA loop												
6. Final report Phase III												
7. Reporting Requirements												
Travel for LANL for meetings												
TRIP EXPLANATION												
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, 2003).
The Researchers are in continuous contact with our their collaborators from the LANL Laboratory where regular visits from one of the collaborators takes place every two months along with frequent e-mails and phone communications.

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

Date: July 12, 2002

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)