Exercise 7 - Determination of laminar flame speed of premixed methane-air mixture

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1. Introduction & Problem

Flame speed is the measure of the rate of expansion of a flame front in a combustion reaction. It can also be defined as the rate at which the unburnt mixture enters the flame. There are two primary types of flame speeds, laminar flame speed and turbulent flame speed. Laminar flame speed refers to the speed of a flame front propagating through a uniform, un-turbulent mixture. On the other hand, turbulent flame speed contains turbulence, which causes the flame front to behave irregularly such as swirling and eddies.

Accurate determination of flame speed is critical for several applications, including internal combustion engine design, optimization of combustion performance, development of predictive combustion models, and ensuring fire safety and explosion prevention. Additionally, flame speed measurements serve as a valuable tool for validating chemical kinetic mechanisms that describe complex combustion processes. By comparing computational predictions with experimental results, these mechanisms can be evaluated and refined for improved accuracy.

This report focuses on determining the laminar flame speed of a premixed methane-air mixture using numerical methods through Cantera and comparing the results with experimental data. We will examine two cases: the effect of varying initial pressure at constant temperature, and the effect of varying unburned mixture temperature at constant pressure, across an equivalence ratio range of 0.5 to 1.5.

2. Theory and Method

When calculating flame speed, one either chooses to keep the flame front stationary and move the fuel through the flame front or vice versa. In this report, we have chosen to go with the second approach and keep the liquids stationary. Cantera also offers several models to represent the reactive flows. They are:

- Freely propagating premixed flames (chosen model in this report)

- Burner stabilized premixed flames

- Counterflow (strained) premixed flames

Freely propagating premixed flames are flames where the fuel and oxidizer are mixed before ignition and the flame front propagates through the mixture without being stabilized by a burner or other solid structure. Burner stabilized premixed flames are the same with the difference that it's anchored to a boundary instead of being freely propagating.

Counterflow (strained) flames are a type of flame where the premixed fuel and oxidizer is forced to flow against a flow of hot combustion products or an inert gas, creating a stagnation point.
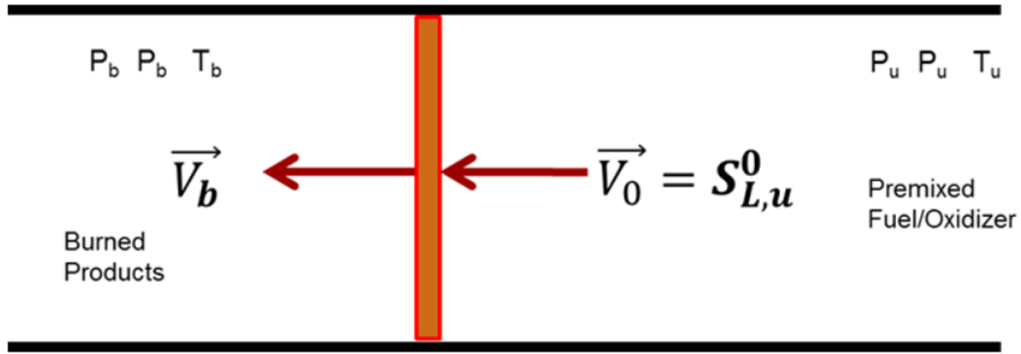
Freely propagating flame

Figure 1: Red illustrates the flame front. Left side is burned reacted products and the right side is the premixed fuel and oxidizer. Red arrows illustrate the path the fuel and oxidizer moves through the flame front.

Appropriate boundary conditions are essential to ensure reliable and meaningful results. For 1D reaction flow simulations, such as freely propagating premixed flames, Danckwerts boundary conditions can be applied.

Danckwerts boundary conditions are a set of conditions used to describe the behavior of concentration profiles at the inlet and outlet of a reactor. It's used when high reaction rates are anticipated near the inlet and calculates the flux of species across the boundaries instead of specifying the concentrations, see equation 1&2

$$\text{Inlet } (x = 0) \begin{cases} T = T_0 \\ \rho u \omega_k + \rho \omega_k V_k = (\rho u \omega)_0 \quad k = 1, ..., N_S \end{cases} \tag{1}$$

$$\text{Outlet } (x = L) \begin{cases} \frac{dT}{dx} = 0 \\ \frac{d\omega_k}{dx} = 0 \quad k = 1, ..., N_S \end{cases} \tag{2}$$

Because the mass flow rate of the mixture is a part of the solution, an additional constraint, temperature, is required. The temperature value is fixed at a specific x-value to ensure that the gradient at the inlet remains zero in order to prevent heat loss, see equation 3.

$$\begin{cases} \frac{dm}{dx} = 0 \\ T(x = x_{fixed}) = T_{fixed} \end{cases} \tag{3}$$

Where $\frac{dm}{dx} = 0$ ensures that there is no mass flux and T(x=x_{fixed}) = T$_{fixed}$ gives the specific coordinate the required temperature to fulfill the conditions.

Cantera's calculations of the flame speed follows the thermal theory of Mallard-Le Chatelier. The Mallard-Le Chatelier theory views flame propagation as a process of heat transfer. The heat conducted from the burning zone is equal to the heat required to raise the premixed mixtures temperature to the ignition temperature, from T$_0$ to T$_{ignition}$, see figure 2.
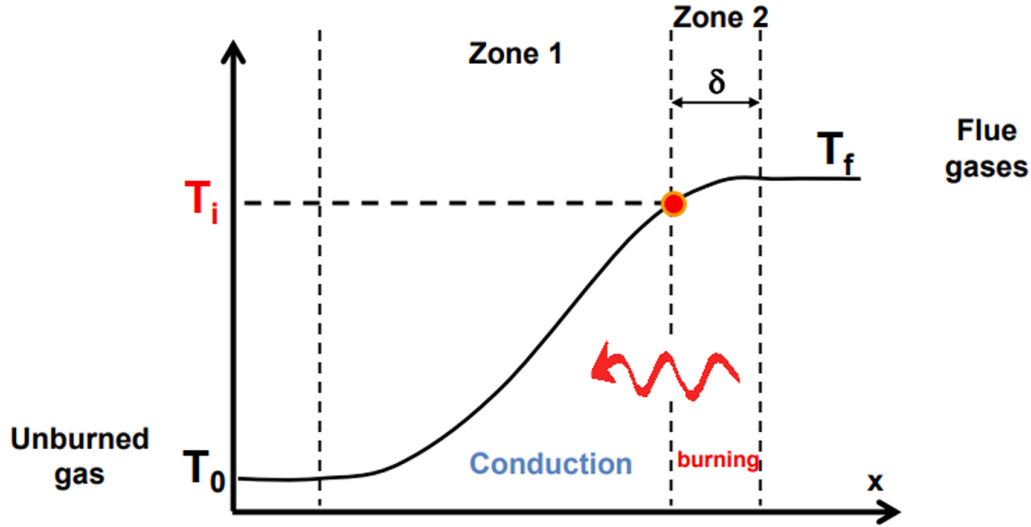
Figure 2: Visual illustration of Mallard-Le Chatelier thermal theory. T_0 equal the initial unburned temperature, T_f is the flue gases exiting temperature. Zone 1 represents the unignited mixture and zone 2 represents the burning zone where the mixture has been ignited. T_i represents the ignition temperature when crossing from zone 1 to zone 2.

By approximating the slope of the profile presented in figure 2 linearly, the enthalpy balance can be written as an equation 4 & 5. Where λ is the thermal conductivity, $\dot{m}$ is the mass flow rate per unit area, ρ is the unburned gas density and δ is the flame thickness. S_L is laminar flame speed, c_p specific heat capacity and T_0, T_i and T_f represent the initial-, ignition- and final temperature (AFT).

$$\dot{m}c_p(T_i - T_0) = \lambda(T_f - T_i)/\delta \tag{4}$$
$$\dot{m} = \rho \cdot S_L \tag{5}$$

3. Results

Two cases for laminar flame speed were calculated and compared to experimental results. Both cases calculated the laminar flame speed in the equivalence ratio range of 0.5-1.5.

Case 1 was calculated with an constant unburnt mixture temperature of 298 K with varying initial pressure at 1, 2, 5 and 20 atm, see figure 3.
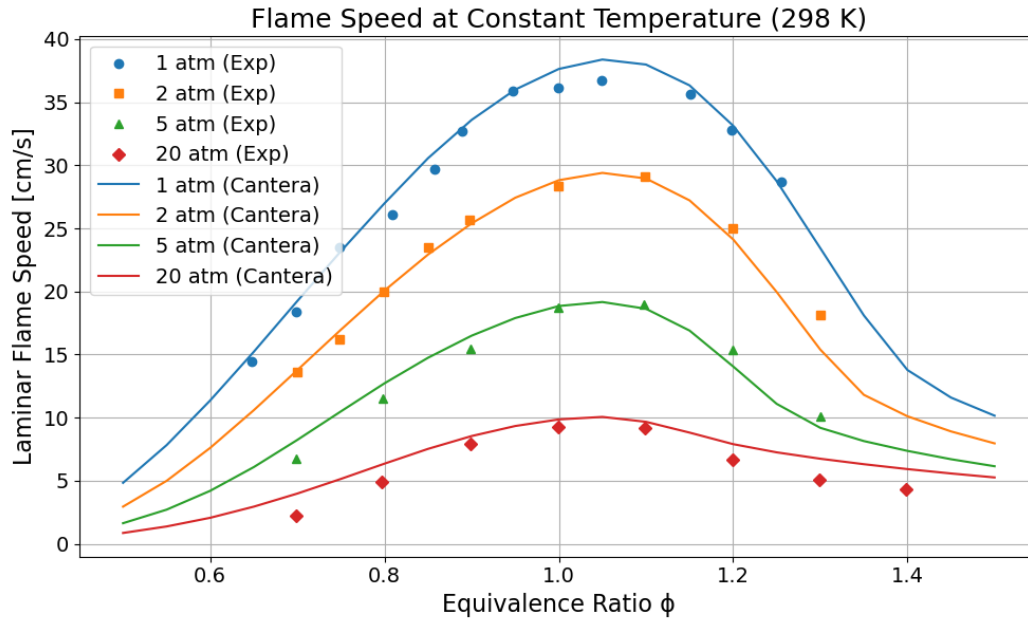
Figure 3: Cantera calculations for laminar flame speed against experimental data with constant temperature. Lines represent Cantera's calculated values and markers represent experimental data.

Case 2 was calculated with an constant initial pressure of 1 atm and with varying unburnt mixture temperatures of 358 K, 393 K and 428 K, see figure 4.
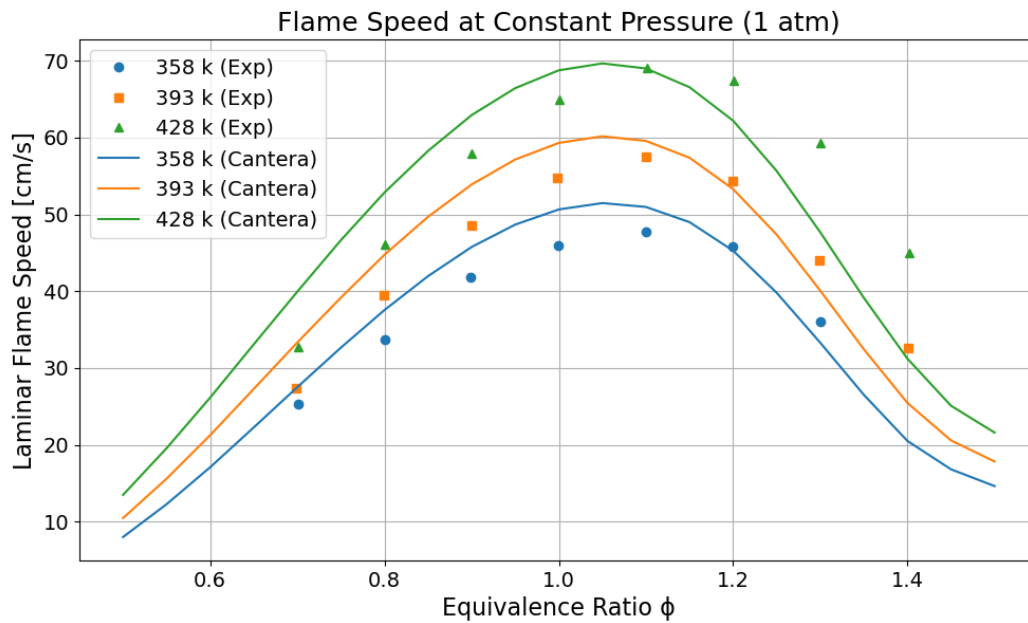

Figure 4: Cantera calculations for laminar flame speed against experimental data with constant pressure. Lines represent Cantera's calculated values and markers represent experimental data.

4. Discussion and Conclusion

For both cases, the maximum laminar flame speed is near stoichiometric conditions, between equivalence ratio 1∼1.1. This is consistent with other experiments that show the fuel and oxidizer are optimally balanced for complete combustion and maximal heat release within this range.

We see in Figure 3 that at constant temperature, increasing pressure leads to a decrease in laminar flame speed. This is likely because higher pressure shifts the reaction equilibrium toward radical termination reactions, such as $CH_4 \rightleftharpoons CH_3 + H*$, favoring the reverse direction. The increased collisional frequency at higher pressures enhances three-body recombination and termination reactions, reducing the concentration of key radicals like H, O, and OH that are essential for sustaining flame propagation. The higher pressure also increases the density of the unburned gas mixture. Limiting the ability of heat and reactive radicals to diffuse ahead of the flame front.

In figure 4, we see that at constant pressure, increasing temperature leads to an increase in laminar flame speed. An increase in initial temperature results in an increase in adiabatic flame temperature for the whole combustion. According to the Arrhenius equation, the reaction rate is proportional to the temperature, so a higher temperature leads to a higher reaction rate which increases the flame speed as more energy is released in a shorter amount of time.

The higher temperature also leads to a higher thermal diffusivity, which allows the heat to be transported more effectively between the flame front and the unburned mixtures, resulting in faster ignition and propagation.

The comparison between Cantera simulations and experimental data shows that Figure 3 matches the experimental data more closely than Figure 4. This discrepancy in Figure 4 may be attributed to limitations in the GRI-3.0 mechanism for small hydrocarbon chemistry (C1-C4). While the mechanism includes these several reactions for small chemistry, it might have incorrect values or pathways. This could be improved with examinations into the path flux or sensitivity analysis to see which reactions are missing or have incorrect values. By addressing the species and reactions that have the greatest impact on the model, we can increase the accuracy of our model.