Advancing CFD Approaches for Jet-Stirred Reactors

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Efficient combustion is vital for optimizing fuel efficiency and minimizing emissions in industries like transportation, manufacturing, and energy production, with hydrocarbons accounting for 80% of global energy consumption. Despite the rise of alternative energy sources, hydrocarbons remain dominant due to their high energy density and established infrastructure. Jet-stirred reactors (JSRs), a subclass of continuous stirred tank reactors (CSTRs), are ideal for studying combustion kinetics of hydrocarbons by varying parameters such as pressure, temperature, and mixing conditions. JSRs are favored for their efficient mixing and ability to operate at dilute reaction conditions, making them crucial for investigating fuel-oxidizer interactions and reaction mechanisms. Computational modeling of flow conditions aids in determining optimal conditions for chemical and thermal homogeneity, as temperature gradients and incomplete mixing are potential sources of uncertainty. This research aimed on replicating and validating prior simulations at 1 atm conditions, focusing on the impact of temperature on mixing efficiency, thermal uniformity, and combustion kinetics. Using Computational Fluid Dynamics (CFD) with Ansys Fluent, this research focused on refining models by assessing how temperature variations influence flow patterns, turbulence, and thermal distribution. Special attention is given to the secondary mixing region, where chemical kinetics are key for reaction completion and product formation. The validated models will contribute to advancing CFD techniques, benefiting combustion research, chemical engineering, and aerospace applications.

I. Introduction

Research in combustion has experienced significant growth over recent decades, driven by increasing demands for low-emission, high-efficiency combustion technologies in transportation and energy sectors. Reactors play a crucial role in this research by facilitating the study of chemical homogeneity, reaction rates, and other variables essential for optimizing combustion processes.

Chemical reactors encompass various model types, each with their own designated purpose. In essence, all reactors have some form of fluid flow, an ensured method of mixing, and ultimately a contained chemical reaction. These allow for a myriad of studies to be performed such as characterizing flow patterns and predicting rates of reactions. The three most popular chemical reactor models are Batch reactors, Continuous stirred-tank reactors, and Plug flow reactors (PFR). Batch reactors are closed vessel tanks without a continuous flow where reactants are pumped in simultaneously while being mixed by an agitator as shown in Fig. 1. These types of reactors heavily mimic fermenters as they can produce a large number of products when effective. They also share a drawback in that a lot of effort must be placed in combining reactants, releasing products, and having to clean the reactor between runs. Continuous stirred-tank reactors on the other hand are different from batch reactors in that they allow for a continuous flow of reactants whilst being agitated, and a continuous outflow of products simultaneously. Fig. 2 shows how this allows for massive product volume, especially in industrial processes. Plug flow reactors, seen in Fig. 3, are cylindrical reactors that allow

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for chemical reactions in continuous “plug” flows. They tend to be convenient for smaller volume kinetic studies, however, are difficult at controlling exothermic reactions.

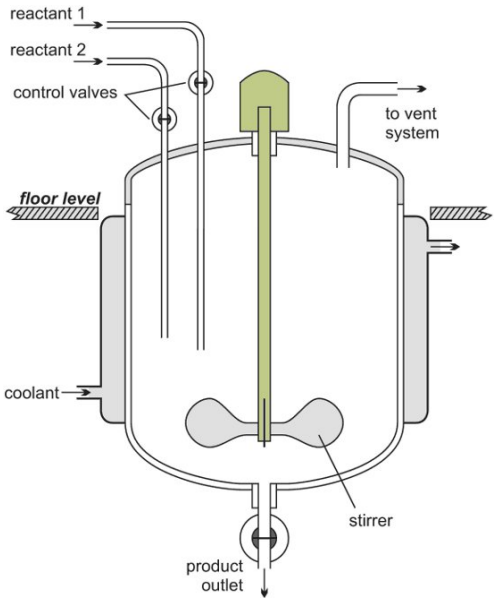

Fig. 1 Batch reactor

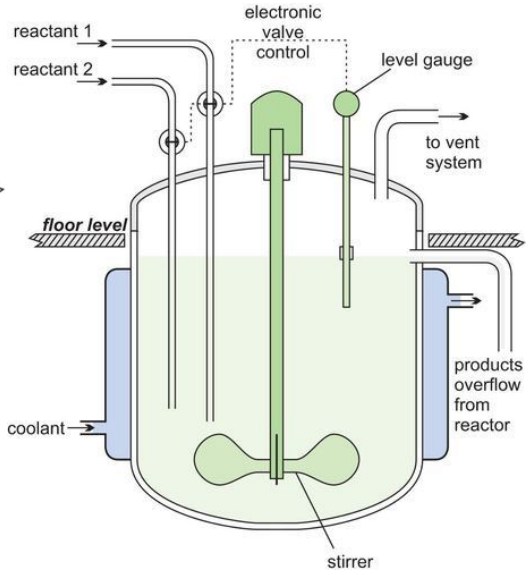

Fig. 2 Continuous stirred-tank reactor

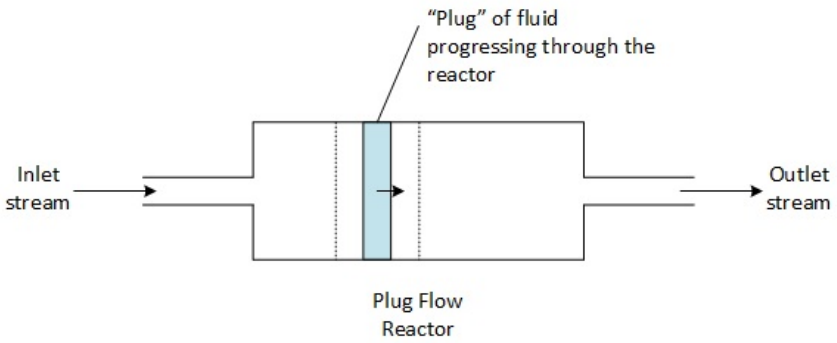

Fig. 3 Plug flow reactor

In our case, continuous stirred-tank reactors are preferred due to their efficient mixing capabilities whilst handling relatively high exothermic reactions. More specifically, the jet stirred reactor (Fig. 4), a class of reactor evolved from continuous stirred-tank reactors, is a more efficient apparatus used to study flow patterns of combustion reactions. They are typically made of fused silica to prevent reactions with the walls of the vessel and are shaped spheres that contain nozzles for reactant injection. These reactors are pivotal in studying combustion flow patterns, as they create a highly turbulent environment conducive to examining mixing efficiencies and reaction dynamics under controlled conditions of pressure and temperature.

The way they operate is through the injection of a fuel via an inlet into a small primary mixing region that also includes the continuous flow of an oxidizer. These reactants can optionally go through a phase of preheating prior to blending in the primary mixing region (PMR). Homogeneity is ensured as the reactants are significantly mixed in the PMR and go through additional mixing in the secondary mixing region. Following the combustion of the reactants, the products are ejected out of the reactor.

Fig. 4 JSR utilized from the Rotavera Group - University of Georgia

The main objective is studying the thermal uniformity throughout the reactor in order to validate results from the Rotavera Group at the University of Georgia. This data can be compared and analyzed to confirm thermal homogeneity predictions within their JSR at various pressure and temperature parameters. We will be focusing on studying the thermal uniformity under a single set pressure and associated inlet velocity parameters while observing fluid flow and temperature patterns in the secondary mixing region. The expectation is to see a relatively constant temperature profile in the secondary mixing region when experiencing a four second residence time. Temperature and pressure contours will be mapped out and studied under variations of wall temperature. As this project is a continuation of DeJongh [1], computer aided design models have already been developed and preliminary simulations have been performed. This project will focus on refining the mesh of previous models and validating data from previous experimental tests along with prior simulations. Upon successful validation of results, further simulations will be performed at higher pressure parameters as an attempt to understand and analyze the issues encountered in higher pressure contours in DeJongh [1].

II. Research Design

Fluid flow in this study is assumed to be nitrogen due to its high concentration in combination with the oxidizer. The fluid is modeled as an ideal gas under steady-state conditions with constant temperature, pressure, and residence time throughout the system. Viscous effects are considered only at the boundaries. Given the low velocities involved, the fluid is treated as incompressible, ensuring a constant density assumption.

The initial conditions include a fuel and oxidizer inlet temperature of 300 K, with the outlet exposed to atmospheric conditions. The oxidizer inlet velocity is set to 1 cm/s, while the fuel inlet velocity is set to 3 cm/s. The wall temperature is maintained at 500 K, and the vessel pressure is set to 1 atm. These velocities were determined using the volumetric flow rate equation (1) and a residence time of 4 seconds with the residence time being the time a fluid portion spends in a certain part of the system. This equation incorporates initial and final, temperature and pressure parameters as well as the volume of the reactor. Additional simulations will be conducted to assess different thermal and flow conditions. A second test case will use a wall temperature of 750 K, with an oxidizer inlet velocity of 1 cm/s and a fuel inlet velocity of 2 cm/s. A third simulation will investigate a wall temperature of 1000 K, with an oxidizer inlet velocity of 0.4 cm/s and a fuel inlet velocity of 1 cm/s.

$$\dot{V}_{total} = \left(\frac{V_{reactor}}{\tau_{residence}}\right)\left(\frac{T_0}{T}\right)\left(\frac{P}{P_0}\right) \tag{1}$$

The CAD files used in this study were originally produced by Joshua DeJongh (Fig. 5) [1]. Upon obtaining these files, few geometric issues were identified, including gaps and overlapping contact fields that required correction. Additionally, filleting was necessary for certain edges within the secondary mixing chamber before proceeding with meshing.

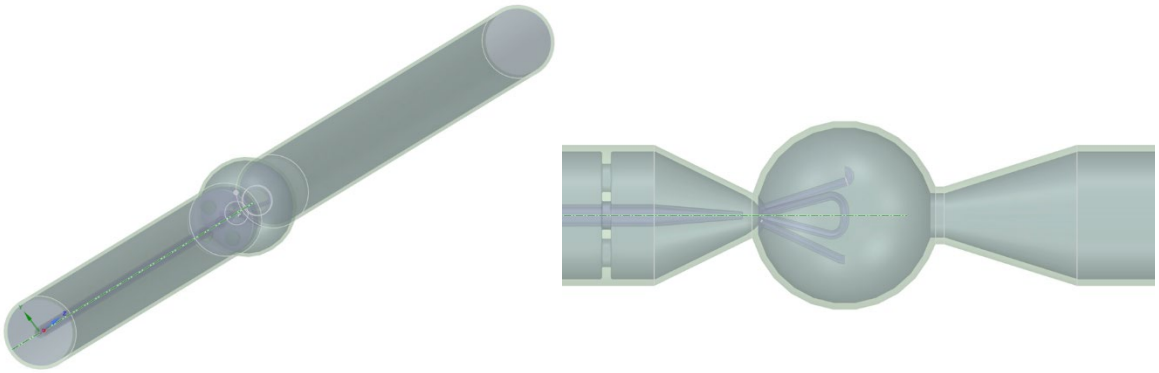

Fig. 5 JSR CAD models. Complete isometric view to the left. xy view of secondary mixing region to the right.

The meshing process initially presented challenges, particularly when automating mesh settings and advancing directly to post-processing. This resulted in erroneous results and jagged contour edges, as shown in Fig. 6. To resolve these issues, the geometry and mesh were carefully reviewed. It was determined that the mesh quality was insufficient, with some regions exhibiting an orthogonal cell quality of zero, as seen in Fig. 7. The primary cause was identified as the need to refine the maximum and minimum cell sizes, which were adjusted to $5.955 * 10^{-5}$ and $4 * 10^{-4}$ respectively. Additionally, the curvature normal angle was reduced from 18 to 12 degrees, eliminating errors and free-floating nodes.

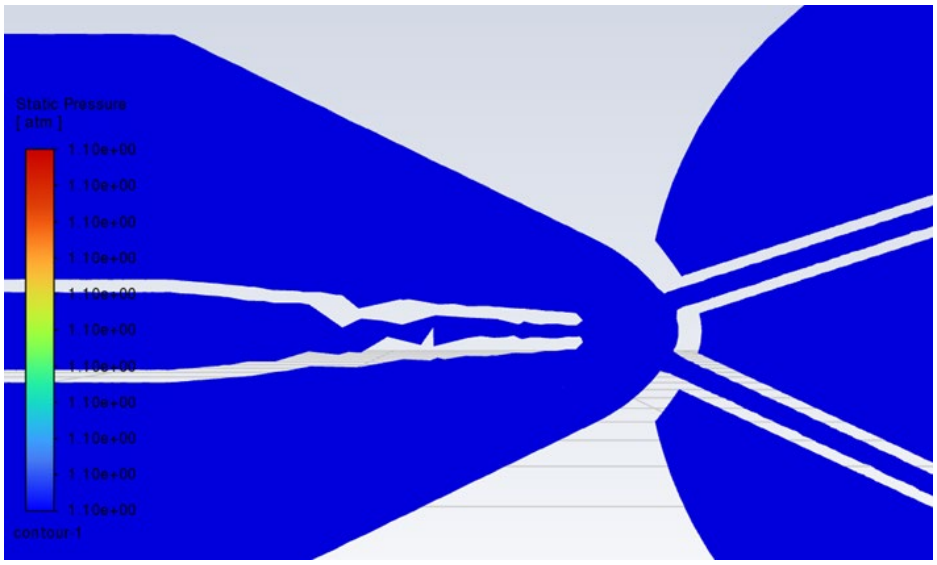

Fig. 6 Erroneous contour with jagged walls.

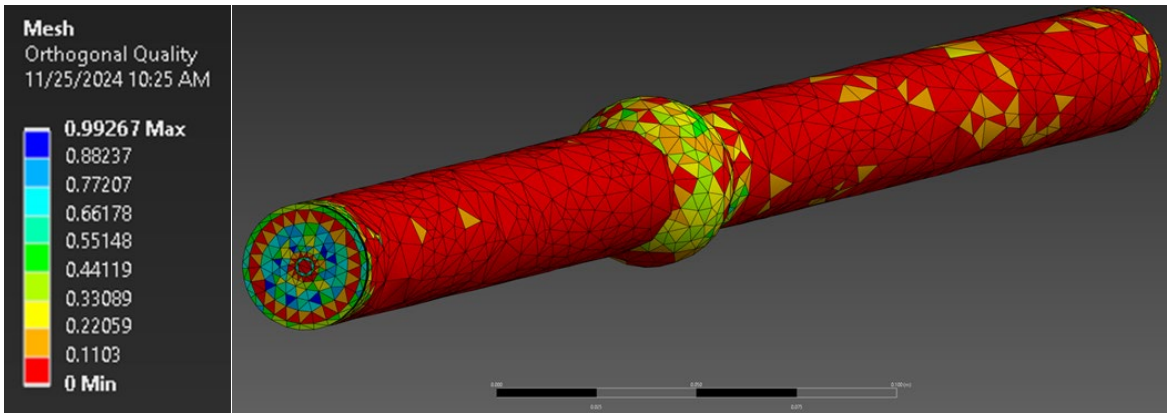

Fig. 7 Initial orthogonal quality readings and mesh.

Due to the increased resolution of the mesh, computational demands were significantly higher, necessitating the use of the UGA GACRC for processing. The final generated mesh was deemed satisfactory, containing approximately 2,262,690 cells with a minimum orthogonal quality of ~0.13—above the minimum threshold of 0.1 (Fig. 8 and 9).

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Surface Diagnostics :

Total Number of Faces          =   276053
Maximum Skewness               =   0.6399
Maximum Aspect Ratio           =    17.73
---------------------------------------
Volume Diagnostics :

Total Number of Cells          =  2262690
Minimum Orthogonal Quality     =   0.1287
Maximum Aspect Ratio           =    64.89
Number of Stair-Step Locations =        2
Number of Isolated Cells       =        0
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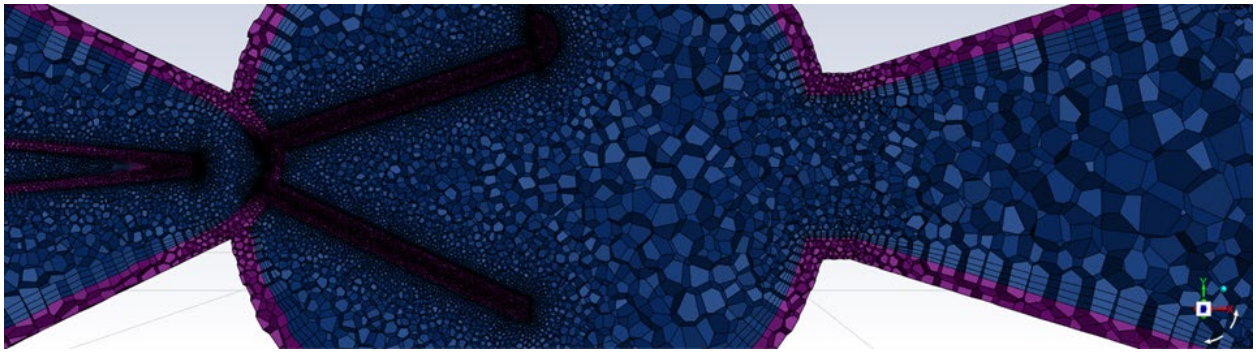
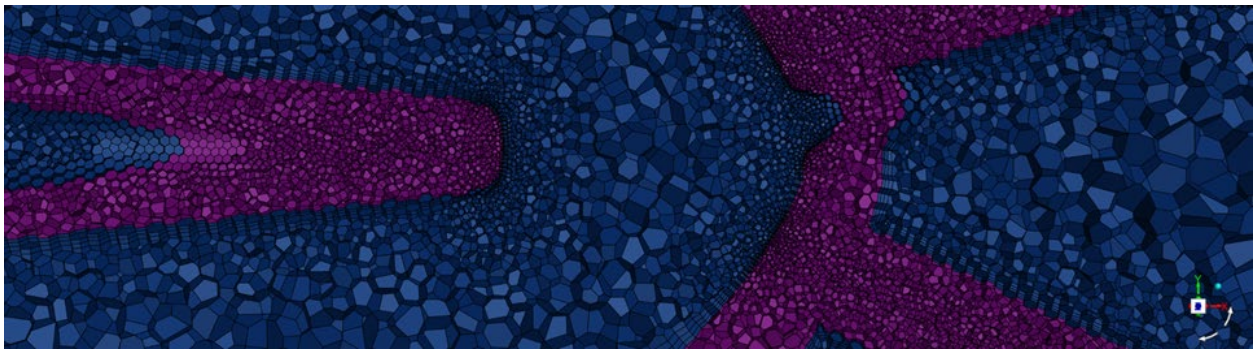
Fig. 8 *Mesh characteristics.*



a)



b)

Fig. 9 Corrected mesh results. a) Secondary mixing region. b) Primary mixing region.

III. Results

Experimental data from the Rotavera Group's Jet-Stirred Reactor (JSR) was analyzed to validate the computational model. A thermocouple was inserted near the center of the secondary mixing region to collect temperature readings. Measurements were taken along a straight line extending to the entrance of the outlet, as illustrated in Fig. 10. The recorded temperature data is presented in Fig. 11.

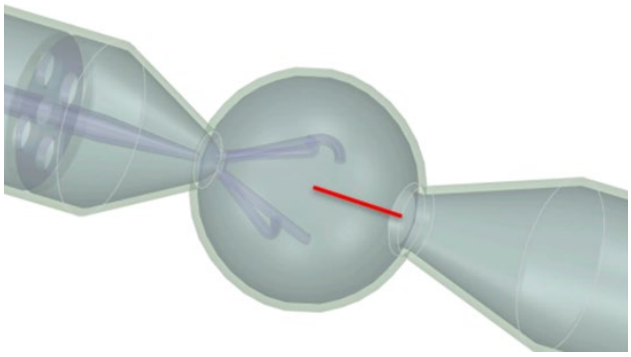


Fig. 10 Region where temperature values were taken.

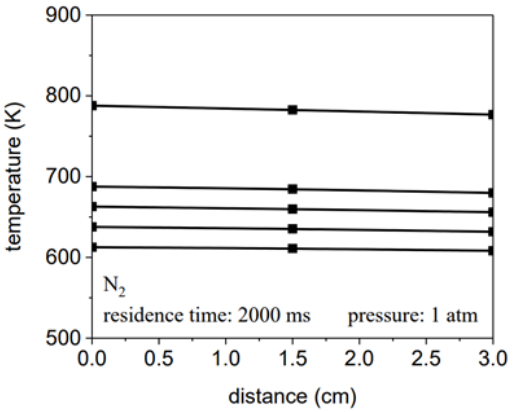


Fig. 11 Measured temperature values.

To compare with the experimental results, a 1 mm line/rake simulation was conducted. The simulation results demonstrated a uniform linear temperature profile at 500 K, closely aligning with the experimental measurements. This agreement confirms the reliability of the computational model in replicating the thermal behavior observed in the JSR (Fig. 12).

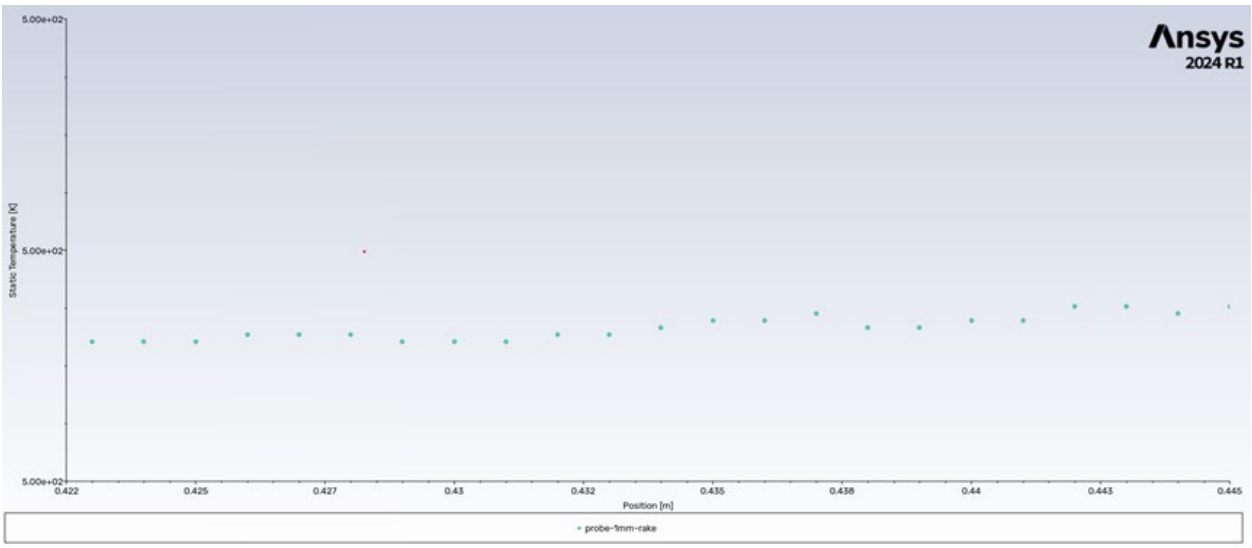


Fig. 12 Simulated probe results.

Following this validation, temperature, pressure, and velocity contours were generated to further examine the flow characteristics. The contour plots, produced using a wall temperature of 500 K, provide insights into the spatial distribution of these parameters within the reactor. All contours are presented as cross-sectional planes along the x-y plane to visualize the internal flow dynamics.

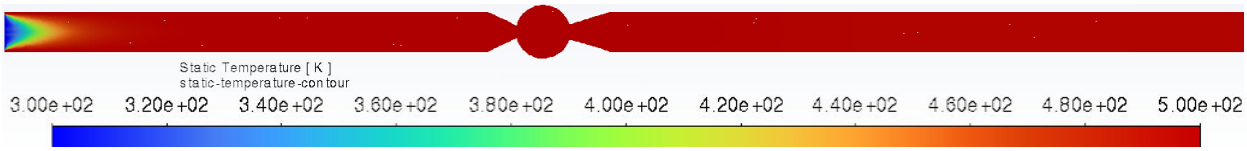


Fig. 13 Temperature contour at 500 K and 1 atm.

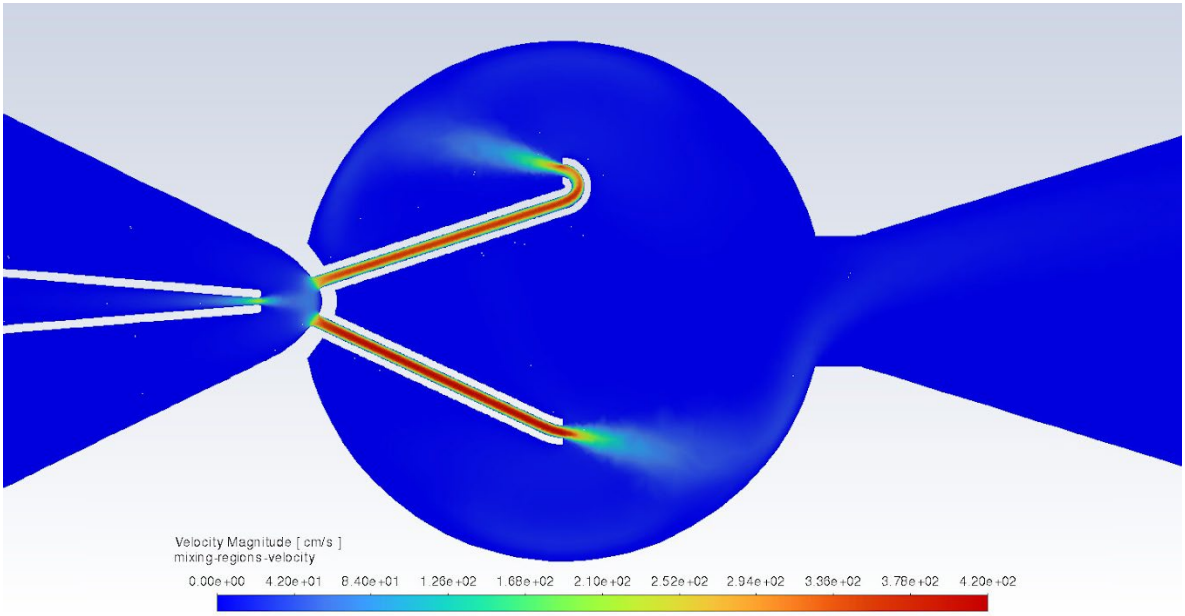


Fig. 14 Velocity contour at 500 K and 1 atm.

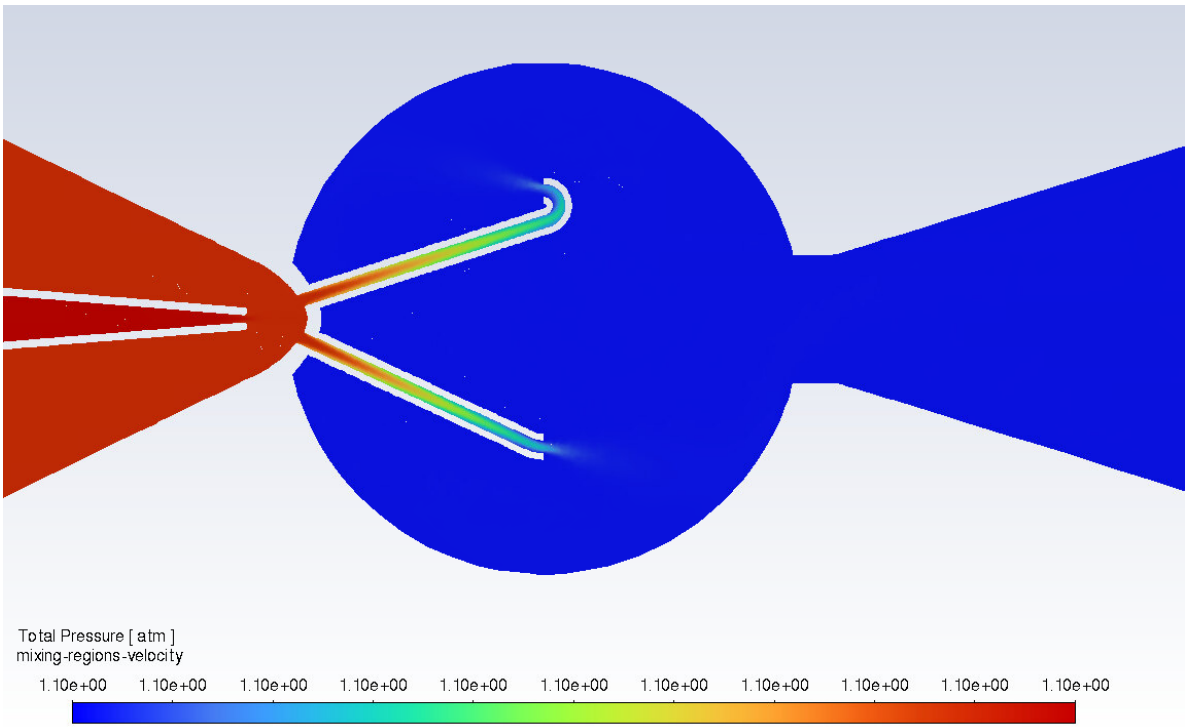


Fig. 15 Pressure contour at 500 K and 1 atm.

The following contours were generated using a wall temperature of 750 K and 1atm.

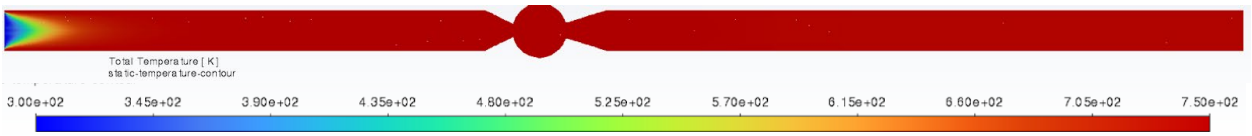


Fig. 16 Temperature contour at 750 K and 1 atm.

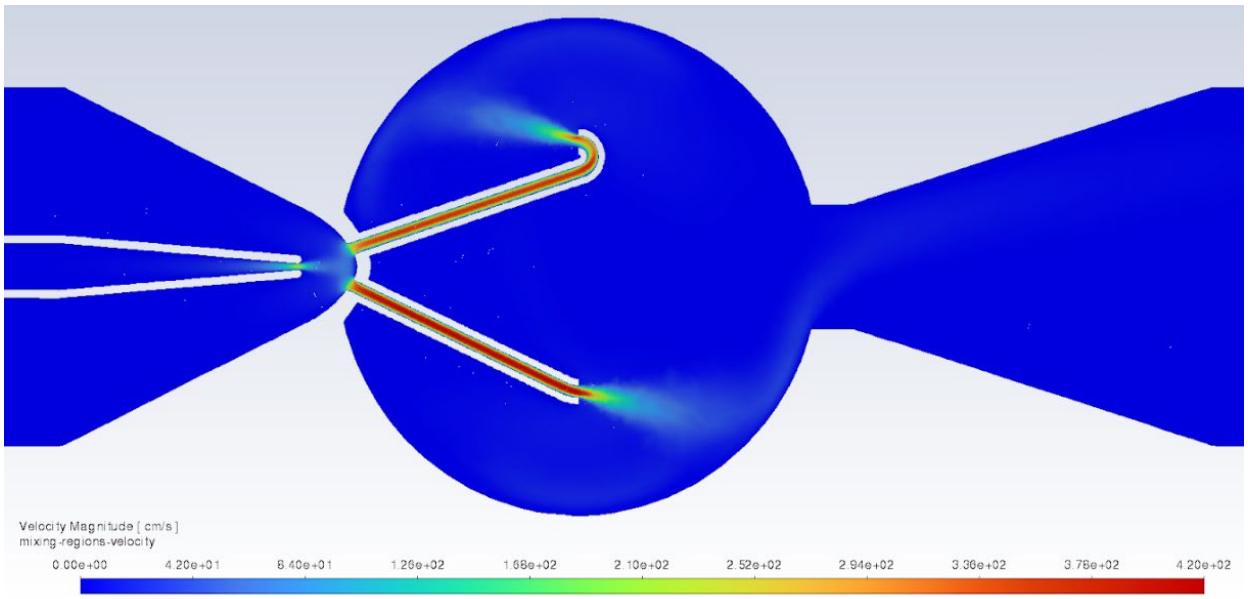


Fig. 17 Velocity contour at 750 K and 1 atm.

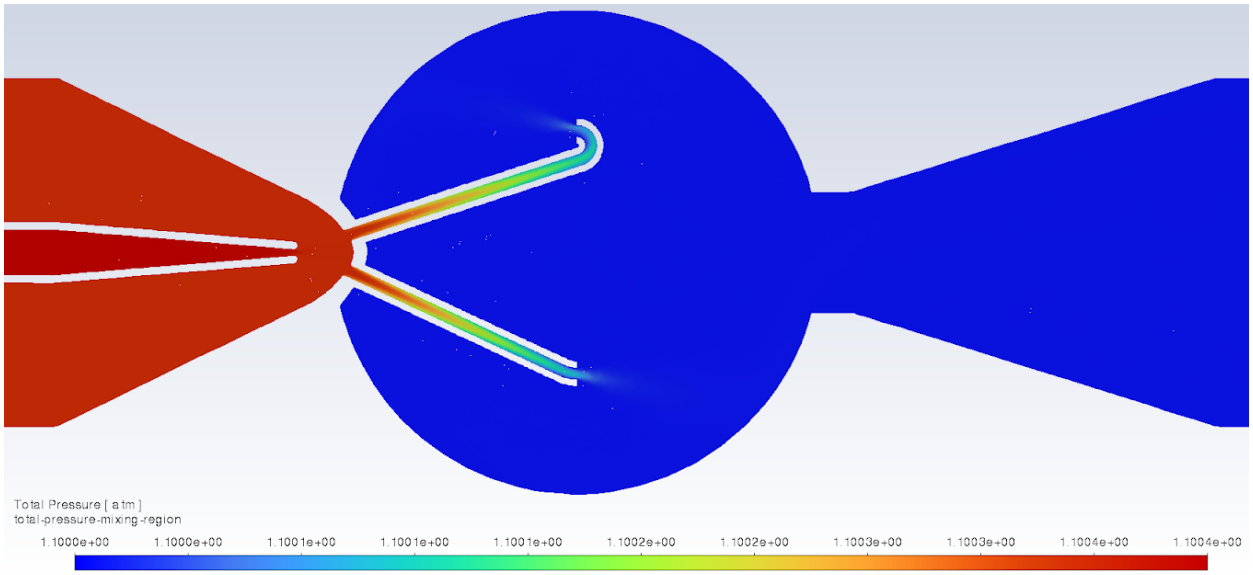


Fig. 18 Total pressure contour at 750 K and 1 atm.

The following contours were generated at a wall temperature of 1000 K and 1 atm.

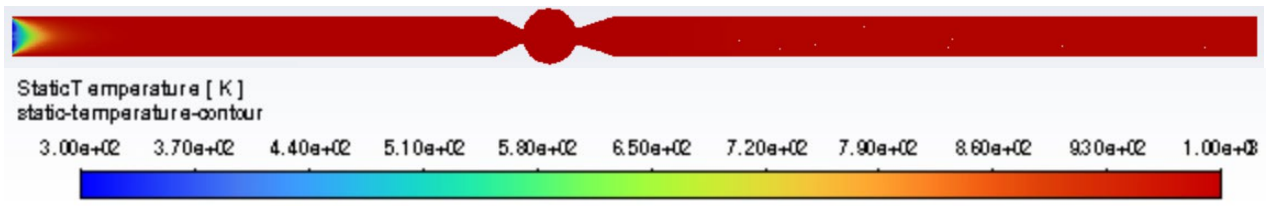


Fig. 19 Temperature contour at 1000 K and 1 atm.

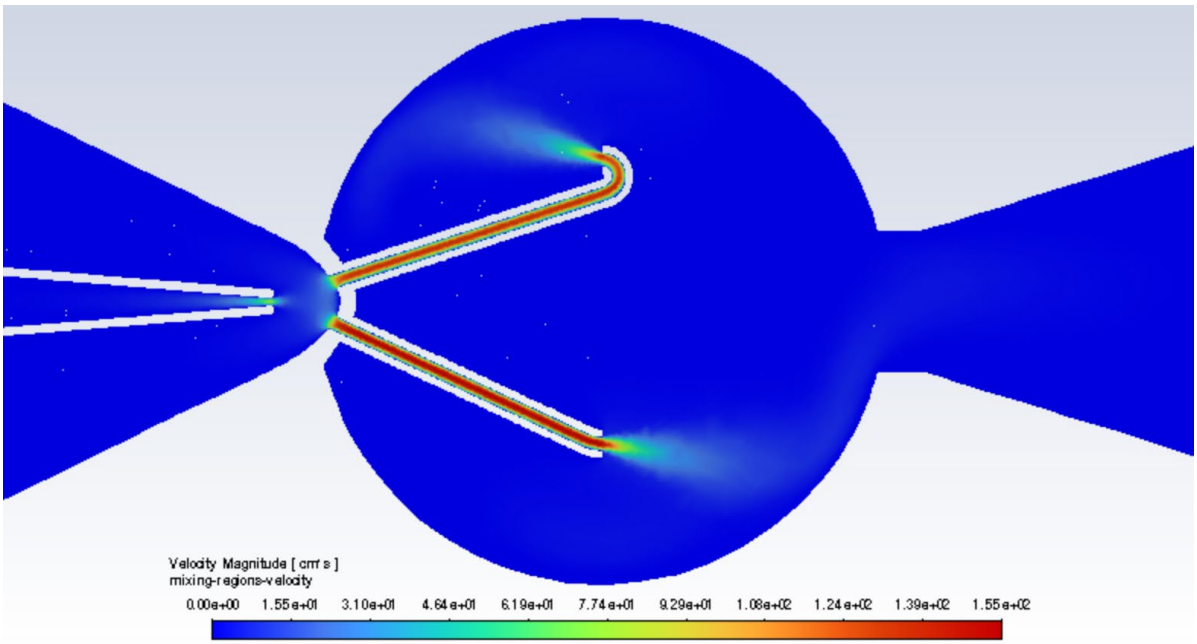


Fig. 20 Velocity contour at 1000 K and 1 atm.

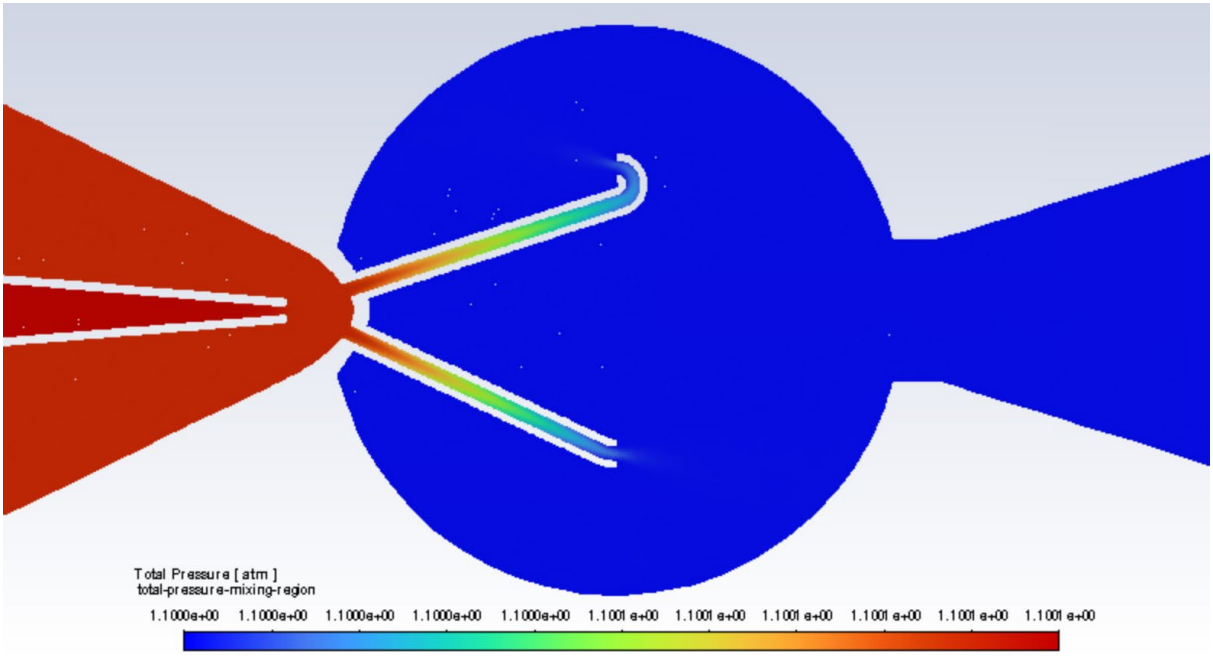


Fig. 21 Pressure contour at 1000 K and 1 atm.

IV. Conclusion

As a replication and refinement of DeJongh's [1] study, the results were compared to his simulations. While both temperature contours reached their respective wall temperatures within the first 2-3 inches of the reactor, my results achieved the wall temperature at a slightly faster rate than DeJongh's [1]. In contrast, the cell Reynolds number contours in my study exhibited lower maximum values compared to his findings. Despite this difference, the results confirm that fluid flow remains the primary transport mechanism, with minimal contribution from diffusion. Additionally, pressure variations between the two studies were relatively minor, with DeJongh's [1] data showing a maximum-to-minimum pressure difference of 0.0012 atm, whereas my study yielded a difference of 0.0004 atm.

Moving forward, future work will involve testing different pressure parameters evaluated in DeJongh's [1] study and extending the analysis using alternative solver methods. This approach aims to generate predictive data for higher-pressure conditions that the JSR may encounter, as well as improve accuracy compared to the results obtained using the Spalart-Allmaras (SA) turbulence model.

Acknowledgments

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