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Modeling Corrosion in Oxygen Controlled LBE Systems with Coupling of Chemical Kinetics and Hydrodynamics: Task V 4th Quarterly Report

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AAA/UNLV
TASK V
4TH QUARTERLY REPORT

Management Issues:

The project is moving on target with the newly realigned objective set for the Phase I. Through close communications with Dr. Li and Dr. Jinsuo Zhang from LANL a realignment of the simulation work has been recommended. The reason for that is the vendor of STAR-CD/CHEMKIN had not perfected yet the final coupling of the post processing of output for any potential surface chemistry reaction taking place on the inside pipe surface of the LBE loop. This is because the coupling of CHEMKIN and STAR-CD has been done fairly recently. This hurdle has already been resolved and through my conversations with the technical people of STAR-CD they are now in the testing phase of this new capability and will let us benefit from these results through a new upgrade to the code. We have hence focused our attention on performing simulations that will allow us to predict the diffusion of the corrosion from the wall by the use of a semi-empirical relationship that is a function of the localized wall temperature. STAR-CD will hence predict the transverse distribution of this concentration in the loop. Finally we can extract the important quantity from this localized profile by evaluating the gradient of concentration at the inner wall surface from which we can deduce the corrosion rate as defined by previous papers of Li.

Technical Issues:

Our final effort has been to generate using an innovative method of simulating a forced flow inside a loop without the
simulation of the pump that creates the flow. The approach allows us to obtain ,after several iterations, the values of the corrosion locally at various axial locations in the loop. To briefly summarize some of our findings, a brief presentation of some of the simulations is made:

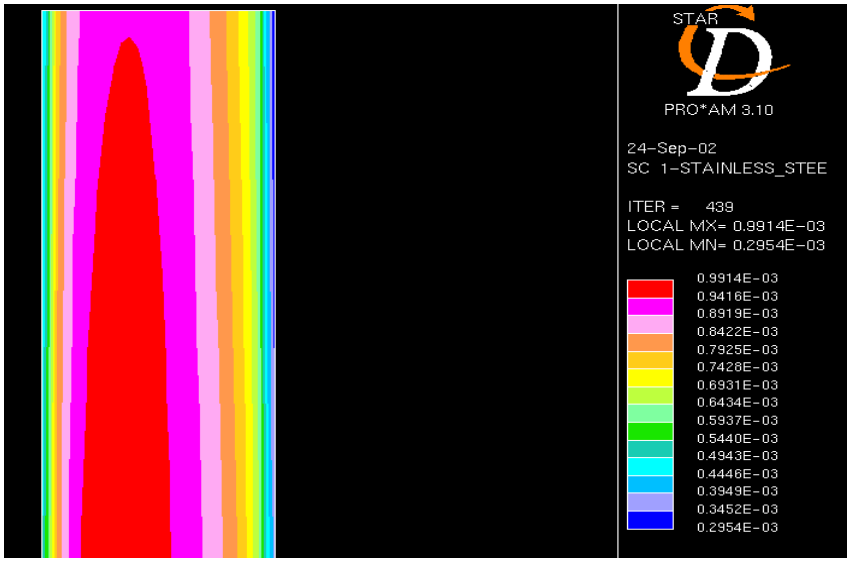

Figure 1. Corrosion Concentration in Fluid at Inlet to Loop II

Figure 1. depicts the transverse profile of concentration from corrosion taking place at the LBE wall. Where a prescribed wall boundary condition of the concentration was inputted. Figure 2 shows the concentration at an elbow of loop II.

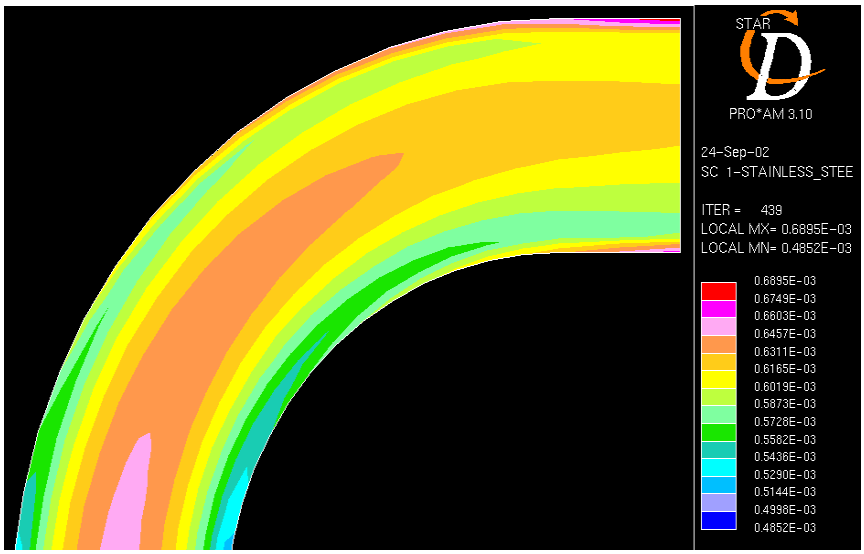

Figure 2- Corrosion Concentration at First Elbow of Loop II

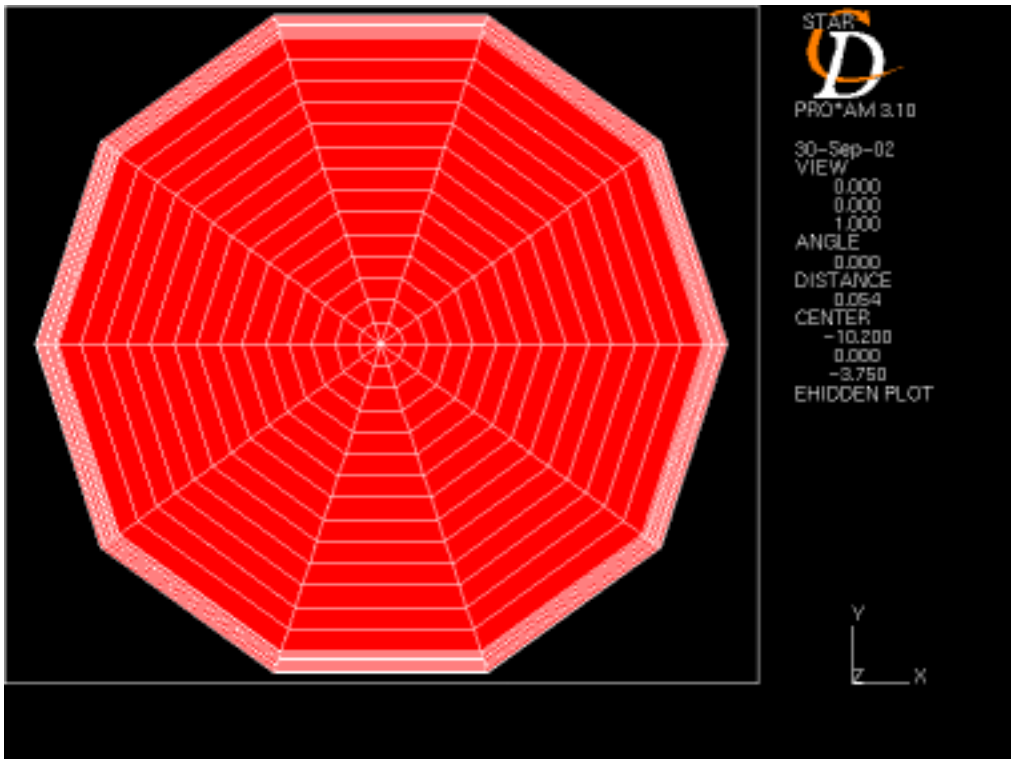

Figure 3. Details of Nodal Arrangement Close to Wall

Figure 3 is a refinement of the nodal arrangement to obtain more detailed information of the concentration profile close to the wall.

Finally a couple of view graphs are shown in Figures 4&5 which depict the transverse diametral concentration profiles for two locations in the loop one with a high wall concentration and one with a very low concentration at the wall respectively.

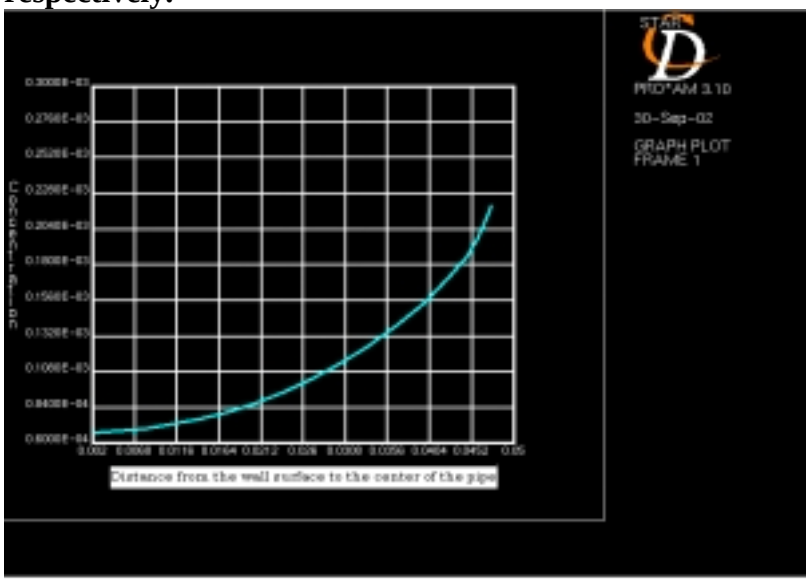

Figure 4. Radial Profile of Concentration with a High Value at Wall

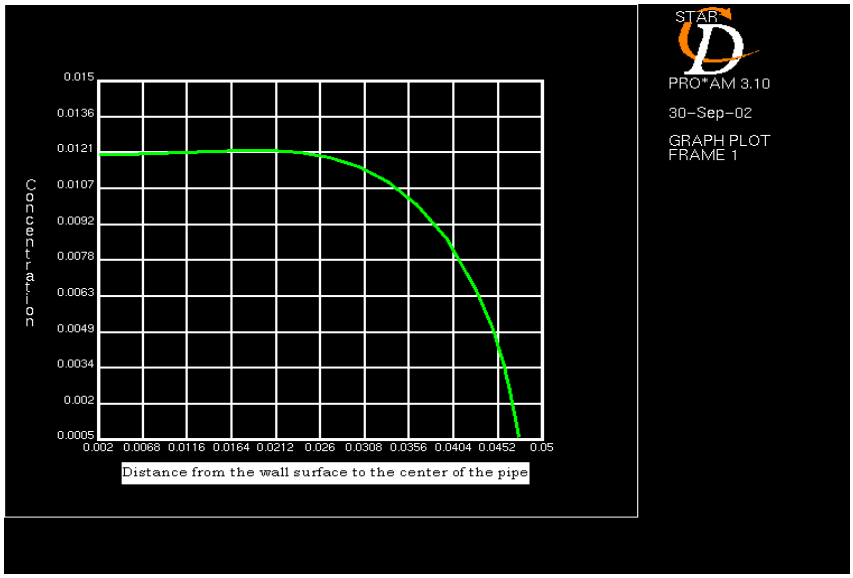

Figure 5. Radial Concentrations in the Fluid with a Low Value of Concentration at Wall

Future Work:

One of my students Chao Wu attended a workshop on STAR-CD in Plymouth Michigan recently. Work is proceeding on obtaining more results from the simulations that are being executed. Some of these runs are taking 15 hrs of CPU time to complete. We are looking at speeding up the process by using more parallel processing on the new machine at the SuperComputing Center.