

Implementation of Strong Acid and CO₂ Corrosion in CFD Software

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ABSTRACT

To properly understand the necessary steps in implementing corrosion modeling into existing CFD software, it is necessary to verify the accuracy of the corrosion predictions made by the software. To do this, simulations are created that replicate experimental work performed in well understood geometries. The corrosion models are implemented in these simulations, and the resulting corrosion rates, as well as hydrodynamic and mass transfer characterizations, are compared to results from the experimental work. Presented herein is work investigating corrosion phenomena in a thin channel flow cell apparatus, as well as single phase straight pipe flow. In both geometries hydrodynamics, mass transfer, and electrochemistry have been simulated at a variety of conditions; the accuracy of the results were confirmed through comparison with experimental data and well tested correlations. Both geometries showed a high degree of agreement between the simulations and the experimental work, indicating that the methodology is viable to be used in other geometries.

Key words: Corrosion mechanisms, Corrosion rate, Oil and gas, Carbon dioxide, CFD

INTRODUCTION

In the oil and gas industry, use of models for prediction of corrosion to develop appropriate mitigation strategies is widespread. There are various models available for this purpose, one commonly used is MULTICORP^{TM†}, which is a mechanistic corrosion prediction model. This is a 1-dimensional mechanistic model meaning it works by predicting corrosion at points along the length of a pipeline, making its predictions based on the actual corrosion mechanisms taking place as opposed to using empirical or semi-empirical models. 1-dimensional models rely on dimensionless number mass transfer correlations

[†] Trade Name

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in order to predict pipe flow conditions which are used to make the corrosion predictions. These correlations are effective in laminar and turbulent, single phase, straight pipe flow.

Using a 1-dimensional system gives the advantage of having significantly fewer points at which calculations must be performed. It also avoids performing complex calculations to account for the flow values, instead replacing them with dimensionless number correlations. The downside to this approach is that in systems where these correlations do not currently exist, such as for many multiphase flow systems or when a more complex geometry is present (bends, valves, fittings, obstacles), these models cannot accurately predict corrosion.

To model corrosion in such systems, CFD (computational fluid dynamics) software can be implemented along with the appropriate understanding of the corrosion mechanisms. CFD software functions by taking a 2D or 3D geometry and breaking it down into a system of points at which flow variables and other system variables like temperature, pressure, species concentration will be calculated; this process is also known as discretization or meshing. Once the mesh has been created for the system the software then solves a number of equations simultaneously at each point inside the system using numerical methods. The equations solved will partly depend on what system variables are of interest to the user, those that must always be solved are the continuity equation, and the Navier-Stokes equation which are shown below.

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_i)}{\partial x_i} = 0 \quad (1)$$

$$\frac{\partial \rho u_j}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_j u_i) = \rho f_j - \frac{\partial P}{\partial x_j} + \frac{\partial}{\partial x_i} \left(\mu \frac{\partial u_j}{\partial x_i} \right) + \frac{1}{3} \frac{\partial}{\partial x_j} \left(\mu \frac{\partial u_i}{\partial x_i} \right) \quad (2)$$

In the case of a corrosion calculation the only thing left out in the above equations are the concentrations of species which are relevant to the corrosion reactions. These can be solved by including the species conservation equation which is shown below.

$$\frac{\partial}{\partial t}(m^s) + \frac{\partial}{\partial x_i}(m^s u_i) = \frac{\partial}{\partial x_i} \left(D^s \frac{\partial m^s}{\partial x_i} \right) + R^s \quad (3)$$

From this point the local concentration of species at any point inside the system can be calculated and utilized in the calculation of the corrosion rate. To calculate the corrosion rate itself, another equation must be solved, this time at the wall where the corrosion occurs. For this the Butler-Volmer equation, which can be seen below, is implemented as what is known as a boundary condition. Boundary conditions play a big role in CFD simulations as these are the ways in which information is transferred into the system, such as specifying a particular velocity or flow rate at an inlet, or a pressure at an outlet.

$$i_F = i_0 \left(\frac{c}{c_{ref}} \right)^n \left[\exp \left(\frac{2.303 \eta}{\beta_a} \right) - \exp \left(\frac{2.303 \eta}{\beta_c} \right) \right] \quad (4)$$

This implementation allows for the calculation by the CFD software of the current density of the electrochemical corrosion reaction, which can then be transformed into a corrosion rate.

EXPERIMENTAL PROCEDURE

For the purposes of this project, the current focus is the verification of the hydrodynamics, mass transfer, and electrochemical and chemical reactions in two experimental geometries, the thin channel flow cell (TCFC), and straight pipe flow. In order to verify these parameters in these experimental systems, first literature sources are found which provide either experimental data in these systems, or

correlations which can be used to calculate these parameters based on the conditions tested. When direct comparison with experimental data is to be performed, the experimental systems are designed carefully replicating the significant physical dimensions of the experimental systems used in the literature source. The parameters of the simulation are input to exactly recreate the conditions seen in the experiments being referenced. The relevant simulation results are then compared with the data present in the literature to determine the accuracy of the simulated results. If a correlation is being used for verification, the experimental system is created to satisfy any requirements that the correlation might have to ensure its validity in the simulated system. A range of conditions may then be simulated by changing the simulation parameters such as flow rate and the trend of relevant parameters can be compared against the trend predicted by the correlation. The CFD software used for all simulations is Ansys FluentTM§.

RESULTS

Thin channel flow Cell (TCFC)

The thin channel flow cell (TCFC) is a piece of experimental equipment commonly used to perform experiments involving high shear stress conditions. The piece of equipment that was used to gather the experimental data which will be later be used for comparison to simulations had a height of 3.57mm, and a length of 3m, although only 200mm was simulated in order to limit the size of the geometry and allow for greater mesh refinement. The simulations were 2-dimensional based on the assumption that the flow across the width of the TCFC would be constant. The mesh generated for the simulations can be seen below in Figure 1.



Figure 1: TCFC mesh.

Inflation was used near the walls of the TCFC to ensure that multiple control volumes inside the mass transfer boundary layer. The inflation utilized a specified first layer thickness and growth rate to gradually increase in size until it matched the bulk mesh size. The refined mesh section can be seen below in Figure 2.

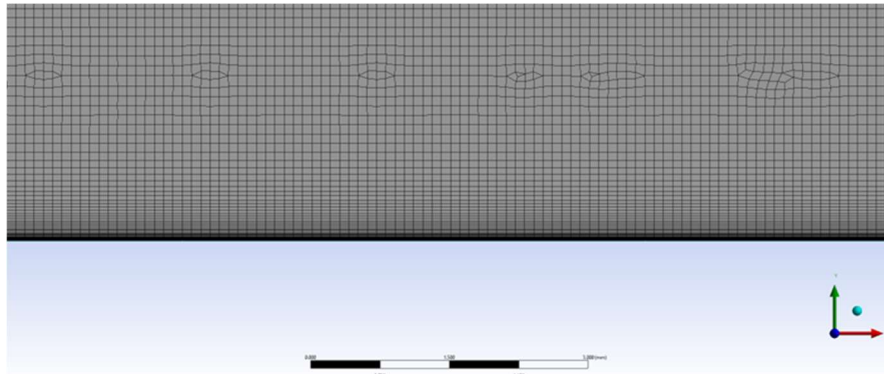


Figure 2: Inflated portion of mesh.

The inlet had a specified value of velocity that was uniform across the boundary, after a certain distance the flow will fully develop into a more realistic flow profile. All data discussed will be taken from regions downstream from the fully developed flow profile. The stable velocity profile can be seen below in Figure 3.

§ Trade Name

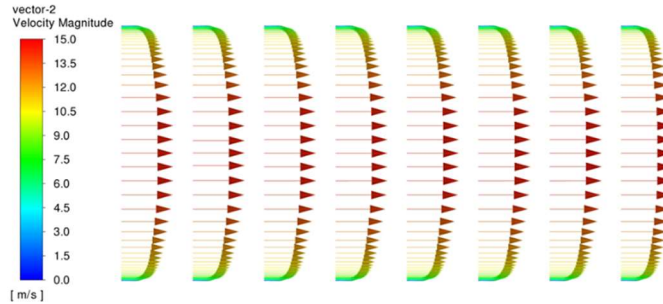


Figure 3: Fully developed flow profile for inlet velocity of 12.9 m/s.

As can be seen in Figure 3 the peak velocity in the flow profile is higher than the inlet velocity, this is due to a combination of the no-slip boundary condition used at the walls and the incompressible nature of the fluid.

Various parameters were checked to ensure the accuracy of the simulations, the first of which was the hydrodynamic characteristics of the flow. Experiments were carried out where the wall shear stress was monitored at various flow velocities, which lead to the development of the equations shown below.¹

$$\tau = \frac{1}{2} \rho C_f V^2 \quad (5)$$

In this equation τ is the wall shear stress in Pa, ρ is the fluid density in kg/m^3 , C_f is the fanning friction factor, and V is the mean flow velocity in m/s. The fanning friction factor for channel flow can be calculated using the Patel correlation.²

$$C_f = 0.0376 Re^{-1/6} \quad (6)$$

A comparison of the calculated wall shear stress and shear stress obtained from CFD simulations at a variety of flow velocities can be seen below in Figure 4.

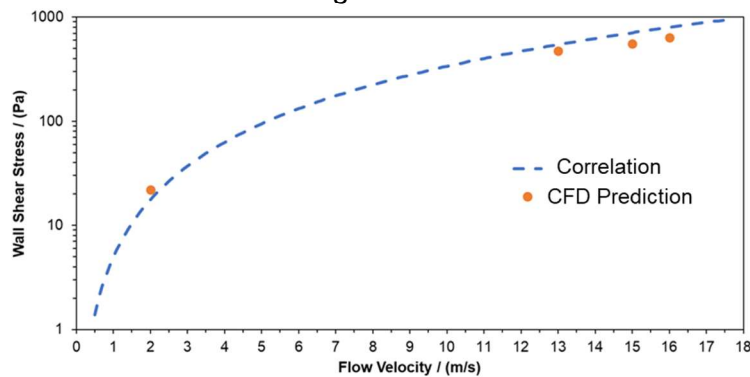


Figure 4: Comparison of theoretical and simulated wall shear stress in TCFC.

Given the good agreement between the CFD simulations and the correlation, it is determined that the CFD simulations are hydrodynamically accurate in this geometry. The next step is to confirm the ability of the CFD software to simulate mass transfer of species in this geometry. Potentiodynamic sweep data was collected in a TCFC and can be seen below in Figure 5.³

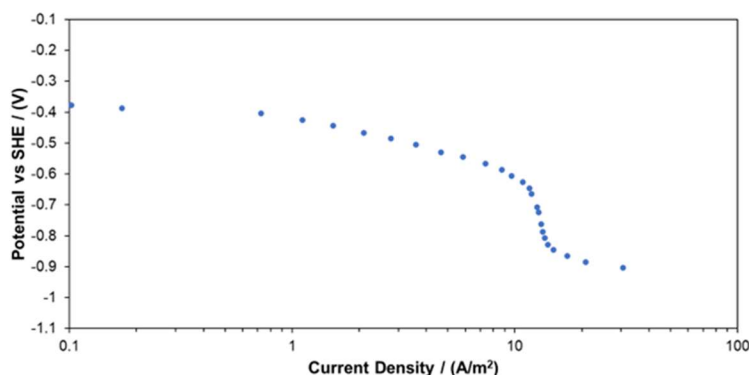


Figure 5: TCFC experimental data during cathodic potentiodynamic sweep at pH 4, V=12.9 m/s, T=30°C.³

From the experimental data the mass transfer limited current is seen to be 13.4 A/m², and from this information the mass transfer boundary layer can be calculated using the following equation.

$$\frac{D_{ab}nFC_b}{i_{lim}} = \delta_m \quad (7)$$

Where D_{ab} is the diffusivity of H^+ in water, n is the electrical charge of H^+ , F is the Faraday constant, C_b is the molar concentration of H^+ in the bulk solution, i_{lim} is the mass transfer limited current density in A/m², and δ_m is the mass transfer boundary layer thickness in meters. From this calculation the mass transfer boundary layer thickness is found to be 7 μ m. A subsequent CFD simulation of the same conditions where a portion of the TCFC wall is designated as having a concentration of H^+ of 0 M. This represents the conditions in a mass transfer limited scenario where all the H^+ that reaches the surface is consumed, as would happen in a cathodic potentiodynamic sweep. The species concentration profile from the CFD simulation is shown below in Figure 6.

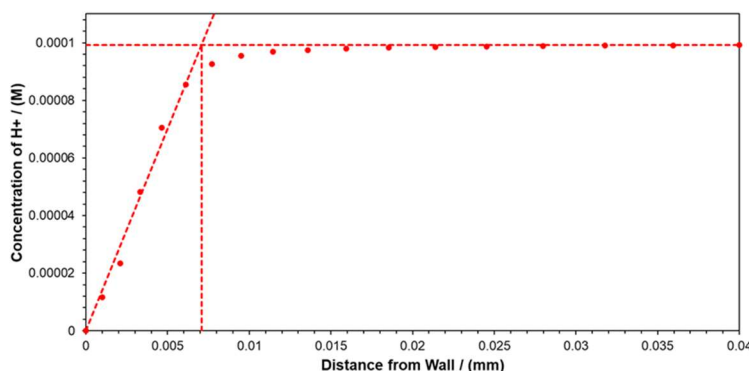


Figure 6: Species concentration profile from CFD simulation of the TCFC and the graphically obtained mass transfer boundary layer thickness.

From the simulated concentration profile and observing the intersection of the two lines shown in Figure 6, the simulated thickness of the mass transfer boundary layer is 7 μ m, exactly matching the calculation made based on the experimental data.

The next step was to replace the specified species concentration for H^+ used in the previous simulation with the actual electrochemical reaction that would be occurring and the associated Butler-Volmer parameters.

