Mixing Length of Hydrogen in an Air Intake

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Due: 5/1/07
EGEE 520

Abstract

Hydrogen is currently being examined as a transportation fuel. One example of the way in which hydrogen has been examined is in diesel pilot ignited hydrogen combustion. This is achieved by injecting hydrogen into the air intake of an engine. The mixing of fuel and air greatly effect the polluting emission created during combustion. The hydrogen and air should be mixed homogenously to reduce polluting emission.

A two-dimensional jet in a cross flow model was created to examine the mixing length of hydrogen being injected into the air intake of an engine. The model was created in Comsol Multiphysics 3.3 and was governed by the turbulent incompressible Navier-Stokes equation and the convection diffusion equation. Given the parameters used in the model, hydrogen and air move at a rate of 14.98 m/s homogenously mix in 0.052 s at a length of 0.77 m. The model was qualitatively compared to experimental results from a jet in a cross flow experiment and both appeared to agree with each other.

1. Introduction

In recent years, advanced combustion modes, such as dual fuel combustion and homogenous charge compression ignition (HCCI) combustion, have gained interest [1-3]. Hydrogen has been researched as a dual combustion fuel, in particular, in diesel pilot ignited hydrogen combustion [4-6]. Diesel pilot ignited hydrogen combustion is of particular interest because it utilizes hydrogen as an alternative energy source and lowers emissions from diesel combustion.

In diesel pilot ignited hydrogen combustion, hydrogen gas is fumigated into an engine's air intake, either before or after the turbocharger. The hydrogen and air are assumed to homogenously mix before reaching the combustion chamber. The hydrogen-air mixture then is drawn into the combustion chamber during the intake stroke. The pressure and temperatures of the hydrogen-air mix increase during the compression stroke. However the hydrogen-air mixture can not ignite due to hydrogen's low cetane number [7, 8]. Therefore the diesel fuel injected during the compression acts as a pilot to ignite the hydrogen [9, 10].

Combustion efficiency can be increased, and emission can be created, suppressed or consumed during the combustion process. It has been shown in numerical studies that premixed hydrogen-air flames show a greater amount of heat release compared to diffusion hydrogen-air flames. [11] Emissions such as high particulate are produced if the hydrogen and air are not mixed well in a HCCI-like mode [12].

In HCCI, combustion mode fuel and air are mix homogenously before high temperature and pressure cause combustion in patches through the air-fuel mixture. HCCI differs from classical compression ignition combustion where a prorogating diffuse flame burns. The air-fuel mixture in HCCI combustion are fuel-lean which provides a better fuel efficiency and lower emissions [2, 13].

Previous work has been conducted on the topic of gas-mixing using numerical models. When compared, these models from earlier studies agree with experimental data. Some of the pervious work dealt with hydrogen and air mixing [14, 15]. Other studies gave exact solutions to mixing problems[16]. In one study, an advective-diffusive model (ADM) was compared to a dusty-gas model (DGM). The DGM was found to be a better model [17]. Furthermore, a numerical model was developed by Kamali using a compressible turbulent Navier-Stokes equation in curvilinear coordinates. Kamali concluded that thermal mass diffusion has a large effect on flow fields when there is a large temperature gradient and secondly, that pressure mass diffusion is negligible for most conventional problems [18].

The mass diffusion equation and the incompressible turbulent Navier-Stokes equations are the primary equations for this model [19]. The model will examine hydrogen being injected into an air flow traveling through the pipe. The objective is to determine the length required for the hydrogen and air to homogenously mix, in a given pipe geometry. The concentration of hydrogen will range from levels at and below the lower explosion limit of hydrogen, which is 4.1% of the volume of air [20].

2. Governing Equations

Figure 1 is a depiction of the system being modeled. In the figure, hydrogen is being added to a length of pipe in which air is flowing. This system is known as a jet in a cross flow. The hydrogen and air will completely mix downstream at some length of pipe.

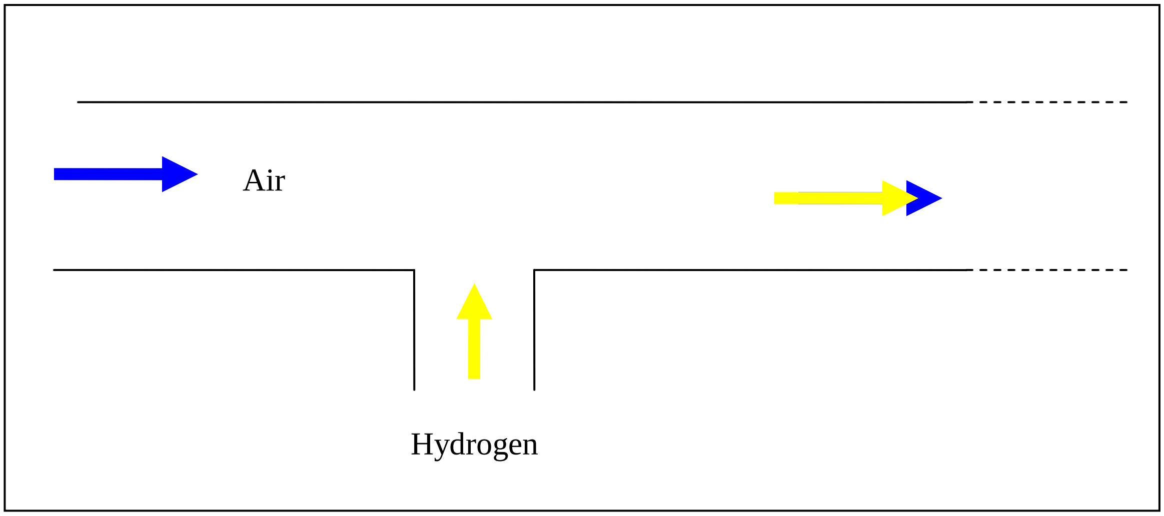

Figure 1. Setup of hydrogen jet in an air crossflow

The system is a two-dimensional model. The motion of air and the flow of hydrogen through the system will be governed by a momentum balanced equation, the turbulent incompressible Navier-Stokes equation.

$$\rho u \cdot \nabla u = \nabla \cdot [-pI + (\eta + \eta_T)(\nabla u + (\nabla u)^T)] + F \qquad (1)$$

$$\nabla \cdot u = 0 \qquad (2)$$

$$\rho u \cdot \nabla k = \nabla \cdot [(\eta + \eta_T / \sigma_k) \nabla k] + \eta_T P(u) - \rho\varepsilon \qquad (3)$$

$$\rho u \cdot \nabla k = \nabla \cdot [(\eta + \eta_T / \sigma_k) \nabla \varepsilon] + C_{\varepsilon 1} \varepsilon \eta_T P(u) / k - C_{\varepsilon 2} \rho \varepsilon^2 / k \qquad (4)$$

Where:

$$P(u) = \nabla u : (\nabla u + (\nabla u)^T) \qquad (5)$$

and

$$\eta_T = \rho C_\mu k^2 / \varepsilon \qquad (6)$$

Where η is dynamic viscosity, ρ is the density, u is the velocity field, P is pressure, U is the averaged velocity, k is the turbulent energy, ε is the dissipation rate of turbulence energy, and C_μ is a model constant.

The boundary conditions of the system for the Navier-Stokes equation are equations (7) to (15). The inflow boundary condition used for the hydrogen jet and air cross flows are equations (7) to (9).

$$u = u_0 \qquad (7)$$

$$k = (3 I_T^2 / 2)(u_0 \cdot u_0) \qquad (8)$$

$$\varepsilon = C_\mu^{0.75} [(3 I_T^2 / 2)(u_0 \cdot u_0)]^{1.5} / L_T \qquad (9)$$

Where I_T is turbulent intensity scale and L_T is the turbulent length scale. Equation (10) and (12) are the logarithmic wall function boundary conditions used for the walls of the system.

$$n \cdot u = 0 \qquad (10)$$

$$K = [\rho C_\mu^{0.25} k^{0.5} / (\ln(y^+) / 0.42 + 5.5)] u \qquad (11)$$

$$\varepsilon = C_\mu^{0.75} k^{1.5} / (0.42 \delta_w) \qquad (12)$$

where

$$K = [(\eta + \eta_T)(\nabla u + (\nabla u)^T)] n \qquad (13)$$

$$y^+ = \delta_w \rho C_\mu^{0.25} k^{0.5} / \eta \qquad (14)$$

δ_w is the layer thickness. Equation (15) is the neutral boundary condition used for the out flow of the system.

$$[-pI + (\eta + \eta_T)(\nabla u + (\nabla u)^T)] n = 0 \qquad (15)$$

The initial conditions are:

$$u(t_0) = u_0 \qquad (16)$$

$$v(t_0) = v_0 \qquad (17)$$

$$p(t_0) = p_0 \qquad (18)$$

Hydrogen mixing in air is governed by a mass balanced equation, the convection diffusion equation.

$$\delta_{ts}\frac{\partial c}{\partial t} + \nabla \cdot (-D\nabla c + cu) = R \tag{19}$$

Where δ_{ts} is the time scale coefficient, c is the concentration, D is the diffusion coefficient, u is the velocity and R is the reaction rate. Equation (20) is the conservative version of the convection diffusion equation. The convection diffusion equation can be further simplified by setting the time scale coefficient to 1 and setting the reaction rate to 0. The diffusion coefficient is assumed to be isotropic.

$$\frac{\partial c}{\partial t} + \nabla \cdot (-D\nabla c + cu) = 0 \tag{21}$$

The Navier-Stokes and the convection diffusion equation are coupled to each other through velocity. The boundary conditions of the system for the convection diffusion equation are equations (22) and (23).

$$c = c_0 \tag{22}$$

$$n \cdot (-D\nabla c) = 0 \tag{23}$$

Equation (22) represents the concentration of the inlets and outlet. Equation (23) represents the insulation in the tube. The initial condition is:

$$c\ (t_0) = c_0 \tag{24}$$

3. Solution

Comsol Multiphysics 3.3 was used to model the mixing of a jet of hydrogen entering a cross flow of air. The model consists of two sets of parallel plates. These plates represent the cross-sectional view of the pipes containing air and hydrogen. The model was set to run at steady state, since engine testing is done at steady state. Table 1, Table 2 and Table 3 provide the values of fluid properties and pipe dimensions used in the model.

Table 1. Values used for hydrogen jet.

Velocity *[m/s]*	**Pipe dia.** *[m]*	**Pipe length** *[m]*	**Concentration of H^2** *[mol/m^3]*	**Reynolds number**	**Turbulence length scale** *[m]*	**Turbulence intensity**
20	0.01	0.04	1	13,688	0.0007	0.0314

Table 2. Values of air cross flow.

Velocity *[m/s]*	**Pipe dia.** *[m]*	**Pipe length** *[m]*	**Concentration of H^2** *[mol/m^3]*	**Reynolds number**	**Turbulence length scale** *[m]*	**Turbulence intensity**
10	0.05	4	0	34,229	0.07	0.0434

Where turbulence length scale is:

$$\iota = 0.07\, d_h \tag{15}$$

Where turbulence intensity is:

$$I = 0.16\ \mathrm{Re}_{d_h}^{-\frac{1}{8}} \qquad (16)$$

Table 3. Shared values of flows at 25 ^{o}C and 1 atm.

Dynamic viscosity *[Pa*s]*	**Density** *[kg/m^3]*	**Diffusion coefficient** *[m^2/s]*
5.79E-07	1.29	7.56E-03

The dynamic viscosity and density used in Table 3 are for that of air. Both inlet flows are assumed to have the same dynamic viscosity and density since air makes up the largest constituent of the system. The diffusion coefficient is the hydrogen in air diffusion coefficient.

The model was configured so that a four meter pipe containing air was intersected by the hydrogen inlet in the middle of the pips length. Using this configuration, the turbulent flow of the air is fully developed at the point that the hydrogen inlet intersects and creates a cross flow.

Figures 2 to Figure 7 are Comsol for the model solutions. Figure 2 is a surface plot of hydrogen concentration in the cross flow. The hydrogen mixes into the air flow in approximately 0.77 meters of distance from the hydrogen inlet. Given the speed of the flow in the x-direction, the mixture is homogenous within 0.052 s of the hydrogen entering the flow. It is important to note that the maximum possible concentration is 1 mol/m^3, yet the model gives a value of 1.015 mol/m^3. This inaccuracy stems from the inability to create a mesh fine enough for the model. The density of the mesh is limited by the computer system memory.

Figure 3 is a line plot of concentration at the center of the cross flow verses pipe length. This line plot displays the model having a maximum concentration of 0.45 mol/m^3 at the point of hydrogen injection. The air-hydrogen mixture is homogeneous at a concentration of 0.38 mol/m^3 at 0.77 m.

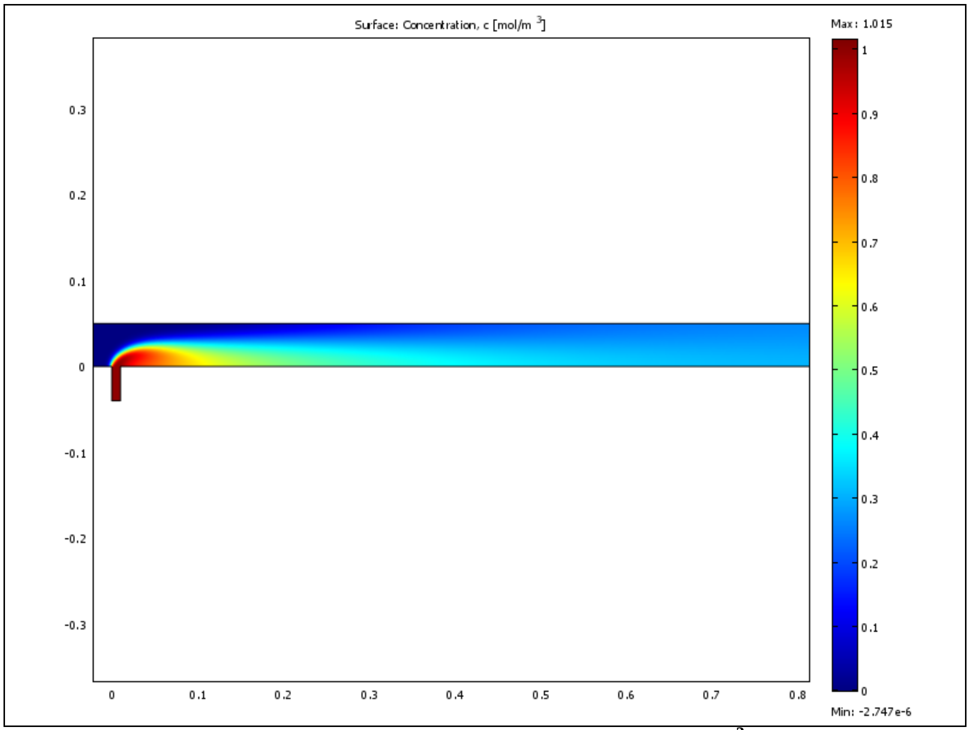

Figure 2. Surface plot – Concentration [mol/m^3].

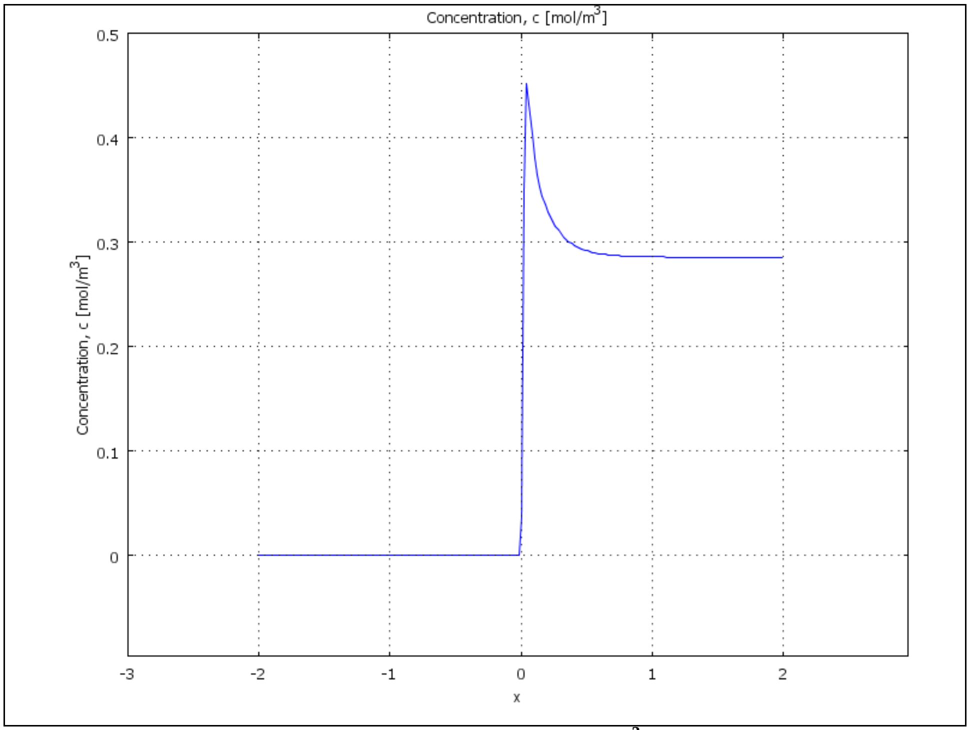

Figure 3. Line plot- concentration [mol/m^3] vs. length [m]

Figure 4 displays the flow's turbulent kinetic energy. This plot shows the model having the largest amount of turbulent kinetic energy after the point of hydrogen injection. The turbulent kinetic energy then disperses as the flow travels along the pipe.

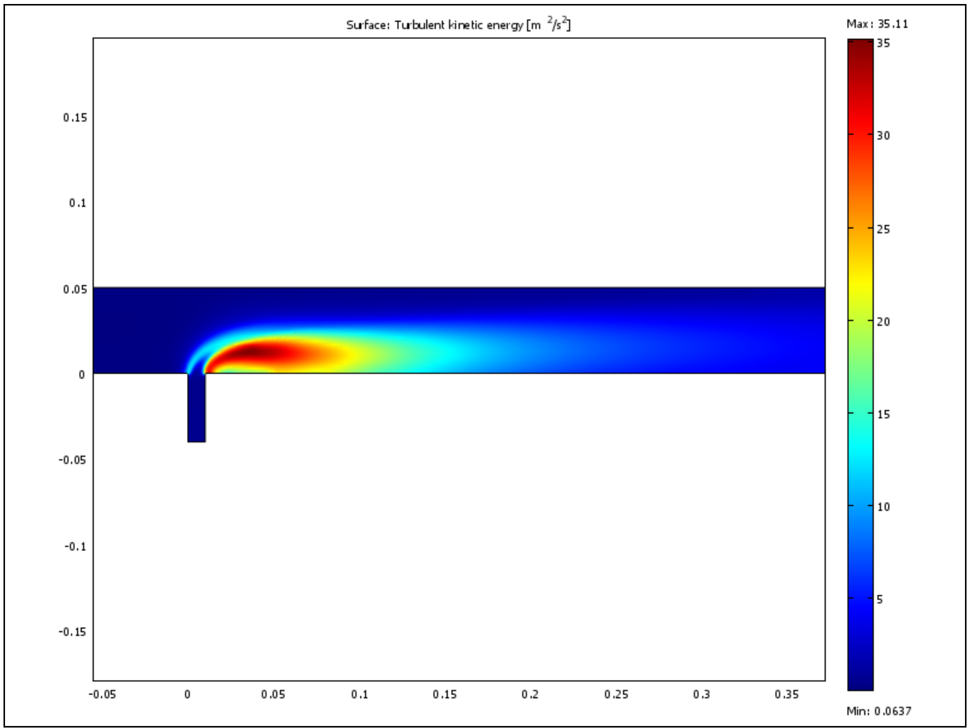

Figure 4. Surface plot – Turbulent kinetics energy [m^2/s^2].

Figure 5 is a surface plot of the system pressure. The system reaches a maximum pressure of ~198 Pa at the point hydrogen is injected. The jet of hydrogen creates a wall of flow in the vertical direction which the cross flow must build up pressure to breach. A negative pressure zone also develops to the right of the hydrogen jet. A vacuum is created by the flow moving quickly at the top of the pipe.

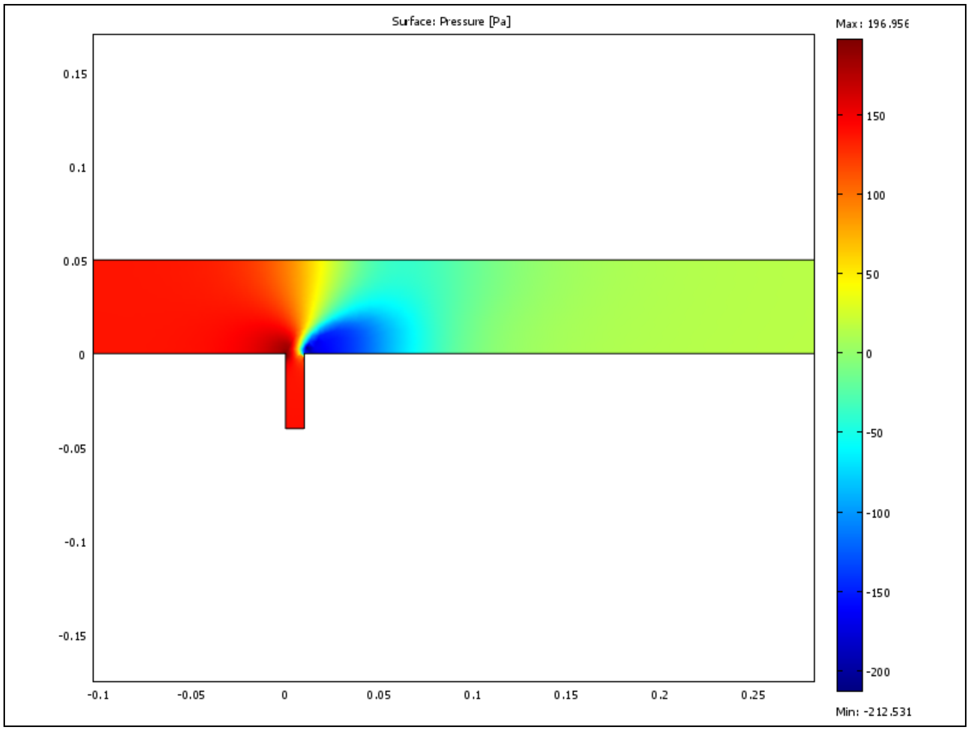

Figure 5. Surface plot – Pressure [Pa].

Figure 6 is a surface plot of the velocity field of the system. The greatest velocity is at the point at which hydrogen enters the air cross flow. Figure 7 is an arrow plot of the velocity field, which reflects the results from Figure 6.

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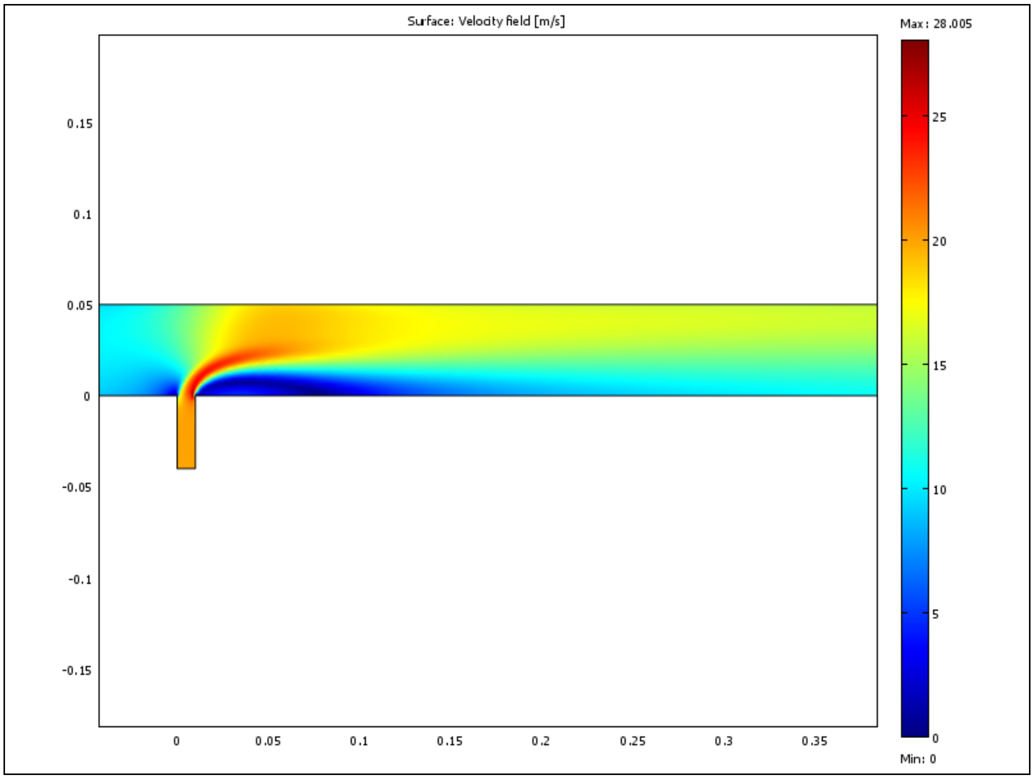

Figure 6. Surface plot – Velocity field [m/s].

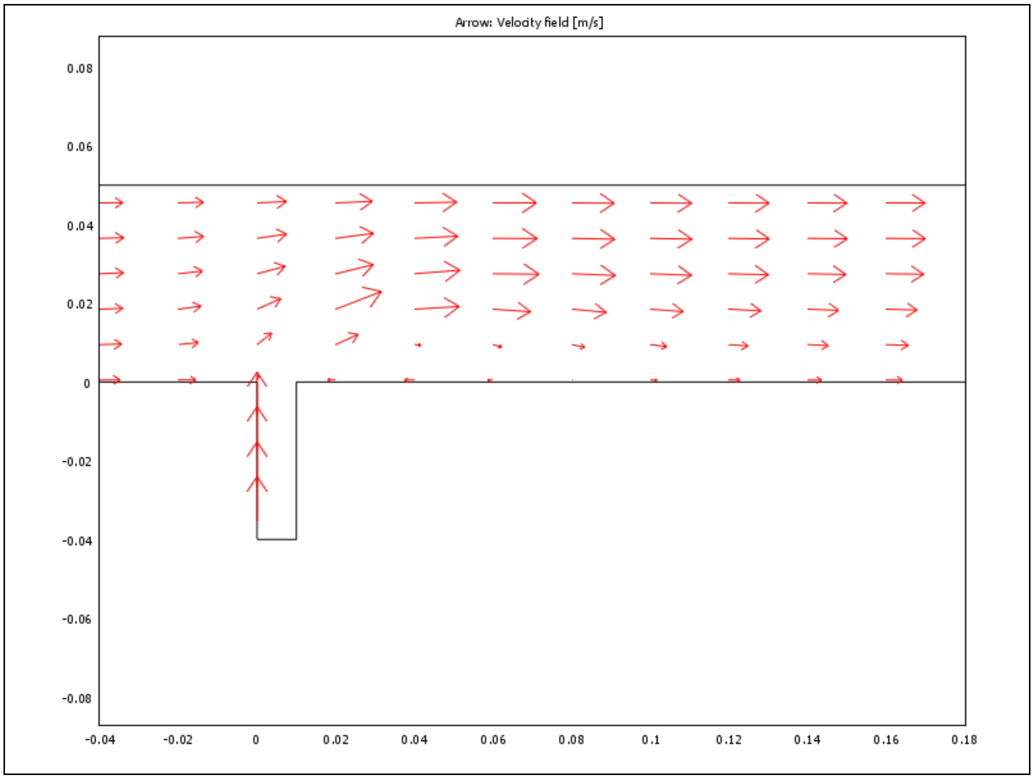

Figure 7. Arrow plot – Velocity field [m/s].

4. Validation

Literature containing numerical data on the mixing length of a hydrogen jet in an air cross flow could not be found. However, the results of this model can be qualitatively compared to figures of experiments from Smith et al. for validation [21]. In this paper, a jet of air concentrated with acetone vapor was introduced into a cross flow of air. The fluorescence of the acetone was measured with a laser to create visualizations. The experiments from Smith et al. used nearly the same dimensions of pipe diameter and similar flow rates as the model created in the project, which makes for an excellent comparison between the two.

Smith et al. uses a jet-to-crossflow velocity ratio, r, to compare flows of equal densities. In this equation U_j is the velocity field of the jet and U_{cf} is the velocity field of the cross flow.

$$r = \frac{U_j}{U_{cf}} \tag{17}$$

The model parameter of cross flow velocity was lowered to better compare it to the experimental results from Smith et al. Unfortunately the model would not converge if the jet velocity was increased to a value greater then 20 m/s due to a high Peclet number. Nonetheless, comparisons can be made.

Table 4. Parameters of model with adjusted velocity and parameters from Smith et al.

	r	U_{cf}	U_j	Jet dia.	Cross flow dia.
		[m/s]	[m/s]	[m]	[m]
Model w/ adj. vel.	4	5	20	0.010	0.050
Smith et al. (A)	10	5	50	0.005	0.054
Smith et al. (B)	10	5	50	0.010	0.054

Figures 8 and 9 are from Smith et al. Figure 8 is the side view of an ensemble-averaged concentration. Figure 9 is side view image of another experiment from Smith et al. only with a smaller jet diameter. These two figures look very similar to the concentration surface plot in Figure 10. Figure 10 shows more mixing than the figures of Smith et al., especially in the area to the lower right of the jet. This is due to the diffusion of hydrogen included in the model. Smith et al.'s experiments were air to air flows, which do not diffuse well. Figure 11 is the model without diffusion. Figure 11 has a more defined concentrated arc like the figures from the experiments. Figure 12, the velocity field of the model, shows the arc with even more definition. Overall, the experiential results from Smith et al. qualitatively validate the model created to measure the mixing length of a hydrogen jet in an air cross flow.

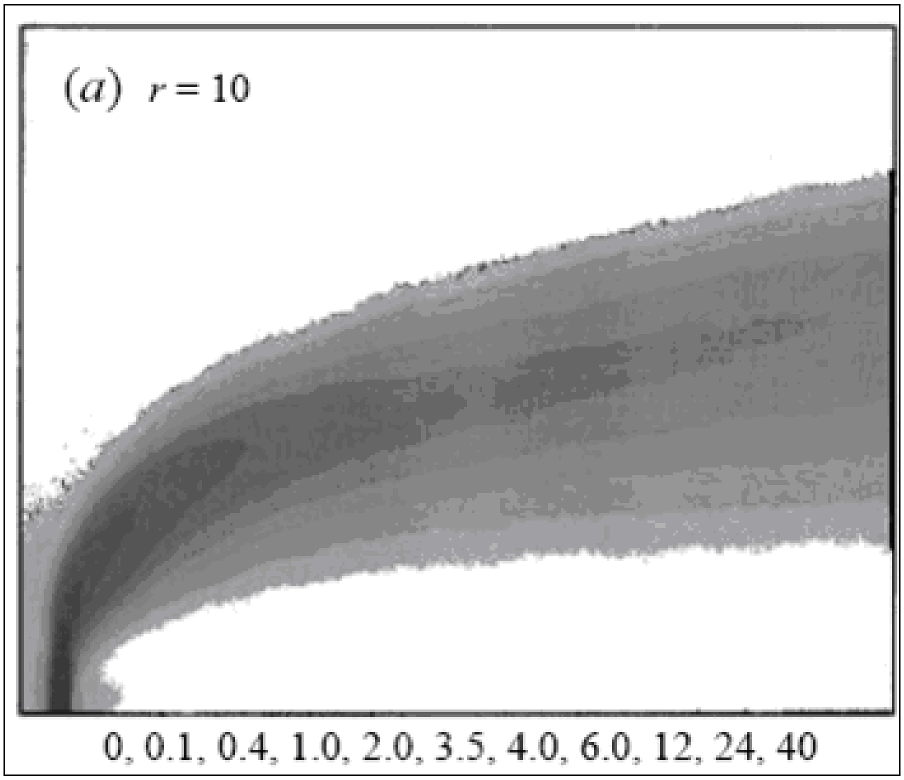

Figure 8. Smith et al. (A): Side-view ensemble-averaged concentration. Contour levels are given below each image in percent jet fluid concentration.

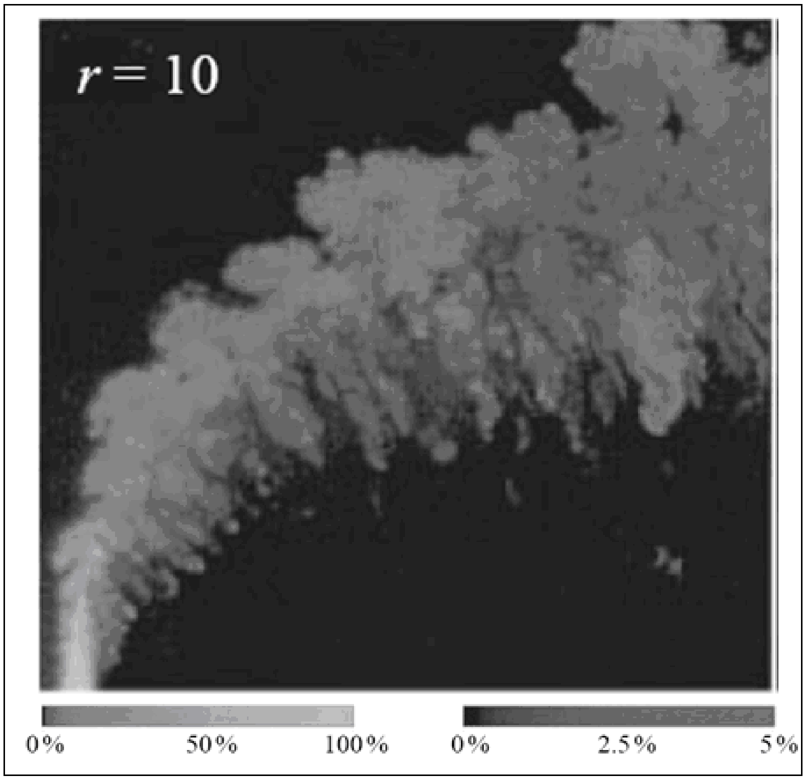

Figure 9. Smith et al. (B): Side-view images.

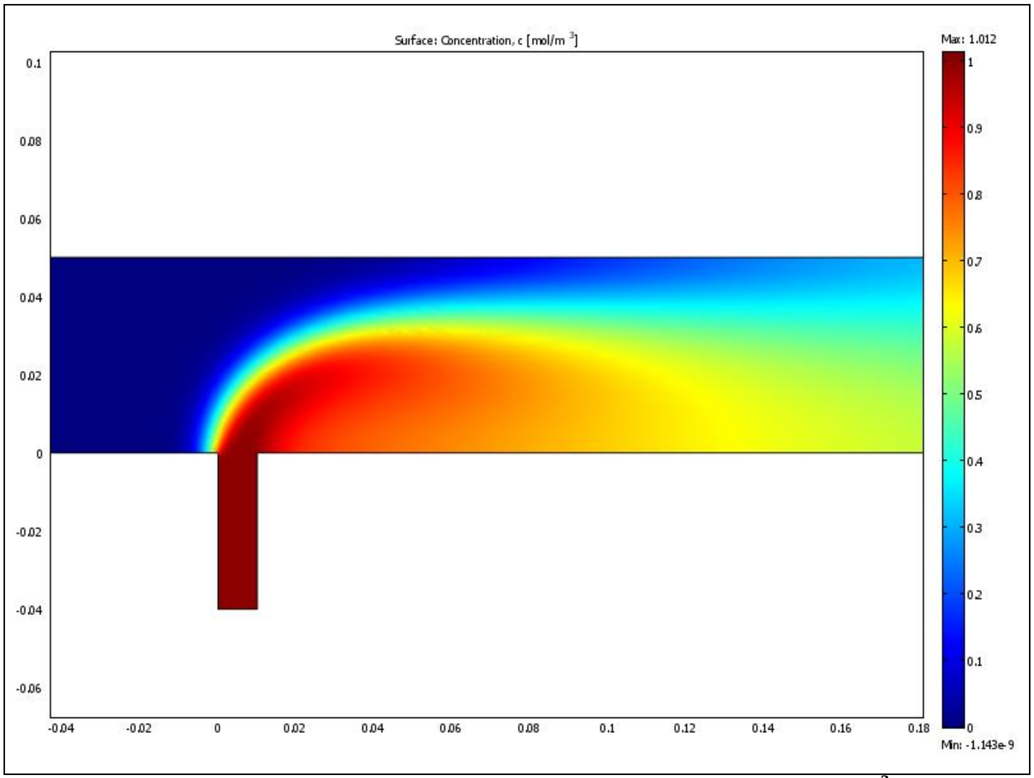

Figure 10. Surface plot with adjust speed – Concentration [mol/m^3]

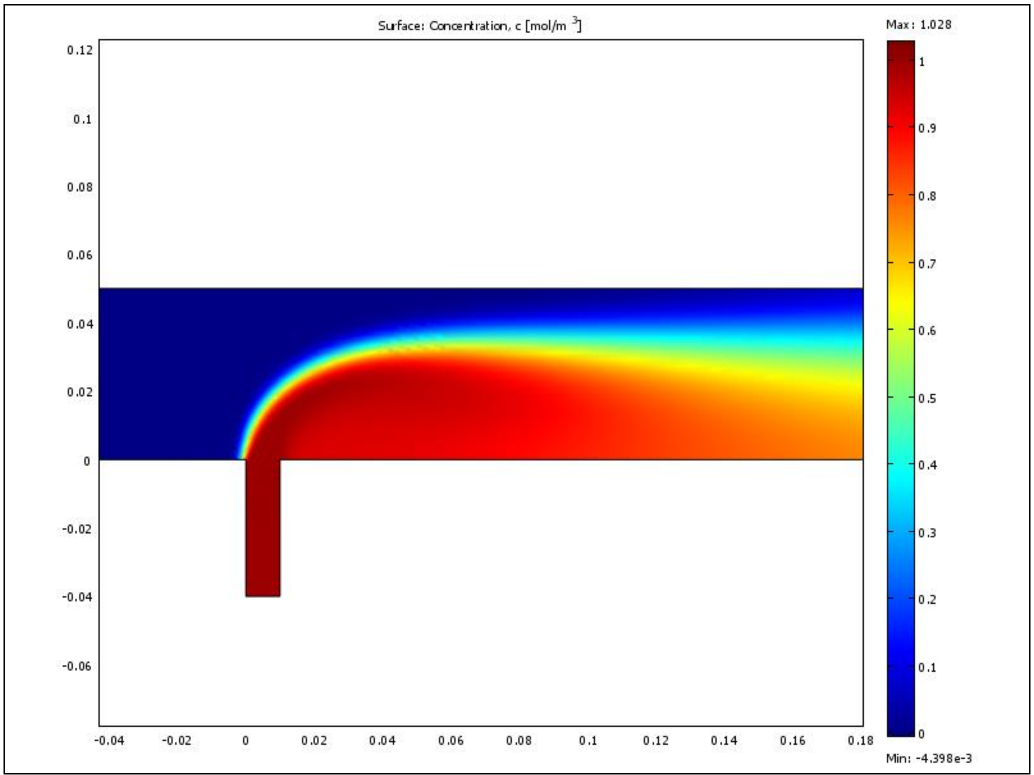

Figure 11. Surface plot with adjust speed – Concentration [mol/m^3]

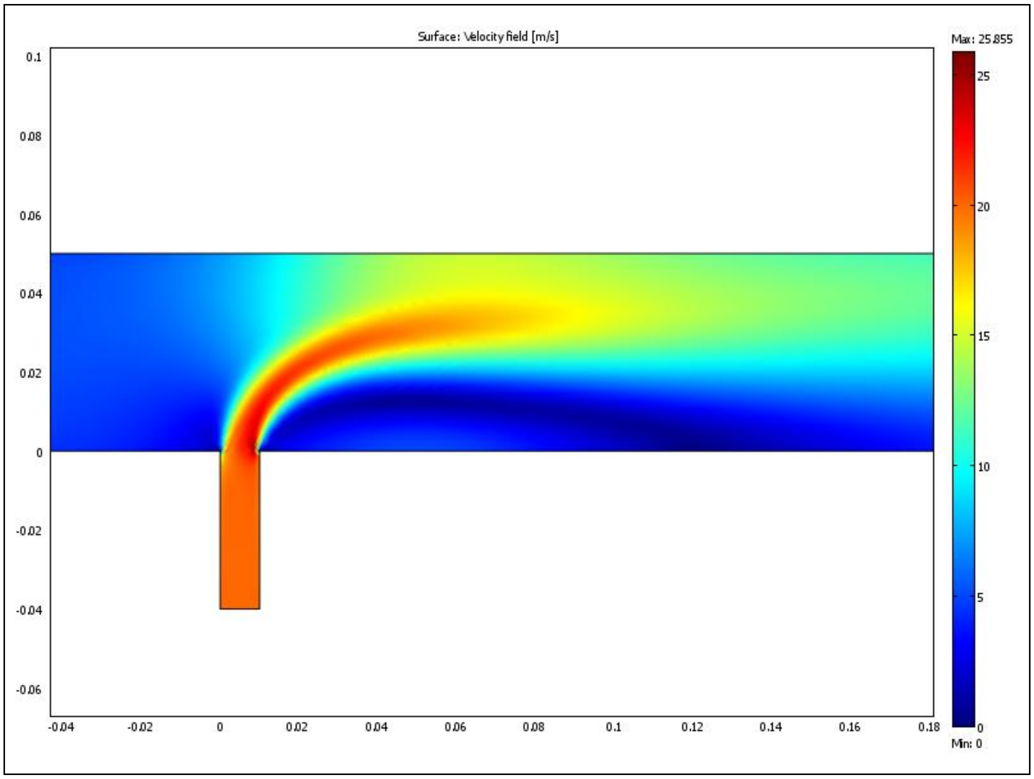

Figure 12. Surface plot – Velocity field [m/s]

Parametric study

Three parameters of the model were altered individually to complete a parametric study. The parameters were adjusted to see how the concentrations of hydrogen in the system would be affected. These parameters are flow velocity of the air cross flow, the velocity of the hydrogen jet and the diameter of the hydrogen jet. Each parameter was adjusted above and below that of the model's control settings. The cases of each parameter change made in the parametric study are given in Table 5.

Table 5. Control and cases for parametric study.

	U_{cf} *[m/s]*	**U_j** *[m/s]*	**Jet dia.** *[m]*
Control	10	20	0.01
Case 1	**5**	20	0.01
Case 2	**15**	20	0.01
Case 3	10	**15**	0.01
Case 4	10	**25**	0.01
Case 5	10	20	**0.005**
Case 6	10	20	**0.015**

Figure 13 gives the result of the parametric study in terms of concentration vs. pipe length. The results in this figure are predictable, such that cases which increase the volume of hydrogen versus air would increase the hydrogen concentration. In the figure, the point at which the parabola becomes a horizontal line is the mixing length.

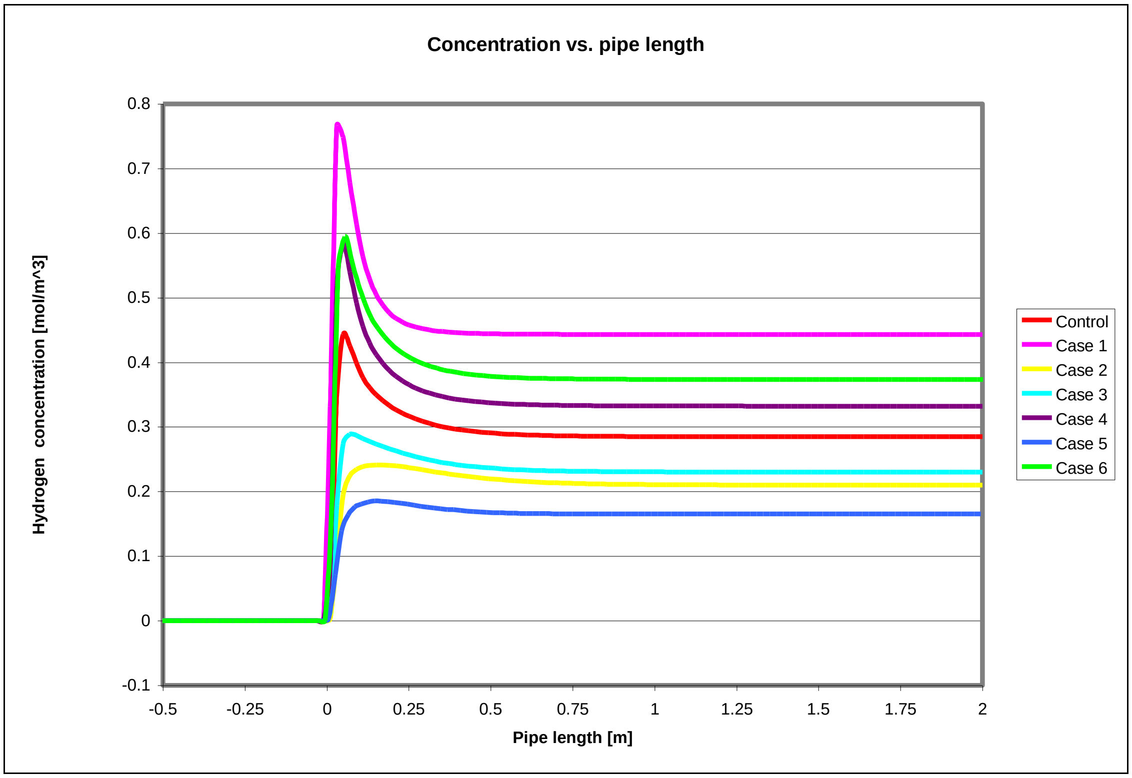

Figure 13: Concentration of case verses pipe length.

The mixing time of the cases was calculated. To do so, exact mixing length for each case was extracted from the data of Figure 13. The mixing length was assumed to be the point at which the standard deviation between data steps of 0.02 meters was less then 0.0001 for the concentration. Next the average velocity in the x-direction was extracted from the data of each case. Then the mixing time was calculated by dividing the mixing length by the average velocity. These results are given in Table 6.

Table 6: Mixing length, Average velocity and mixing time of parametric study cases.

	Mixing length *[m]*	**Average velocity** *m/s*	**Mixing time** *[s]*
Control	0.77	14.96	0.052
Case 1	0.55	9.99	0.055
Case 2	0.87	20.06	0.044
Case 3	0.79	13.79	0.058
Case 4	0.73	16.19	0.045
Case 5	0.65	13.03	0.050
Case 6	0.74	16.92	0.044

It can be concluded from Table 6 that the best mixing time occurs in Case 2 and Case 6. In Case 2 the cross flow velocity was increased to from 10 m/s to 15 m/s. In Case

6 the jet diameter is increased from 0.01 m to 0.015 m. These results show that the fast mixing is due to increased jet velocity and jet diameter.

Conclusion

A jet in a cross flow model was created to simulate the mixing of hydrogen being injected into the air intake of an engine for hydrogen assisted combustion. The model was governed by the turbulent incompressible Navier-Stokes equation and the convection diffusion equation. Given the parameters used in the model, hydrogen and air at a rate of 14.98 m/s homogenously mixed in 0.052 s at a length of 0.77 m. The model was found to qualitatively agree with results from a jet in a cross flow experiments which used air flowing into air. However, an experiment using hydrogen flowing into air with matching parameters is necessary to more completely validate the results of this model.

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