Modeling Corrosion in Oxygen Controlled LBE Systems with Coupling of Chemical Kinetics and Hydrodynamics: Quarterly Progress Report 11/16/01-2/15/02

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

Quarterly Progress Report
11/16/01- 2/15/02

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. 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.

The first subtask of this project 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 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

Principal Investigator:
- Dr. Samir Moujaes (Mechanical Engineering)

Co-Principal Investigator:
- Dr. Yitung Chen (Mechanical Engineering)

Students:
- Mr. Chao Wu, M.S. Graduate Student, (Mechanical Engineering)
- Mr. Kanthi Kiran, M.S. M.S. Graduate Student, (Mechanical Engineering)

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

Management Progress

Budget Issues:
- Salary expenditures has been adjusted in January according to the proper account number.

Management Problems

We have encountered so many problems in using STAR-CD + CHEMKIN software since CHEMKIN is a beta version from Adapco company. We have been working with their technical groups to help them to debug those library links errors in order to make the program running in the SGI Origin 2000 at NSCEE.

Technical Progress

As specified earlier, STAR-CD+CHEMKIN has been chosen as the CFD tool for analyzing the fluid flow and chemical reactions. The method of solvability used in STAR-CD is a Control Volume Method or finite-volume method. The governing equations followed by STAR-CD for fluid analysis and mass transfer are shown below.

Continuity:
\[ \nabla \cdot \rho V = 0 \]  \hspace{1cm} (1)

Momentum:
\[ \rho \frac{DV}{Dt} = \rho g - \nabla p + \mu \nabla^2 V \]  \hspace{1cm} (2)

Energy:
\[ \rho C_p \frac{DT}{Dt} = k \nabla^2 T + \mu \Phi_v \]  \hspace{1cm} (3)
Species transport:

\[
\frac{DC}{Dt} = D_{\text{eff}} \nabla^2 C + R
\]  

For testing the chemistry and fluid analysis solvability strengths of the STAR-CD, a simple model involving the surface chemistry has been chosen and the results analyzed. A flow over a flat plate has been considered as the test model. A section of the plate has been chosen with dimensions of 2mm x 100mm for the analysis. Air along with propane is allowed to flow over a Vanadium plate. The fluids at a temperature of 600K are allowed to flow over the plate with temperature at 1290K. The mesh has been refined at the wall surface for clear depiction of the surface reactions. The propane gas disassociates by reacting with air at high temperatures and also reacts with the vanadium surface resulting in the formation of various chemical species which are described in more detail using the figures. The fluids are allowed to flow at a velocity of 5m/s in the turbulent regime. The initial concentrations of the species of the gases are given below.

- \( \text{C}_3\text{H}_8 \)  
- \( \text{O}_2 \)  
- \( \text{N}_2 \)

The values are specified in terms of weight percent.

The results are depicted in the form of figures and followed by an explanation. Figure 1 shows the geometry of the model that has been considered. Figure 3 describes the velocity variation of the fluids along the surface of the flat plate. The values vary from 5m/s at the inlet to 13m/s at the outlet. The velocity of the fluid in more detail at a particular section of the considered geometry is shown in Figure 4. The profile and the formation of the boundary layer can be seen more clearly in this figure. The variations of the temperature along the lateral direction of the plate is shown in Figures 5. The variations of concentration of oxygen due to the reaction with propane are shown in Figure 6. The final concentration of the oxygen comes down to 0.2240 weight percent, the initial concentration being 0.2392. Figure 6 shows a closer view of the variation of oxygen concentration.
Figure 1: Geometry of the example model

Figure 2: Mesh refinement at the wall surface
Figure 3: Velocity profile along the surface of the plate

Figure 4: Velocity profile along the longitudinal direction to the surface
Figure 5: Temperature profile

Figure 6: Oxygen concentration diagram