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## Modeling Corrosion in Oxygen Controlled LBE Systems with Coupling of Chemical Kinetics and Hydrodynamics: Quarterly Progress Report 12/1/02- 2/28/03

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# **N bModeling Corrosion in Oxygen Controlled LBE Systems with Coupling of Chemical Kinetics and Hydrodynamics**

## **Quarterly Progress Report 12/1/02- 2/28/03**

UNLV-AAA University Participation Program

Principle Investigator: Samir Moujaes  
Co-Principle 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**

Principle Investigator:

- Dr. Samir Moujaes (Mechanical Engineering)

Co-Principle Investigator:

- Dr. Yitung Chen (Mechanical Engineering)

Students:

- Mr. Chao Wu, M.S. Graduate Student, (Mechanical Engineering)
- Mr. Kanthi Dasika , M.S. Graduate Student, (Mechanical Engineering)

National Laboratory Collaborator:

- Dr. Ning Li, Project Leader, Lead-Bismuth Material Test Loop, LANL

## **Management Progress**

Budget Issues:

- Monthly research expenditures are reasonable and on schedule

## **Management Problems**

Some questions that created initial problems as to what kinds of analyses need to be made for some of the deliverables. The team is working on it.

## **Technical Progress**

### **Hydrodynamics:**

Concentration Flux profiles have been obtained for a straight pipe for both laminar and turbulent profiles to test as a prelude to the complete chemical kinetics analysis for corrosion on the inside walls of the LBE loop. The results of the wall flux values are summarized in figures 1 and 2 respectively.

The ordinate of both of these graphs shows the magnitude and the sign of the flux. Some of the values are positive and some are negative indicating corrosion flux and precipitation flux respectively at different axial pipe locations. The abscissa is the nodal location over the length of the pipe. The length of the pipe is about 5.0 m. The k-ε turbulent modeling is used for the turbulent case. A distinct difference is seen in the “sharpness” of the variation of the different values of the flux at different axial locations. Although the main peak and valley in both graphs are predicted at the same locations axially there is a marked difference in the values. It is expected that the turbulent flow will show somewhat more rounded peaks and values as opposed to laminar flow and that could be partially explained due to the fact that more convection is taking place in the core flow of the turbulent as opposed to laminar flow. In these runs the values of the wall concentrations are calculated as prescribed functions of temperature on the wall.

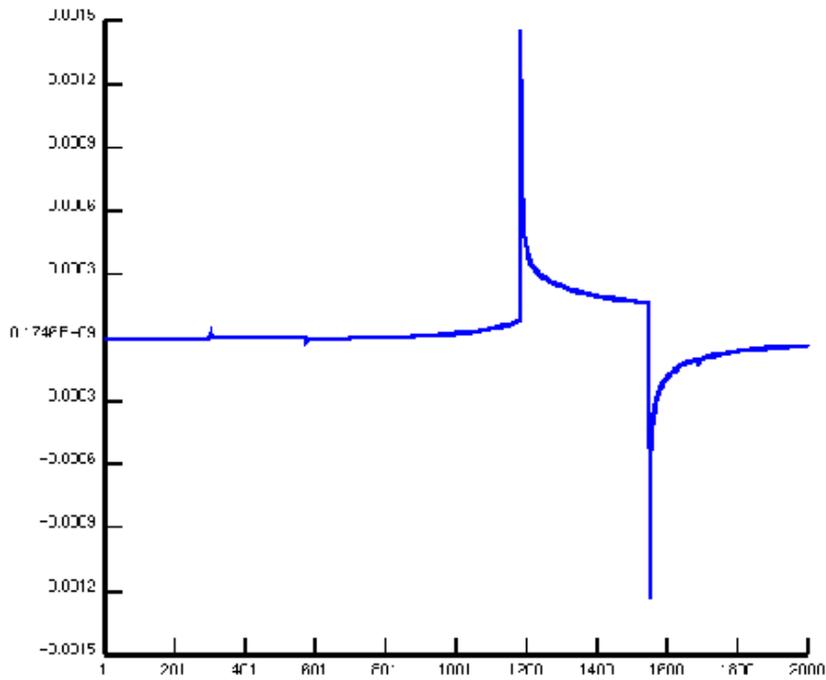


Figure1. Concentration Wall Flux for A straight pipe-Laminar flow(Re=2,000)

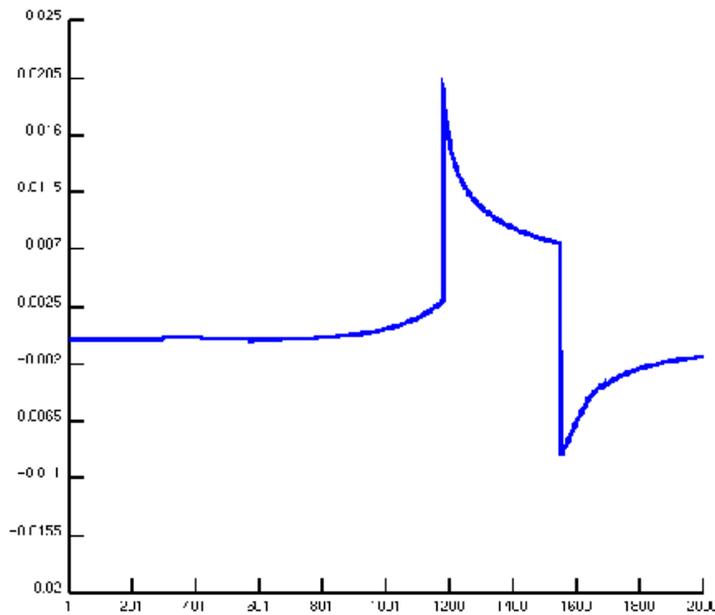


Figure 2. Concentration Wall Flux variation-Straight pipe-Turbulent Flow(Re=200,000)

The profile of imposed axial wall temperatures and concentrations are shown in Figure 3.

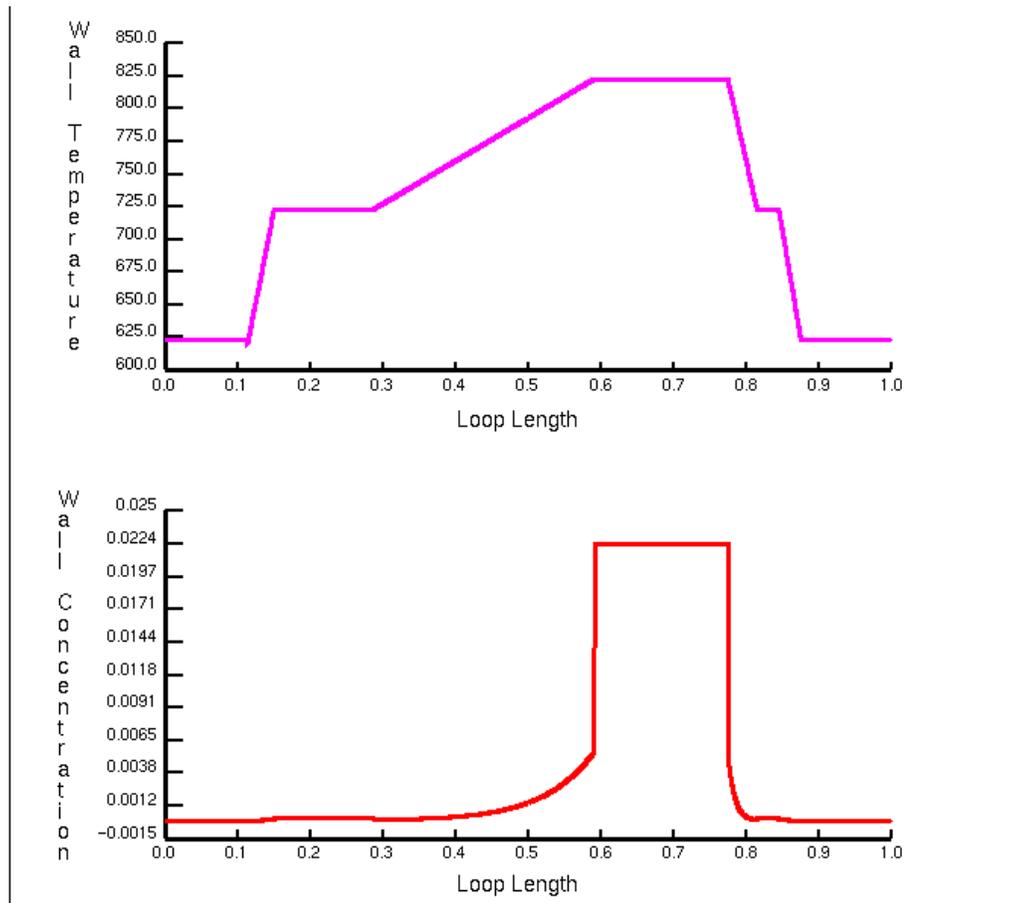


Figure 3. Plots of Imposed Wall Temperatures and Concentrations (SC=36.0,  $D=10^{-8}$  m<sup>2</sup>/s)

The selected Schmidt number for both runs is 36.0 and the selected diffusivity coefficient is  $D=10^{-8}$  m<sup>2</sup>/s. The Schmidt number is defined as the ratio of the molecular kinetic viscosity to the mass diffusivity  $D$ . This temperature profile was provided from the expected temperature profiles to be found in the different locations of the Delta Loop at LANL. Again all our calculations are chosen after careful discussions with the research mentors at LANL Dr. Ning Li and Dr. Jinsuo Zhang.

**Chemical kinetics of corrosions:**

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 reasonably 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. The report from LANL points out that the analytical solution to this problem proves that corrosion rate  $q$  is inversely proportional to  $x^{1/3}$ , where  $x$  is the coordinate in the length direction. By definition,

$$q = -D \frac{\partial C}{\partial x} \approx -D \frac{\Delta C}{\Delta x}.$$

Obviously,  $q$  is proportional to  $\Delta C$  in this expression. As a result,

we can expect that  $\Delta C$  is inversely proportional to  $x^{1/3}$ . Figure 1 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.

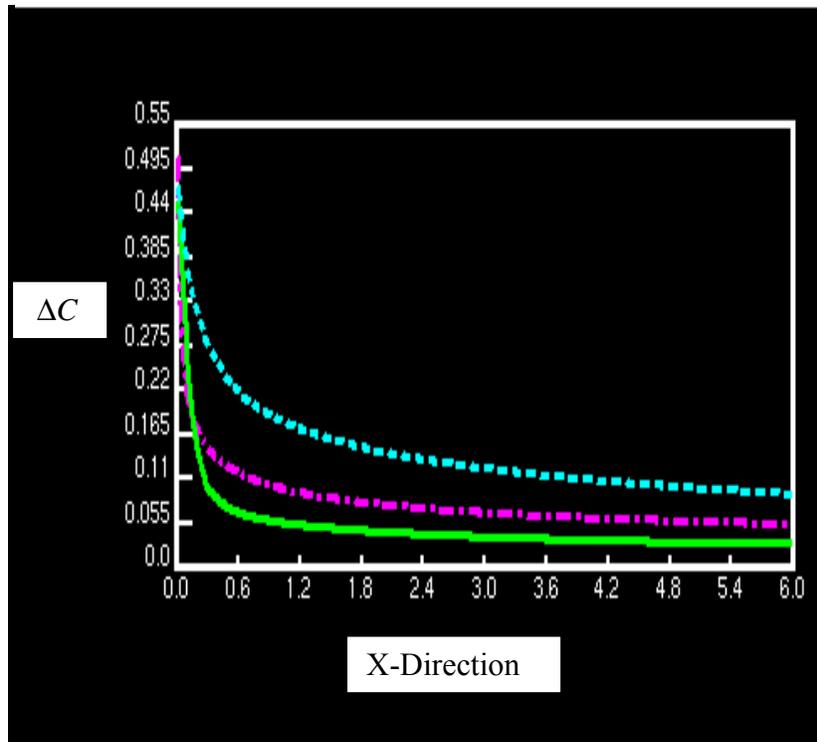


Figure 4. Concentration gradient versus x-coordinate

Another 2-D test case was set up with sudden expansion geometry as shown in Figure 2. 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 5. 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 3.

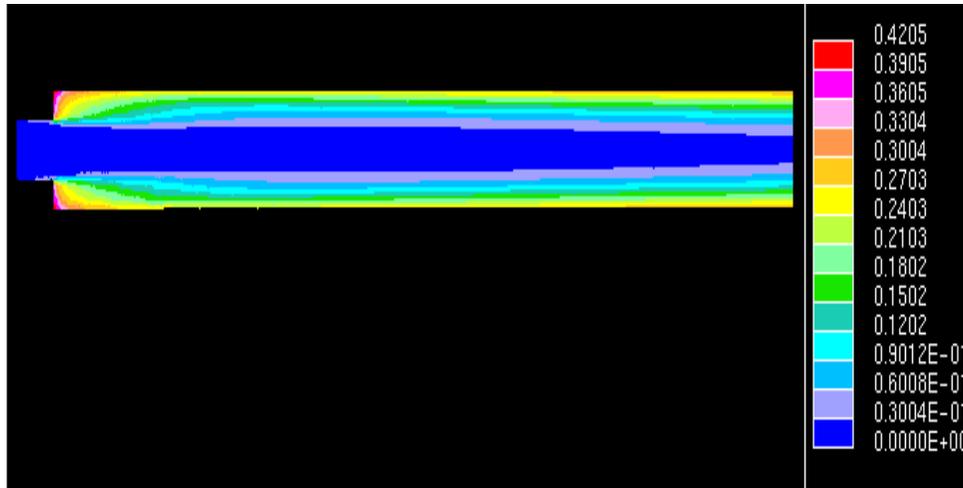


Figure 6. Concentration contours for Re=40

Interesting phenomenon is observed, when Re is equal to 1,000. The concentration difference is shown in Figure 4. Each peak value of concentration on the curve occurs at the location where the separation point exists. Contour of axis component (Z component) of velocity is presented in Figure 5. From the contour, fluctuation of flow in bulk area can be seen. This fluctuation gives rise to the production, propagation and disappearance of vortices 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.*[7] the curve demonstrates a good consistency with experimental results. Since the constantly changing flow condition, data should be averaged over several discrete iterations in order to get reasonable results over a long-term period. It also indicates that detailed research on the geometry effects is important, because of the complicated flow conditions that result from the sudden expansion geometry.

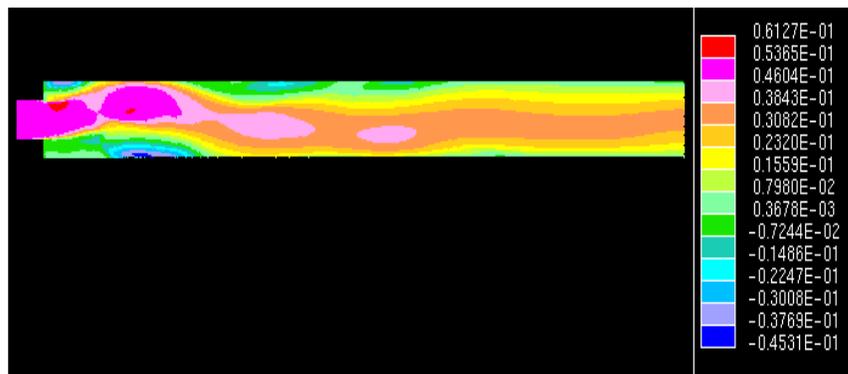


Figure 7. Contour of Axis Component of Velocity for Re=1,000

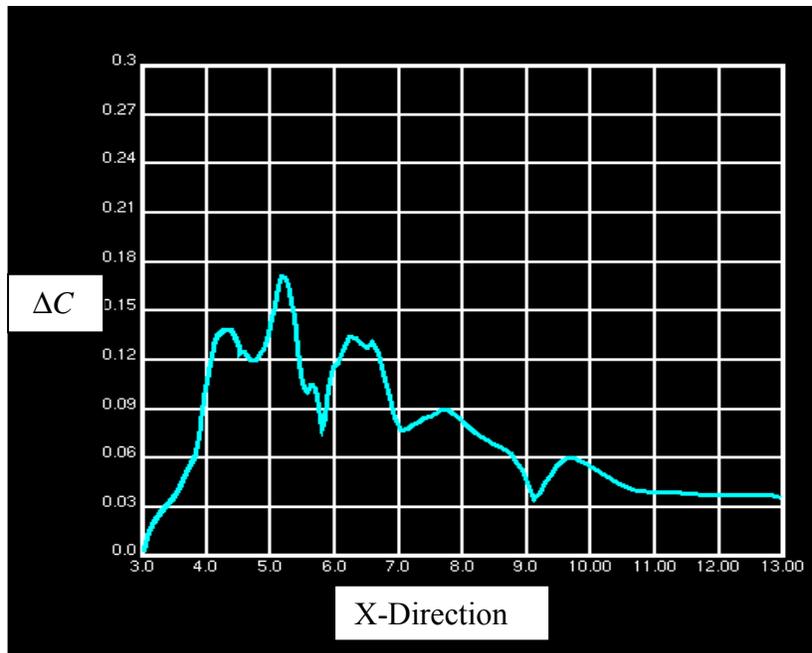


Figure 8. Concentration gradient of expanded area for Re=1000

Additionally, a 3-D gradual expanding pipe model has been built. 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 unequal along the axis direction, namely Z-direction. As a result, the corrosion rate is proportional to  $\frac{\Delta C}{\Delta x}$ , where  $x$  is the direction of radius, instead of  $\Delta C$  only. A run was performed at Reynolds Number equal to 10,000. Figure 6 shows the decrease of  $\frac{\Delta C}{\Delta x}$  along the Z-direction. Compared to the sudden expansion, gradual expansion has relatively simple and straightforward corrosion phenomena. It proves again that corrosion rate is closely related to the flow condition, such as vortexes and separation. For those geometries, which may yield complex distribution of velocity, the research is extremely needed in analyzing the relation between geometry design and corrosion rate.

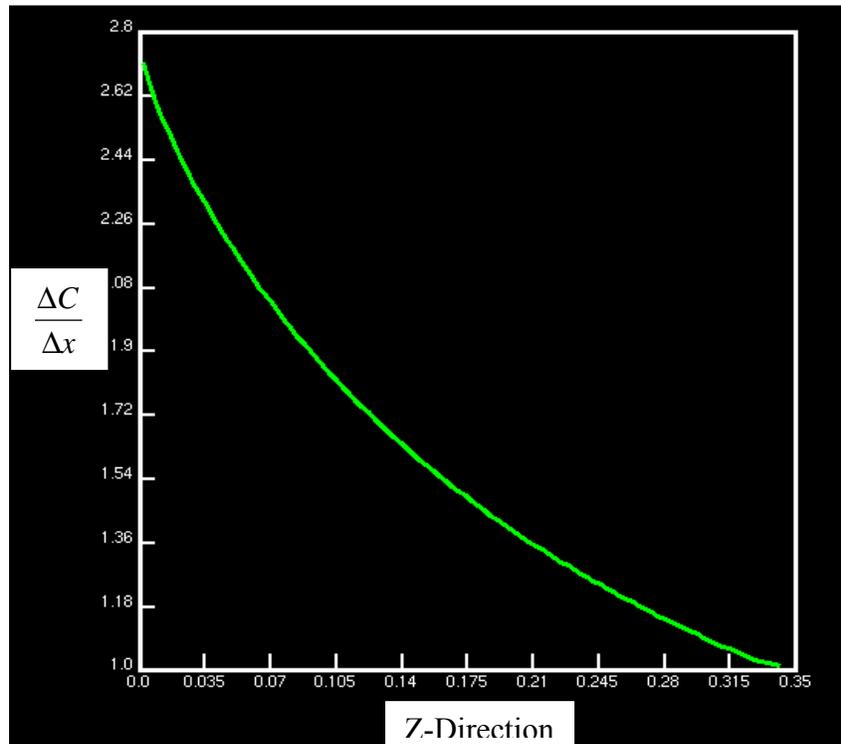


Figure 9. Concentration gradient for the linear expanding geometry

From the study on test cases, it proves that the outcome from STAR-CD is correct and that numerical modeling is applicable to the research in this problem.

In the near future, the problem will be developed into 3-D. The different value of  $\frac{D}{d}$  will be considered as a factor, which may affect the local corrosion rate. Combined with various Reynolds Numbers, temperature and concentration boundary conditions, certain value of  $\frac{D}{d}$  will be able to optimize the design of the Delta Loop by reducing corrosion rate to the minimum.

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