CFD Modeling Ensures Safe and Environmentally Friendly Performance in Shell Claus Off-Gas Treating (SCOT) Unit

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Introduction

Refineries processing high sulfur crude oils produce significant quantities of by product hydrogen sulfide (H_2S), also called acid gas. This gas is often processed in a Claus Sulfur Recovery Unit (SRU). The Claus process converts acid gas (H_2S) into elemental sulfur in an oxygen-deficient combustion process and then liquid sulfur from the condenser runs through a seal leg into a covered pit from which it is pumped to trucks or railcars for shipment to end users. Approximately 65 to 70 percent of the sulfur is recovered.

The SCOT Process (Shell Claus Off-gas Treating Process) was developed by Shell, and introduced in the early seventies as an attractive process for improving the efficiency of a Claus sulfur recovery unit (See Figure 1). The process consists of four combustion processes (as well as catalytic reactors which are not discussed here):

1. Reaction furnace
2. Inline reheater
3. Reducing gas generator
4. Tail gas incinerator

The CFD analysis discussed in this article considers only the second process, the inline reheater. The inline reheater heats the acid gas by mixing it with hot reducing products of combustion. An important design consideration is that the products of combustion being mixed are reducing. If O_2 slip (uncombusted O_2) is available to mix with the acid gas, the H_2S can be oxidized to undesirable compounds (e.g., SO_3, SO_4, H_2SO_4) that can attack refractories and damage the environment.

CFD analysis

The purpose of this CFD analysis was to determine if the proposed burner design for the inline reheater would perform as required. In particular, the client was concerned regarding the following issues:

1. O_2 slip
2. Soot formation in the reactor
3. Flame length
4. Swirl number of the combustion air
5. Uniformity (mixedness) of SRU tailgas and combustion products leaving reheater

These issues were analyzed using CFD at several operating conditions, but only the maximum liberation case is discussed in this article. All calculations were performed with Star-CD version 3.15.

The mesh generation was performed using pro-am, the CD adapco Group's proprietary trimmed cell meshing software. The mesh generated had 1.1 million cells with significant refinement in the combustion zone to resolve the small jets used by the burner designers to produce a short flame.

Figures 2 and 3 show the geometry of the CFD model as well as the flow inlets and outlets considered.

Chemistry

The chemistry has been approximated using the eddy break-up model. This model assumes mixing-limited chemistry, which is appropriate for most hydrocarbon combustion reactions. The included species in the model are H_2, CH_4, CO, CO_2, H_2O, H_2S, O_2, SO_2, and N_2. The chemical reactions considered are:

$$H_2 + ½\, O_2 \rightarrow H_2O \qquad (1)$$

$$CH_4 + 3/2\, O_2 \rightarrow CO + 2\, H_2O \qquad (2)$$

$$CO + ½\, O_2 \rightarrow CO_2 \qquad (3)$$

$$H_2S + 3/2\, O_2 \rightarrow SO_2 + H_2O \qquad (4)$$

The mixture of gases is treated as an ideal gas. The density is computed at each location as a function of pressure, temperature, and species mass fractions. The specific heat of the mixture of gases is computed at each location as a weighted sum of the individual species specific heats, which are themselves a polynomial function of temperature.

Figures 4 and 5 show temperature and oxygen mass fraction results for the maximum liberation case. These figures indicate that the thermal mixing between the SRU tailgas and the products of combustion is sufficient that the exhaust is well-mixed. The figures also show that the near-burner mixing is very thorough and O_2 slip into the SRU tailgas does not occur.

Soot formation potential

Soot formation in the reheater can have significant negative consequences. The model as formulated does not directly compute the formation of soot particles. However, the model does do a good job of computing the major species profiles and temperatures. To estimate the sooting potential in the mixing zone between the SRU tail gas and the products of combustion, we used the equilibrium program CET89 to compute the equilibrium gas composition at locations in the centerplane of the reactor. To do this, we took all 9 species concentrations (H_2, CH_4, CO, CO_2, H_2O, H_2S, O_2, N_2) and the gas temperature and pressure at about 2500 cell locations and fed that data into CET89. CET89 performed the equilibrium calculations at fixed temperature and pressure and predicted the C_2H_2 mole fraction shown in Figure 6. The figure shows that the C_2H_2 mole fraction is at most about 10^{-18}. Experience shows that acetylene levels greater than 10^{-8} are needed to produce observable soot in a flame. The CET89 computations were not carried out for all the cells in the model to minimize the length of the calculations and because the chosen cells are believed to represent the important locations where soot might be formed.

Performance Testing: Additional Cases and comparison to experimental data

Following completion of the base case, five additional cases were identified to demonstrate the capabilities of the current SCOT Burner design. Process conditions for these cases are shown in Table 1. These conditions included high Hydrogen flow rates at two stoichiometric conditions (Cases 1-3), refinery fuel (Case 4), and 100% fuel gas (Case 5). To evaluate the model's ability to predict soot formation potential and performance, an test rig was built and operated at ZEECO. Data collected during the tests included pressure drop at various locations in the reactor. Also, soot formation was measured by visual inspection at the stack. Comparisons between predictions and measurements for Cases 1, 4, and 5 are shown in Table 2 with CFD results for these same cases shown in Figures 7 and 8. Selection of cases for comparison to CFD results were made based on demonstrated data quality. Results in Figure 8 show essentially zero soot formation at the stack which also agreed with visual observations. Comparison between predicted and measured pressure drop through the reactor show good agreement. Based on these comparisons the proposed design was constructed and installed at Ashland-Marathon and is currently operating as expected. Figure 9 shows the installed unit.

Conclusions

This paper has presented the CFD analysis of the inline reheater section of a SCOT system. The present analysis has indicated that the mixing in the near burner zone is very good and that O_2 carryover is not predicted to occur. Analysis of the chemical composition in the reactor using the thermodynamic equilibrium code CET89 facilitated the prediction of equilibrium acetylene mole fractions at locations through out the vessel. These mole fractions indicate that soot formation will not occur in the combustion zone or in the SRU tailgas mixing zone.

The use of CFD analysis during the design phase of industrial combustion systems can significantly reduce the likelihood of startup and operating problems. In this case, issues such as long flames or soot production in the furnace would be very expensive to repair because the unit is operational continuously. System operation was tested via the follow-on performance cases. Data from these cases were also compared against experimental measurements (both measured pressure drop across various portions of the reactor and visual observation of soot formation). Based on these comparisons the reactor was constructed and installed and is successfully operating as expected.

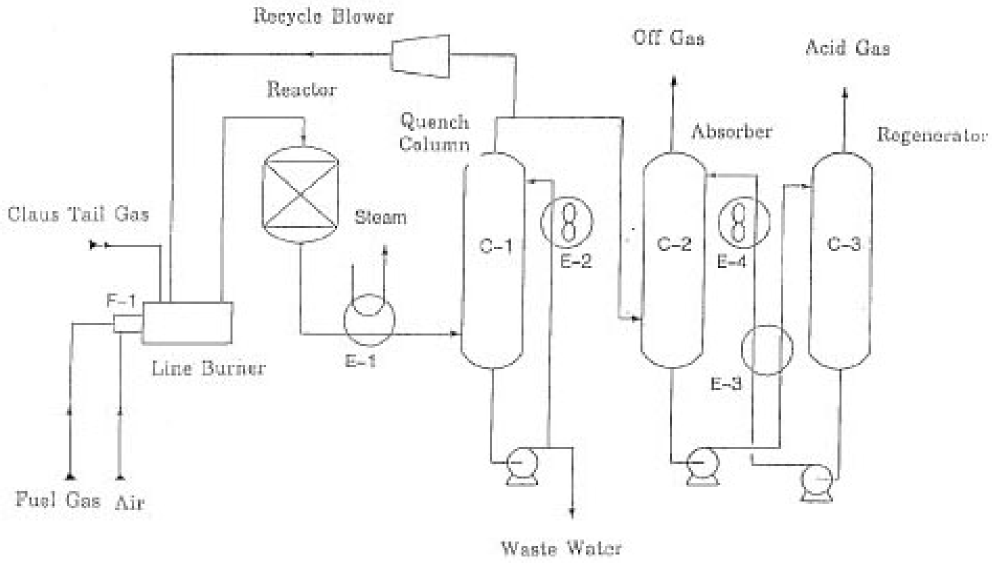

Figure 1: SCOT (Shell Claus Off-gas Treating) process

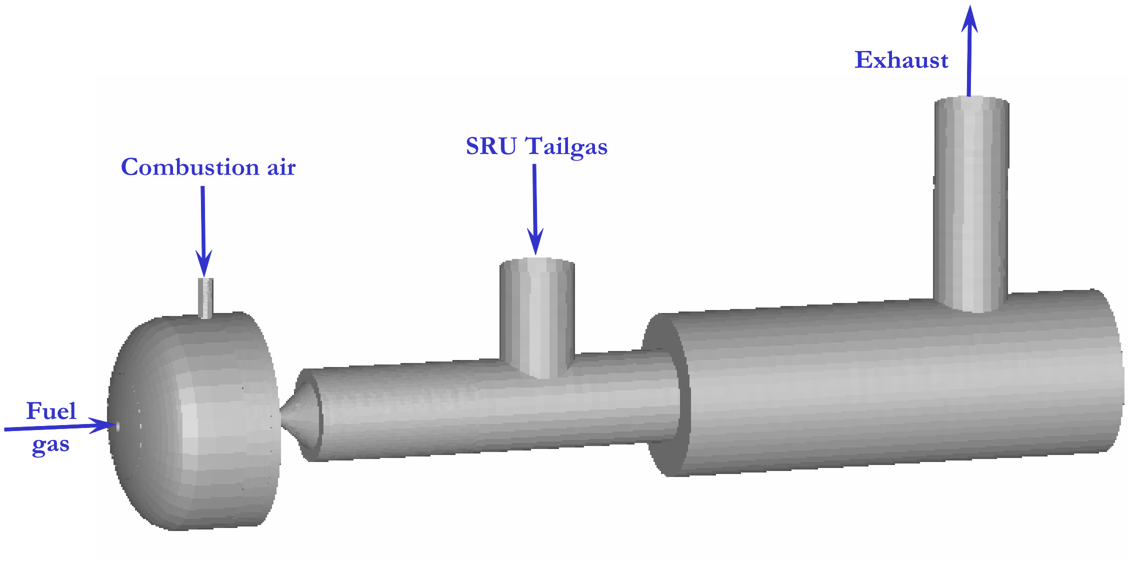

Figure 2: Geometry of inline heater

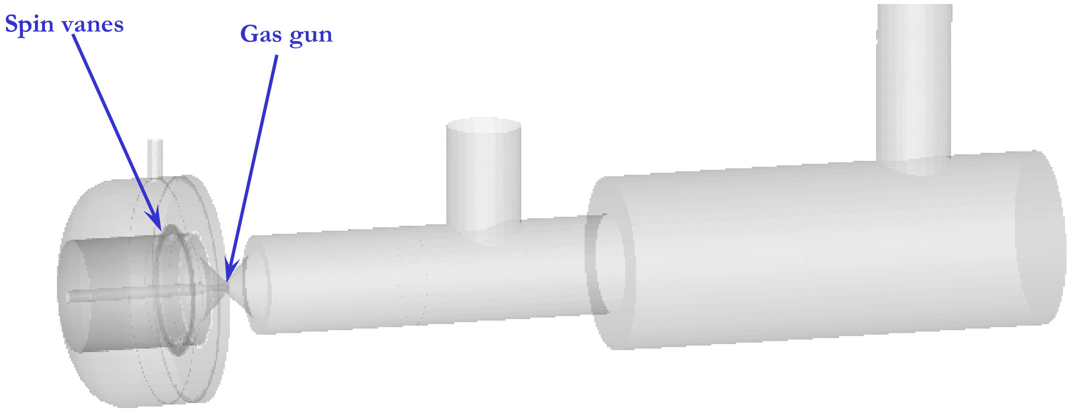

Figure 3: Transparent surface view showing location of gas gun and spin vanes

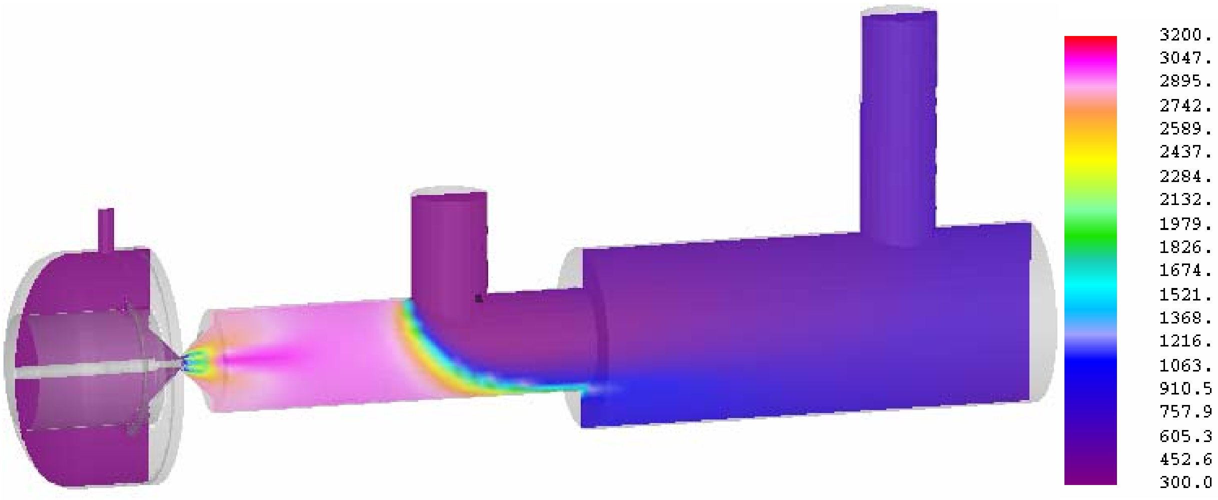

Figure 4: Base case Temperature (°F) contours of on centerline of burner and vessel

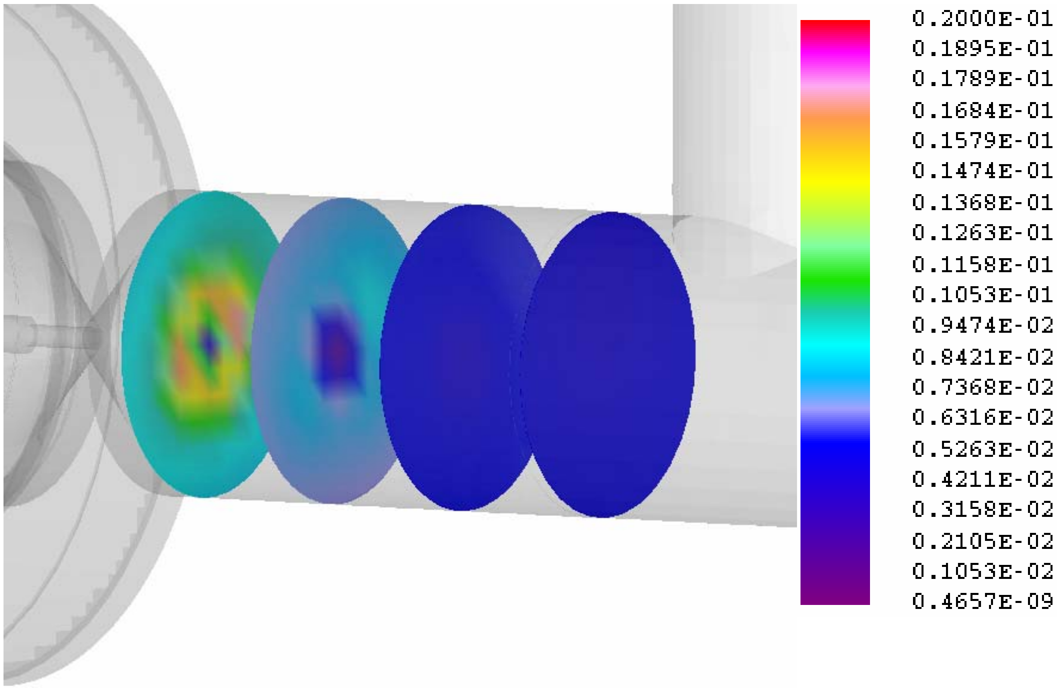

Figure 5: Wet O_2 mole fraction (contours from 0-2%) shown 12”, 24”, 36”, and 48”downstream of fuel discharge. This figure shows the fuel/air mixing and indicates that O_2 carry over does not occur.

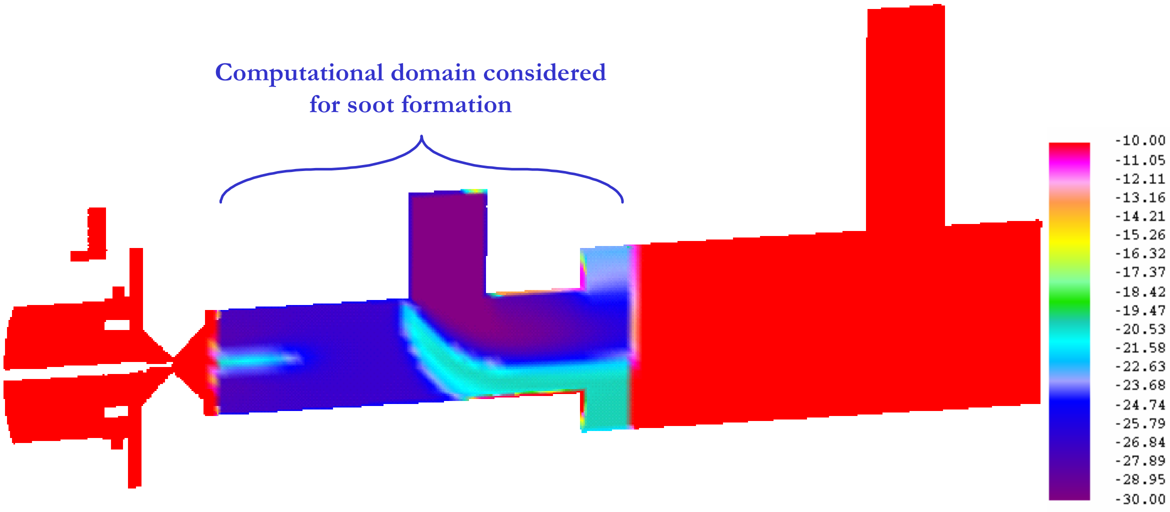

Figure 6: Log_{10} of C_2H_2 mole fraction in the mixing zone between the products of combustion and the SRU tail gas. Note that only the mixing zone where the Claus gas enters has been analyzed. Other parts of the domain are shown in red to distinguish the zone. Also, near the walls, there is an interpolation error (a graphic smoothing issue) that makes the acetylene concentration appear higher. This is because the wall data was not used in the procedure.

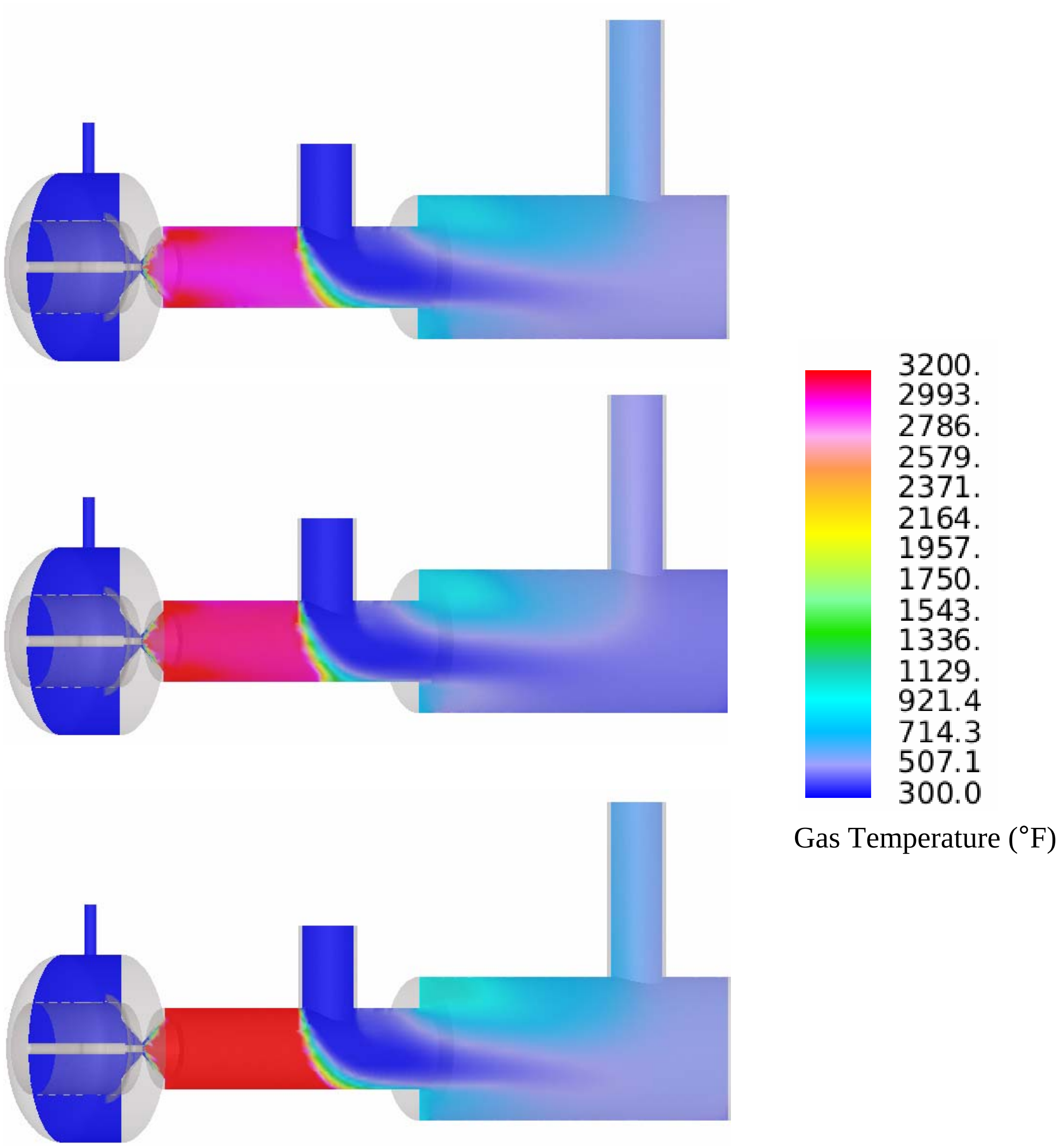

Figure 7: Predicted gas temperature (°F) for Cases 1, 4, and 5.

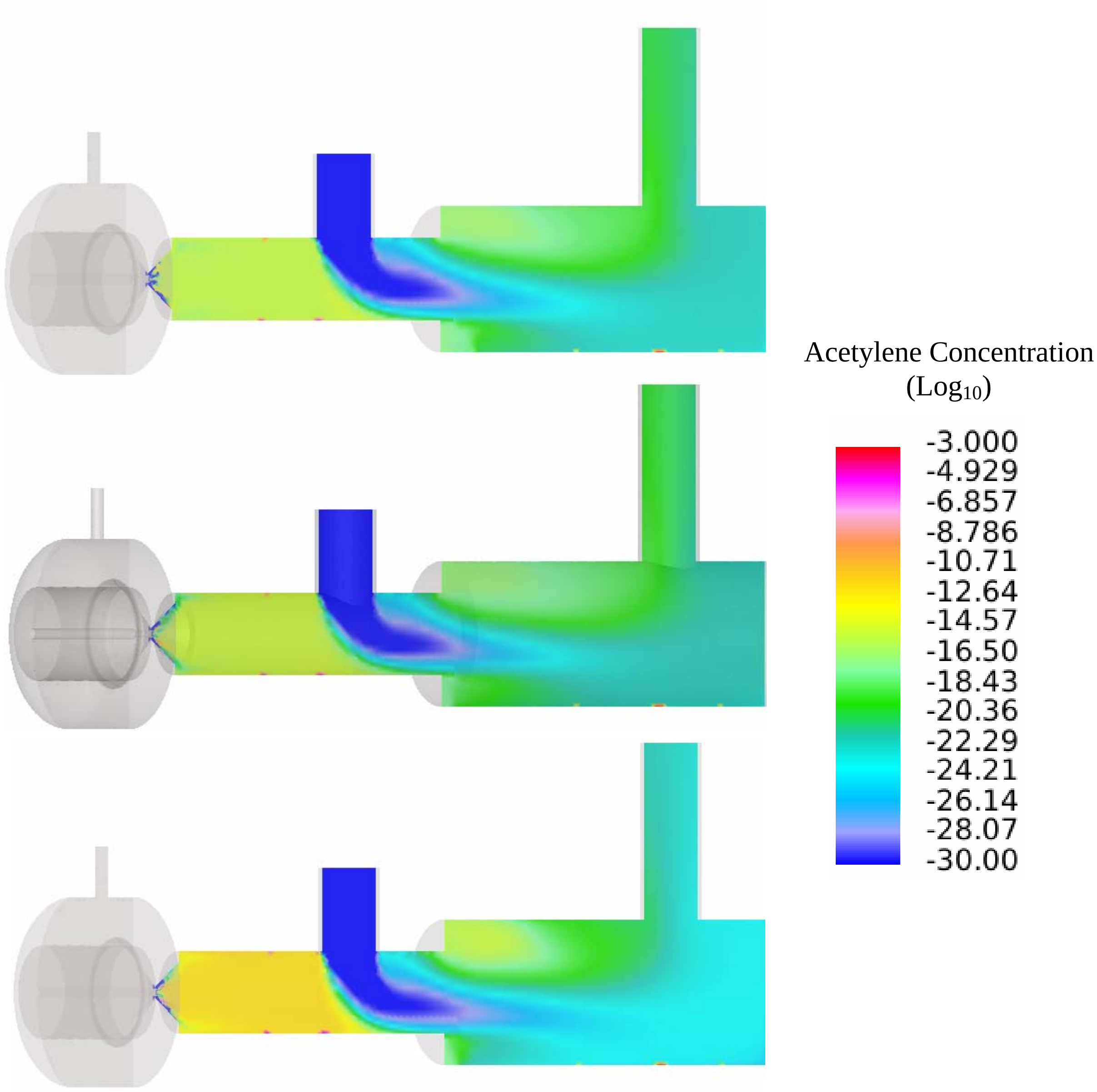

Figure 8: Predicted Acetylene Concentration Profiles (Log_{10}) for Cases 1, 4, and 5.

Table 1. Flow rates for five performance cases used to characterize SCOT unit.

Case	Air (lbm/hr)	Fuel (lbm/hr)	Tailgas (lbm/hr)	%H2	%TNG	%C3H8
1	1437	107	18,105	92.5	7.5	0
2	287	21	3,621	92.5	7.5	0
3	1309	21	3,621	92.5	7.5	0
4	1698	184.5	18,105	25	55	20
5	1254	186	18,105	0	100	0

Table 2. Comparison of predicted/measured pressure drop through reactor for selected cases.

Case	CFD1*	Test 1	Error	CFD4*	Test 60%	Error	CFD5*	Test	Error
Burner delta P, psig	1.06	1.05	1.4%	1.60	1.96	18.6%	1.07	1.1	2.6%
Spin Vane Delta P,psig	0.47	0.45	4.3%	0.75	0.7	6.5%	0.45	0.4	13.0%
Throat Delta P, psig	0.60	0.6	0.7%	0.85	1.25	32.0%	0.62	0.7	11.4%