

Validation of Modern CFD Software in Various Experimental and Complex Flow Geometries

Adam Cutright, Srdjan Nesic, Bruce Brown, David Young
Institute for Corrosion & Multiphase Technology,
Department of Chemical and Biomolecular Engineering,
Ohio University, Athens, OH 45701, USA

Muhammad Sami
Ansys
15915 Katy Fwy #550
Houston, TX, 77094
United States

ABSTRACT

Models are widely used to predict corrosion in pipelines to assist in the development and implementation of appropriate mitigation strategies. These models often rely on dimensionless number mass transfer correlations to account for the fluid flow and associated mass transfer in pipelines. They exist for a limited number of geometries and conditions, mainly single phase, straight pipe flow. By implementing corrosion models into CFD software, the goal is to bypass the necessity of the mass transfer correlations and allow for corrosion predictions in a wider range of geometries. The key issues with the utilization of CFD software for corrosion prediction in complex geometries are the method of implementation and confidence in the results obtained. Using simulations that replicate systems where experimental data has also been obtained allows for direct comparison of the experimental data with predictions obtained from the simulations. The geometries investigated in this paper show a high degree of agreement between the simulations and the experimental work and correlations, indicating that the methodology is viable to be used in other geometries. The overall goal is to develop a procedure for implementing CO₂ corrosion into CFD software and demonstrate the accuracy of the results obtained.

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. These models often rely on dimensionless number mass transfer correlations to predict pipe flow conditions which are used to make corrosion predictions. These correlations are effective in laminar and turbulent, single phase, straight pipe flow. 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 parameters and other system variables like temperature, pressure, and 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. The Navier-Stokes¹ equation is a set of 3 equations which describes the momentum transfer in a fluid system.

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

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

In the above equations ρ is the density, t is the time, u is the velocity, x is the position, f_j is the gravitational force, P is the pressure, and μ is the viscosity.

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 determined by including the species conservation shown in Equation 3 where m is the mass of a species, D is the diffusivity of the species, and R^s is the generation of the species from chemical reactions.

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

Using these equations, 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 metal surface where the corrosion occurs. For this, the Butler-Volmer equation², which can be seen below, is implemented. The Butler-Volmer equation relates the current associated with corrosion, i , with the anodic and cathodic Tafel slopes, β_a and β_c , as well as the potential in the system, η , and concentration of relevant

species, c . This equation is implemented as a boundary condition. Boundary conditions play a governing 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 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

Equipment

- Ansys Fluent* software¹

Procedure

For the purposes of this project, the current focus is the verification of hydrodynamics, mass transfer, and electrochemical and chemical reactions in different experimental systems. In order to verify these parameters in these experimental systems, first literature sources are found which provide matching experimental data. When direct comparison with experimental data is to be performed, the experimental systems are designed in the CFD software, 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.

RESULTS AND DISCUSSION

Thin Channel Flow Cell

The first experimental system simulated is the thin channel flow cell (TCFC), a commonly used experimental system³ in our laboratory designed to provide high shear stress in a small volume. The experimental geometry modeled here has a height of 3.57mm, and the length of the geometry was modeled as 200mm to limit the size of the mesh. The mesh can be seen below in Figure 1.



Figure 1. TCFC mesh where flow moves from left to right.

* Trade name

The inlet had a specified velocity uniform across the boundary, which is unrealistic, however, after a certain distance the flow develops into a more realistic flow profile, and all data shown here is taken after the flow has fully developed. The fully developed velocity profile can be seen below in Figure 2.

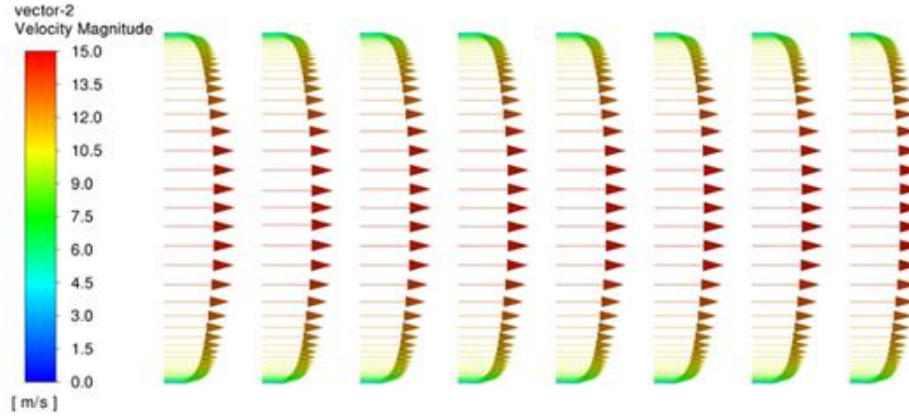


Figure 2. Fully developed flow profile in TCFC

In order to determine the hydrodynamic accuracy of the simulation, the wall shear stress was measured and compared with a model that had itself been developed based on experimental data, which is shown below.

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

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 where Re is the bulk Reynolds number.

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

The simulated wall shear stress compared to the theoretical wall shear stress can be seen below in Figure 3.

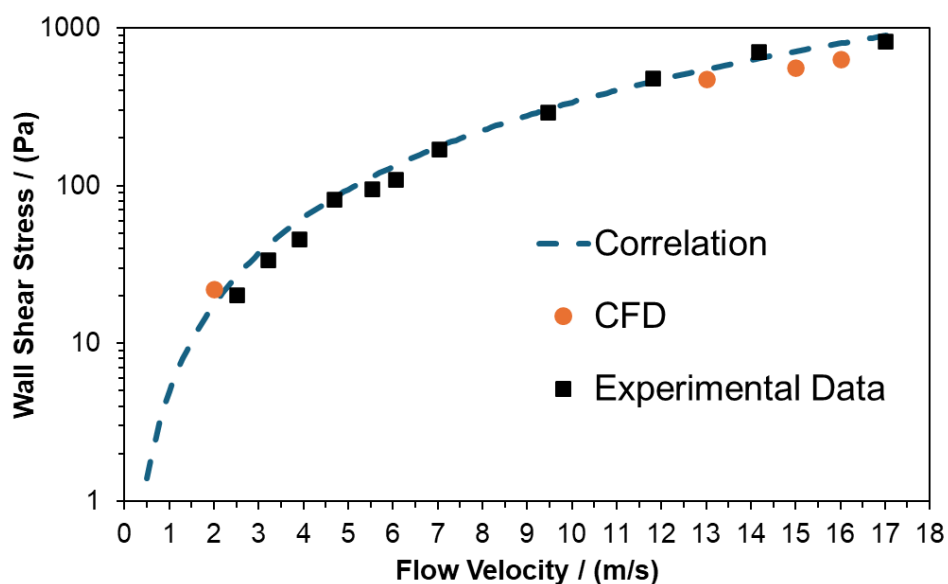


Figure 3. Comparison of wall shear stress at various flow velocities

These results indicate that the CFD simulations are able to accurately predict the wall shear stress over a wide range of flow velocities. The next step was to verify the ability of the CFD software to accurately predict mass transfer in the near wall region, which is highly relevant to corrosion simulations. Using experimental data, the mass transfer limiting current was determined to be 13.1 A/m^2 which corresponds to a mass transfer boundary layer thickness of $6.8 \text{ }\mu\text{m}$. A simulation was created where a portion of the wall in the TCFC was set to have a fixed concentration of H^+ ions of 0 M , which represents a mass transfer limited process. From this simulation a concentration profile was generated which can be seen below in Figure 4.

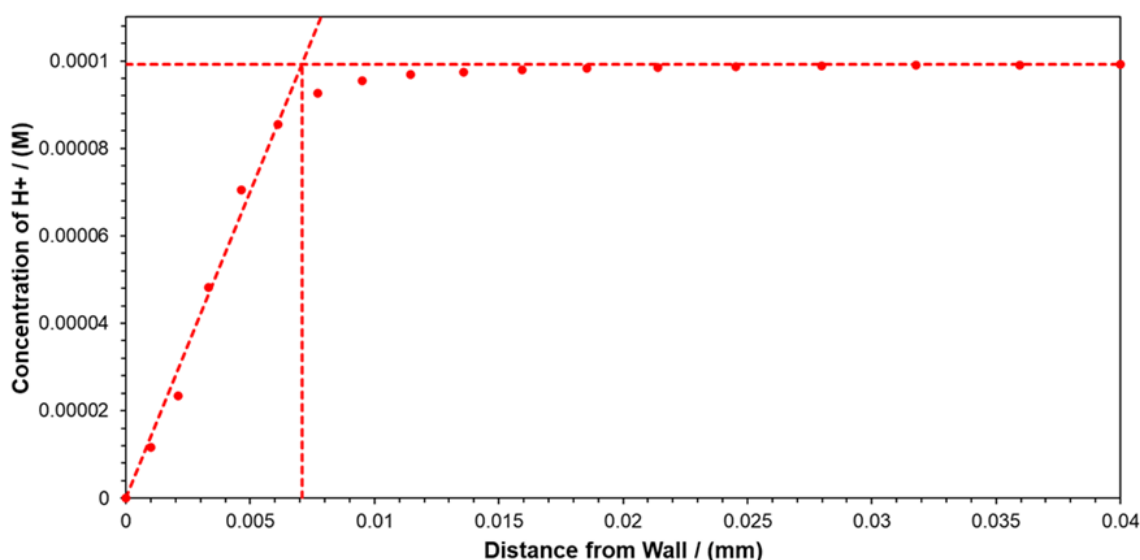


Figure 4. Concentration profile and marking indicating mass transfer boundary layer thickness in the TCFC geometry

Based on this concentration profile, and from the intersection of the lines shown in Figure 4, the mass transfer boundary layer is 7 μm , very closely agreeing with the mass transfer boundary layer thickness found from the experimental data.

The next step forward was to simulate corrosion in the experimental geometry by creating an active surface which allowed for the anodic and cathodic electrochemical reactions associated with corrosion phenomena. The specific values used can be seen below in

Table 1.

Table 1. Reaction parameters for electrochemical reactions in CFD software

	Hydrogen Reduction	Iron Oxidation
Input Variable	Value	
Exchange current density (A/m ²)	0.03	0.005
Species concentration (M)	0.0001, 0.00001	1
Reference mass fraction H ⁺	1E-07	0.001
Reaction order	0.5	0
β_a	0.12	0.04
β_c	0.12	0.04
Equilibrium potential (V)	-0.24	-0.488

Using these parameters, strong acid corrosion was simulated at two different pH values and compared against theoretical calculations of the corrosion rate in the same conditions.

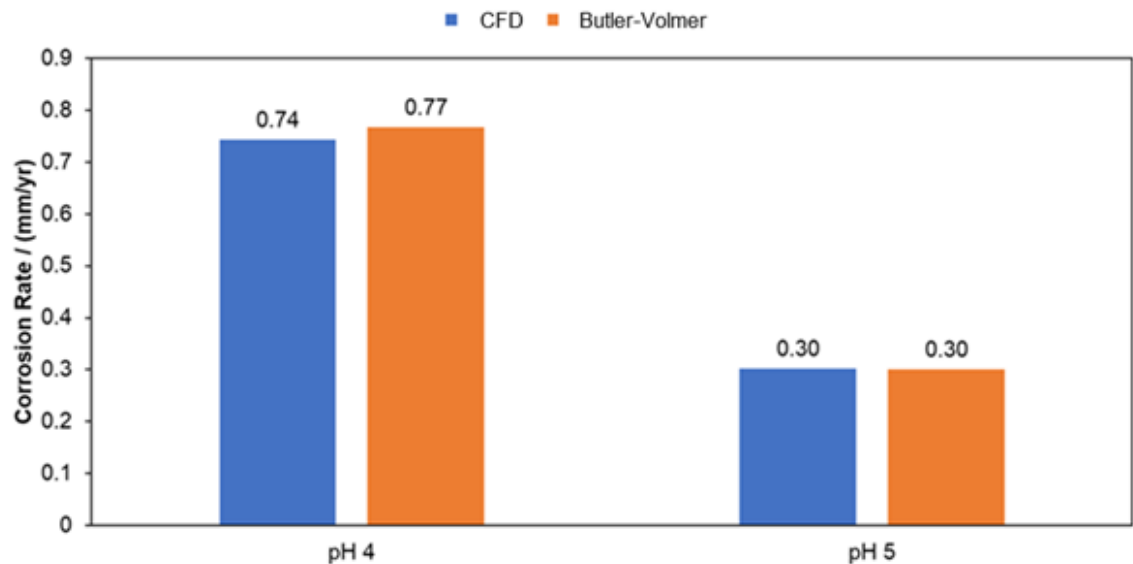


Figure 5. Comparison of strong acid corrosion rates in TCFC geometry at different pH values

As can be seen in Figure 5, the results between the simulations and theoretical calculations match closely indicating the ability of the CFD simulations to predict the corrosion rates under

these conditions. Following this, it is appropriate to move on to CO₂ corrosion which involves additional bulk chemical reactions which are shown below.



To include these chemical reactions in the CFD simulations the forward and backward rate constants must be specified, the values used are shown below in Table 2.

Table 2. Chemical reaction constants related to CO₂ corrosion⁴

Reaction	Forward Rate Constant	Backward Rate Constant
CO₂ Hydration	0.0348 s ⁻¹	24.5 s ⁻¹
H₂CO₃ Dissociation	1.9x10 ⁷ s ⁻¹	4.7x10 ¹⁰ M ⁻¹ s ⁻¹
HCO₃⁻ Dissociation	181 s ⁻¹	3.67x10 ¹² M ⁻¹ s ⁻¹
H₂O Dissociation	0.00126 Ms ⁻¹	1.4x10 ¹¹ M ⁻¹ s ⁻¹

When these chemical reactions are included in the CFD simulations it is possible to simulate CO₂ corrosion and compare against experimental data taken under similar conditions. The results at two different pH values are shown below in Figure 6.

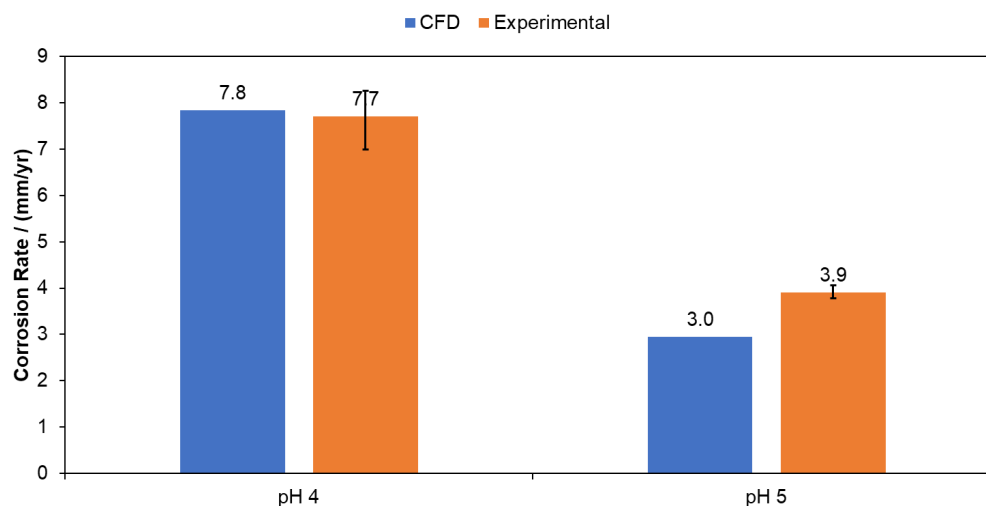


Figure 6. Comparison of CO₂ corrosion rates at various pH values³

Once again it can be seen that the simulated corrosion rates and the experimentally determined corrosion rates agree very well at two different values of pH, indicating that the CFD software is able to accurately predict corrosion rates under these flow conditions.

Submerged Impinging Jet

An impinging jet is defined as a system where a nozzle with a diameter **D** is placed perpendicular to a surface, known here as the impinged surface, at a fixed distance **H** away. To be a submerged impinging jet, the nozzle itself will be submerged in fluid along with the impinged surface. A general drawing of a submerged impinging jet can be seen below in Figure 7.

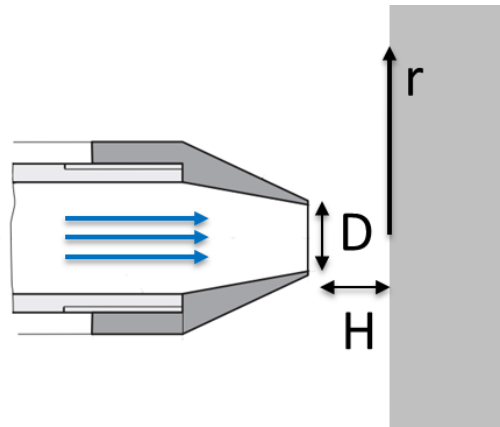


Figure 7. Diagram of a submerged impinging jet

To verify the hydrodynamics in the simulation, experimental values of the skin friction, which is related to the wall shear stress, were found. A comparison of the experimental⁵ and simulated skin friction values on the impinged surface are shown in Figure 8, along with the relevant values used in the simulation. The simulated and experimental values match very well, indicating the accuracy of the simulation results.

Table 3. Relevant simulation parameters for hydrodynamic submerged impinging jet validation

Parameter	Value
Velocity (m/s)	0.0472
Flowrate (ml/min)	500
Reynolds number (Re)	1360
Height (mm)	15.6
Diameter (mm)	7.8
H/D	2

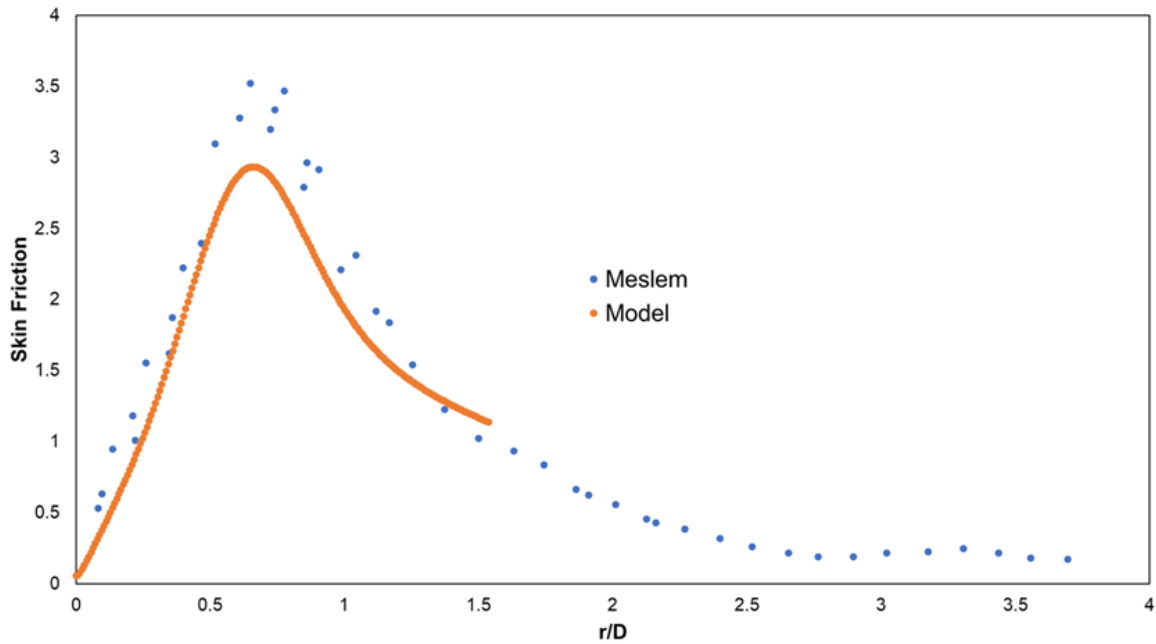


Figure 8. Comparison of experimental and simulated skin friction values along impinged surface⁵

The next step was to validate the mass transfer in the submerged impinging jet geometry. Once again experimental results were found in the literature⁶ that allowed for the calculation of the mass transfer boundary layer thickness which was determined to be 0.0133mm. A simulation was then performed where the impinged surface had a fixed concentration of H⁺ ions of 0 M as would be seen in a mass transfer limited scenario, the particular values used in the simulation are shown below in Table 4. From this simulation a concentration profile is generated, as shown in Figure 9.

Table 4. Relevant simulation parameters for mass transfer validation in submerged impinging jet

Parameter	Value
Diffusivity (m ² /s)	6.54 x 10 ⁻¹⁰
Flow velocity (m/s)	0.1262
Viscosity (kg/m.s)	1.06 x 10 ⁻³
Density (kg/m ³)	1042
Diameter (m)	0.00635
Height (m)	0.00635
Inlet concentration mass fraction	0.01

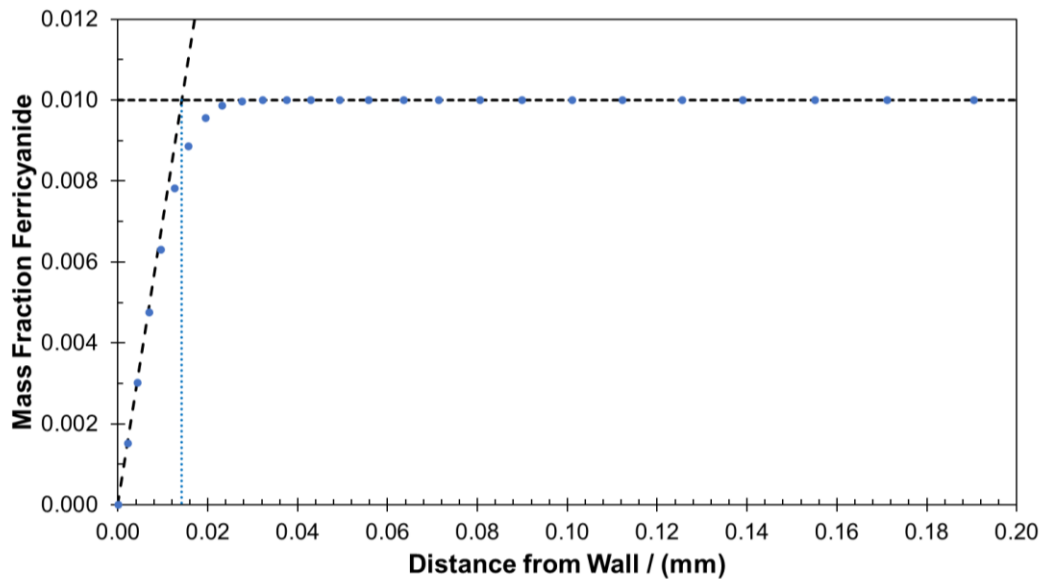


Figure 9. Concentration profile and marking indicating mass transfer boundary layer thickness in the submerged impinging jet geometry

Based on the intersection of these lines the mass transfer boundary layer can be found, in this case it is 0.014 mm, which is very close to the experimentally determined value of 0.0133 mm.

Sudden Pipe Expansion

The next experimental system simulated is the sudden pipe expansion, where a pipe undergoes an immediate increase in diameter. To verify the hydrodynamics of the simulations, data was taken from Khezziar.⁷ The experiments in this work to be compared against were axisymmetric and so a 2D axisymmetric simulation was used. The geometry and mesh along with relevant physical measurements can be seen below in Figure 10 and Figure 11.

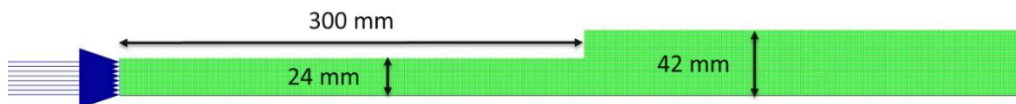


Figure 10. 2D mesh for sudden pipe expansion simulation.



Figure 11. Magnified view of sudden pipe expansion mesh.

To start modeling, only hydrodynamics were considered, where data from Khezzer that indicates the reattachment length after the expansion (see arrow in Figure 12) as a function of the upstream Reynolds number (prior to the expansion) was used.⁷ After the expansion it is expected that the flow will separate causing a recirculation zone, the bulk of the flow towards the center of the pipe will continue moving forward, while the flow near the edges will flow backwards; the reattachment length is the distance after which all of the flow moves forward, with the flow towards the edges that was moving backwards reattaching itself to the bulk flow.

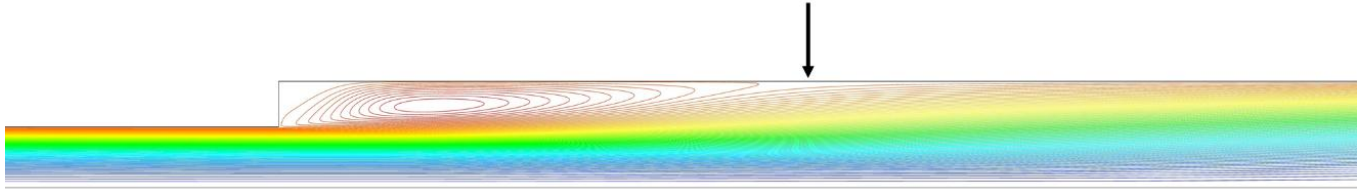


Figure 12. Contour of stream function indicating the general flow pattern with the location of reattachment indicated by arrow.

By using the geometry shown in Figure 10 and specifying the inlet velocity, flow profiles were generated at various distances following the expansion which is denoted by values of x/D where x is the distance after the expansion and D is the diameter of the pipe. These flow profiles are compared against experimental data⁷ which was taken using laser doppler anemometry (LDA). LDA is a non-intrusive technique which provides highly accurate flow information in experimental systems. The comparison of the simulated flow profiles and the experimentally obtained profiles is shown in Figure 13.

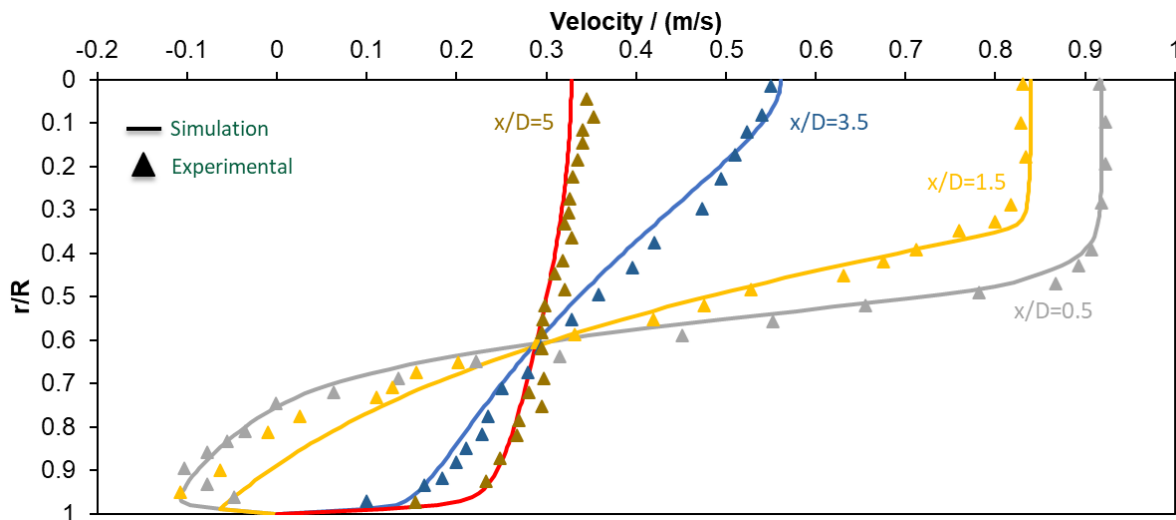


Figure 13. Velocity profile comparison at different values of x/D after the sudden expansion at $Re=40000$ ⁷

In this figure r is the particular value of the radius, while R is the total value of the radius. There is a fairly good agreement between the simulation and the LDA data. This indicates that the simulations are able to accurately simulate the flow in this sudden expansion geometry.

Experimental data was also obtained in a sudden constriction and expansion geometry where the mass transfer coefficient was determined, which is ideal for validating the mass transfer in the geometry. The geometry itself can be seen in Figure 14.

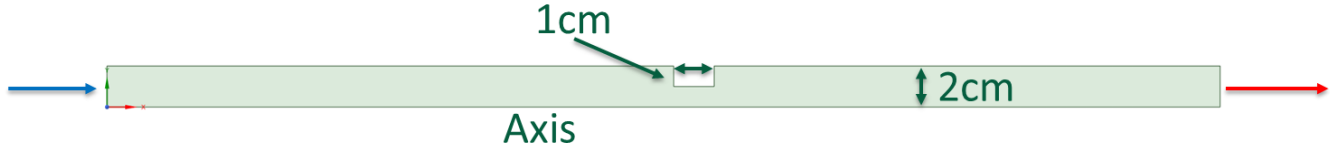


Figure 14. Sudden contraction and expansion geometry used for mass transfer validation simulations

In this geometry, the top wall immediately following the expansion is a reactive surface where all H^+ ions are consumed, making it a mass transfer limited system. From the subsequent concentration profiles the values of the mass transfer coefficient k were determined. A comparison of the experimentally obtained mass transfer coefficient values and those obtained from the simulations can be seen in Figure 15.

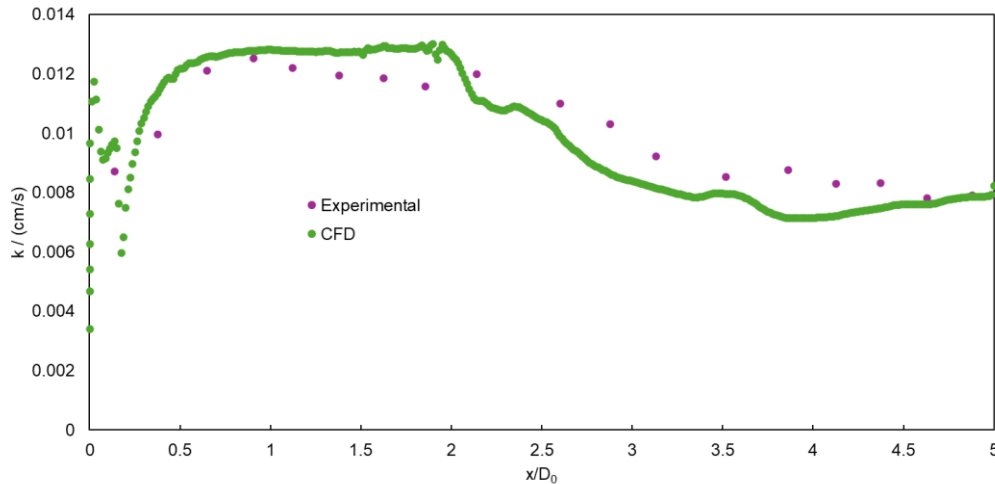


Figure 15. Comparison of simulated and experimental mass transfer coefficient values at $Re=84000$

Once again, there is a very good agreement between the simulation results, and the experimental data indicating that the simulation is able to accurately predict the mass transfer in this highly complex geometry.

2-Liter Glass Cell

Simulations were also performed for the 2-liter glass cell geometry which can be seen below in Figure 16, with the corresponding mesh shown in Figure 17. This geometry is commonly used in laboratory experiments, which consists of 5 sample holders evenly spaced around a central impeller which is intended to provide a uniform flow pattern across all 5 samples.

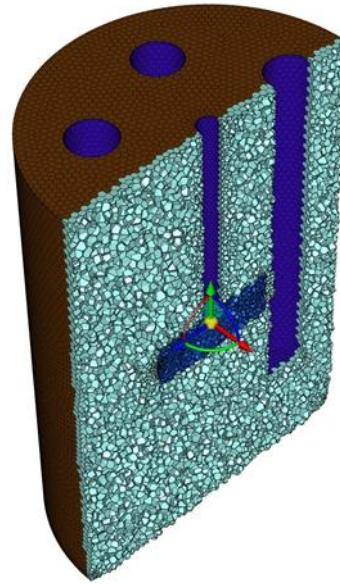
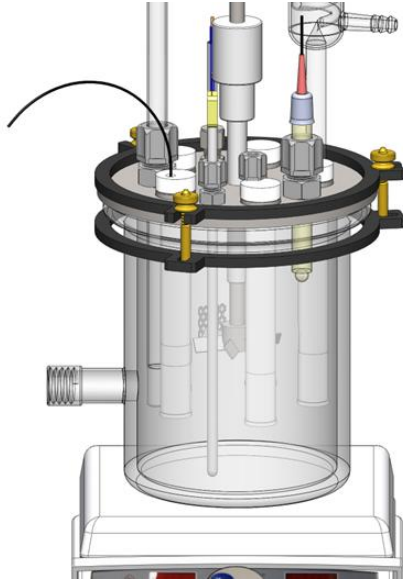


Figure 16. 2 Liter glass cell drawing. Figure 17. 2-Liter glass cell polyhedral mesh.

It can also be seen in Figure 17 that there are two different regions in the geometry, one region closely surrounding the impeller (dark rectangle in center of drawing), and the other consisting of the sample holders (dark blue) and the bulk fluid (light blue). The impeller motion was simulated in the system using the multiple reference frame (MRF) approach, where the entire center region of cells containing the impeller is rotated without having to remesh the system as the impeller moves. This region of cells can be assigned a specific rotational speed allowing for simulations of various impeller speeds. The velocity profile in the ZX plane that contains the impeller moving at 75 rpm can be seen below in Figure 18.

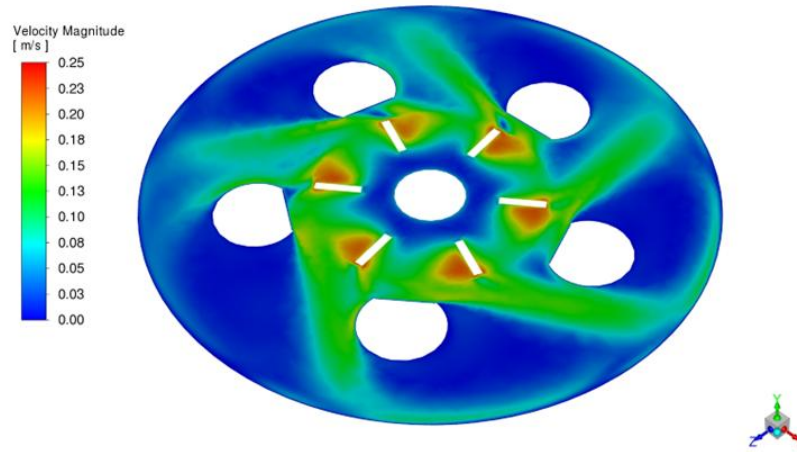


Figure 18. Velocity contour, 75 rpm.

This image shows how the flow is spreading from the impeller and impacting the 5 sample holders spaced evenly around it (colors indicate fluid velocity, so sample holders and metal impeller blades are white). Additionally, the flow appears to be very even across each sample, the velocity magnitude in contact with each sample holder appears to be around 0.13 m/s. It's also important that each sample have a uniform flow across the entirety of its surface, aiming to avoid any uneven corrosion across the samples themselves. In , the wall shear stress on one of the sample surfaces can be seen. While there are some areas around the edges which show lower wall shear stress values, the vast majority of the sample has a uniform wall shear stress of approximately 0.45 Pa.

With the hydrodynamics in the system well studied, the next step was to simulate CO₂ corrosion in the system. The parameters for the electrochemical and chemical reactions are specified as shown in Table 5 and Table 2, respectively. The simulation results were compared with experimental data taken from the corresponding experimental system. A comparison of the experimental data and the simulated corrosion rates can be seen in Figure 20.

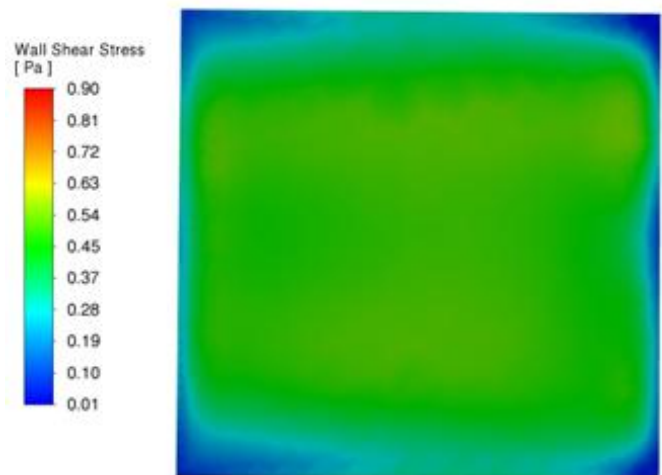


Figure 19. Wall shear stress on sample surface, 75 rpm.

Table 5. Electrochemical parameters for corrosion reactions.⁴

	Hydrogen ion reduction	Iron oxidation
i_0 : exchange current density (A/m^2)	0.03	1
C: species concentration (M)	1E-07	1
Reference mass fraction H^+	1E-07	0.001
n: reaction order	0.5	0
β_a : anodic Tafel slope (V)	0.12	0.04
β_c : anodic Tafel slope (V)	0.12	0.04
Equilibrium Potential (V)	-0.24	-0.488

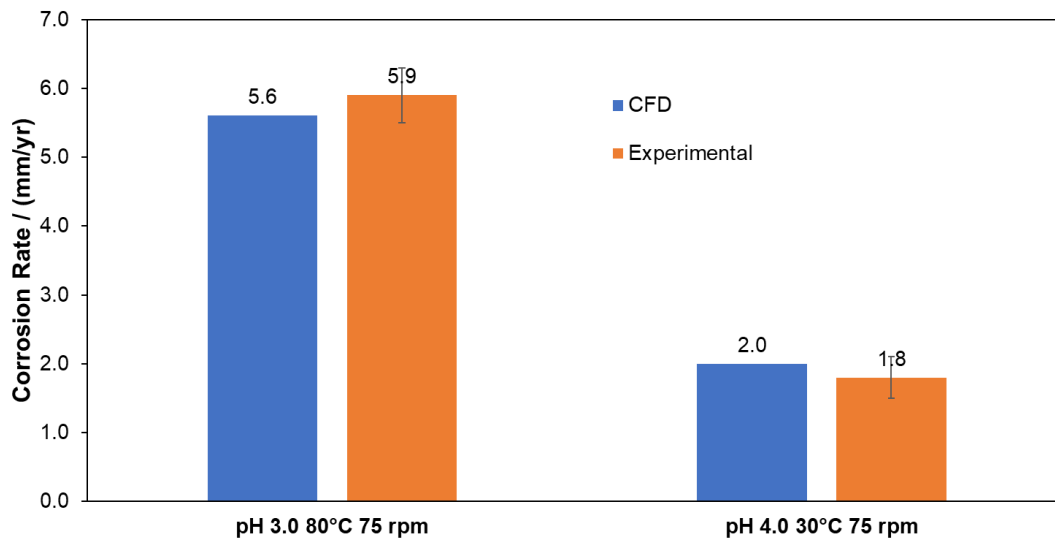
**Figure 20. Average corrosion rate at various pH and temperature vs. experimental results from the 2-liter glass cell with impeller.**

Figure 20 shows the simulated and experimental values of the corrosion rate are very close for both of the conditions shown, indicating a good ability to accurately simulate and predict the corrosion rates in this specified geometry.

CONCLUSIONS

In a wide range of geometries, some simple and some highly complex, similar techniques were used to validate hydrodynamics, mass transfer, and in some cases electrochemical and chemical reactions associated with corrosion. Across all geometries and with regard to all parameters, there was a high degree of agreement between the simulated results from the CFD analysis and the experimental data indicating that the methodology used is a robust and transferable way to model the flow, mass transfer, and reactions needed to simulate corrosion in these and other complex geometries.

REFERENCES

- (1) Bird, R. B. (Robert B., 1924- author. *Introductory Transport Phenomena*; Hoboken, NJ : Wiley, [2015] ©2015, 2015.
- (2) Dickinson, E. J. F.; Wain, A. J. The Butler-Volmer Equation in Electrochemical Theory: Origins, Value, and Practical Application. *Dr Richard Compton 65th Birthd. Spec. Issue* **2020**, 872, 114145. <https://doi.org/10.1016/j.jelechem.2020.114145>.
- (3) Kahyarian, A. Mechanism and Prediction of Mild Steel Corrosion in Aqueous Solutions Containing Carboxylic Acids, Carbon Dioxide, and Hydrogen Sulfide. Dissertation, Ohio University, Athens Ohio, 2018.
- (4) ICMT. *Freecorp 2.0 Theoretical Background*; 2018.
- (5) Meslem, A.; Sobolik, V.; Bode, F.; Sadjavi, K.; Zaouali, Y.; Nastase, I.; Croitoru, C. Flow Dynamics and Mass Transfer in Impinging Circular Jet at Low Reynolds Number. Comparison of Convergent and Orifice Nozzles. *Int. J. Heat Mass Transf.* **2013**, 67, 25–45. <https://doi.org/10.1016/j.ijheatmasstransfer.2013.07.096>.
- (6) Chin, D.-T.; Tsang, C.-H. Mass Transfer to an Impinging Jet Electrode. *J. Electrochem. Soc.* **1978**, 125 (9), 1461. <https://doi.org/10.1149/1.2131697>.
- (7) Khezzar, L.; Whitelaw, J. H.; Yianneskis, M. Round Sudden-Expansion Flows. *Proc. Inst. Mech. Eng. Part C J. Mech. Eng. Sci.* **1986**, 200 (6), 447–455. https://doi.org/10.1243/PIME_PROC_1986_200_154_02.