

Velocity of laminar flame propagation vs pressure, temperature and fuel-to-oxidizer ratio

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1 Introduction

This paper presents results of an investigation of initial conditions' (temperature, pressure and mixture composition) influence on a laminar flame velocity. The calculations are carried out using Cantera 2.2. with Python 2.7, basing on "adiabatic flame.py" example. The hydrogen-oxygen mixture is used.

2 Mathematical model

Cantera models flames which are stabilized in an axisymmetric stagnation flow, and computes the solution along the stagnation streamline ($(r = 0)$), using a similarity solution to reduce the three-dimensional governing equations to a single dimension. The governing equations for a steady axisymmetric stagnation flow follow those derived in Section 6.2 of [1]:

Continuity:

$$\frac{\partial \rho u}{\partial z} + 2\rho V = 0 \quad (1)$$

Radial momentum:

$$\rho u \frac{\partial V}{\partial z} + \rho V^2 = -\Lambda + \frac{\partial}{\partial z} \left(\mu \frac{\partial V}{\partial z} \right) \quad (2)$$

Energy:

$$\rho c_p u \frac{\partial T}{\partial z} = \frac{\partial}{\partial z} \left(\lambda \frac{\partial T}{\partial z} \right) - \sum_k j_k c_{p,k} \frac{\partial T}{\partial z} - \sum_k h_k W_k \dot{\omega}_k \quad (3)$$

Species:

$$\rho u \frac{\partial Y_k}{\partial z} = -\frac{\partial j_k}{\partial z} + W_k \dot{\omega}_k \quad (4)$$

where ρ is the density, u is the axial velocity, v is the radial velocity, $V = \frac{v}{r}$ is the scaled radial velocity, Λ is the pressure eigenvalue (independent of z), μ is the dynamic viscosity, c_p is the heat capacity at constant pressure, T is the temperature, λ is the thermal conductivity, Y_k is the mass fraction of species k , j_k is the diffusive mass flux of species k , $c_{p,k}$ is the specific heat capacity of species k , h_k is the enthalpy of species k , W_k is the molecular weight of species k , and $\dot{\omega}_k$ is the molar production rate of species k . The tangential velocity ω has been assumed to be zero, and the fluid has been assumed to behave as an ideal gas. To help in the solution of the discretized problem, it is convenient to write a differential equation for the scalar Λ :

$$\frac{d\Lambda}{dz} = 0 \quad (5)$$

The boundary conditions are following:

Inlet boundary:

$$T(z_0) = T_0 \quad (6)$$

$$V(z_0) = V_0 \quad (7)$$

$$\dot{m}_0 Y_{k,0} - j_k(z_0) - \rho(z_0)u(z_0)Y_k(z_0) = 0 \quad (8)$$

$$\Lambda(z_0) = 0 \quad (9)$$

Outlet boundary:

$$\Lambda(z_{out}) = T_0 \quad (10)$$

$$\left. \frac{\partial T}{\partial z} \right|_{z_{out}} = 0 \quad (11)$$

$$\left. \frac{\partial Y_k}{\partial z} \right|_{z_{out}} = 0 \quad (12)$$

$$V(z_{out}) = 0 \quad (13)$$

Symmetry boundary:

$$\rho(z_{sym})u(z_{sym}) = 0 \quad (14)$$

$$\left. \frac{\partial V}{\partial z} \right|_{z_{sym}} = 0 \quad (15)$$

$$\left. \frac{\partial T}{\partial z} \right|_{z_{sym}} = 0 \quad (16)$$

$$j_k(z_{sym}) + \dot{s}_k W_k = 0 \quad (17)$$

where \dot{s}_k is the molar production rate of the gas-phase species k on the surface. In addition, the surface coverages θ_i for each surface species i are computed such that $\dot{s}_i = 0$.

3 Results

The calculations were performed mainly using Cantera's "freeFlame" function. The plots show how the flame speed changes with air-fuel equivalence ratio, pressure and temperature. Each plot presents results for one parameter fixed, one changing gradually and one changing continuously. The temperature range is set at 250 - 750K, leaving a safe gap to the self-ignition range. Ranges of pressure and air-fuel equivalence ratio are 0.5 - 4 bar and 0.1 - 3 accordingly.

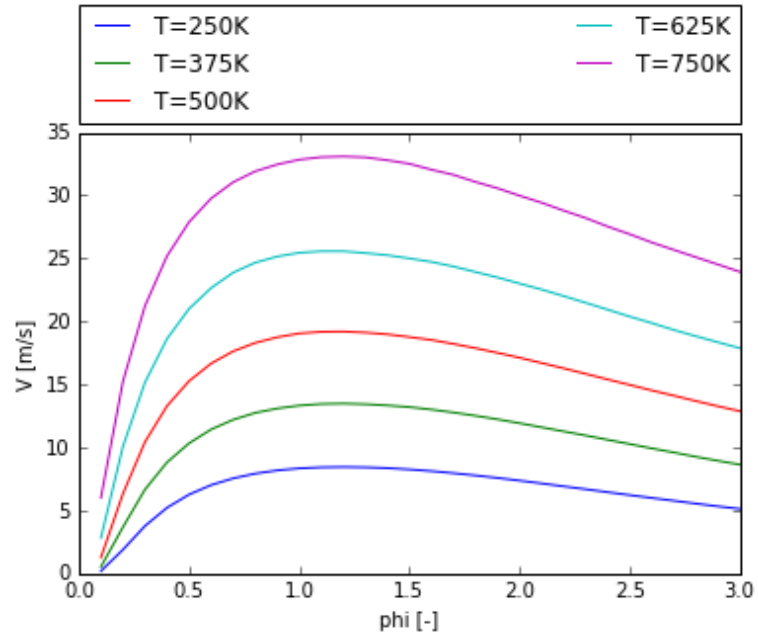


Figure 1: Laminar flame speed vs air-fuel equivalence ratio and temperature.
 $p = 1 \text{ bar}$

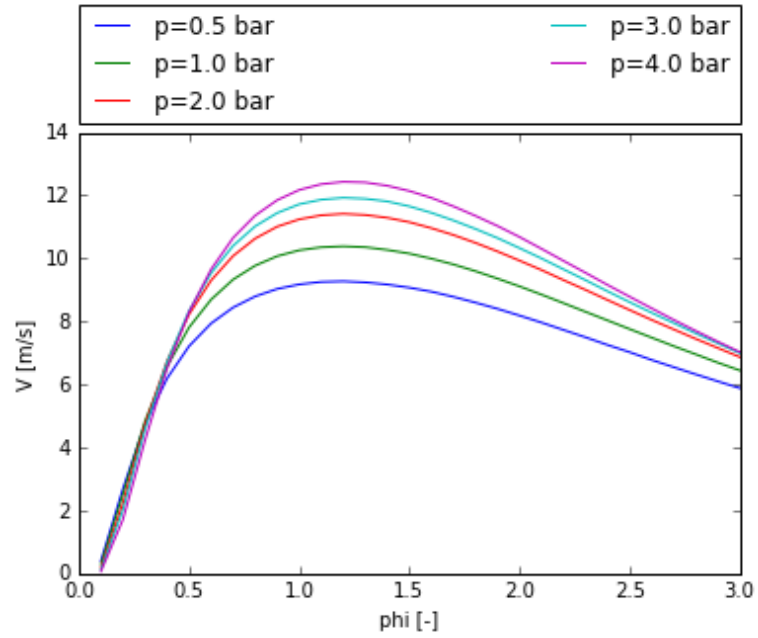


Figure 2: Laminar flame speed vs air-fuel equivalence ratio and pressure.
 $T = 300K$

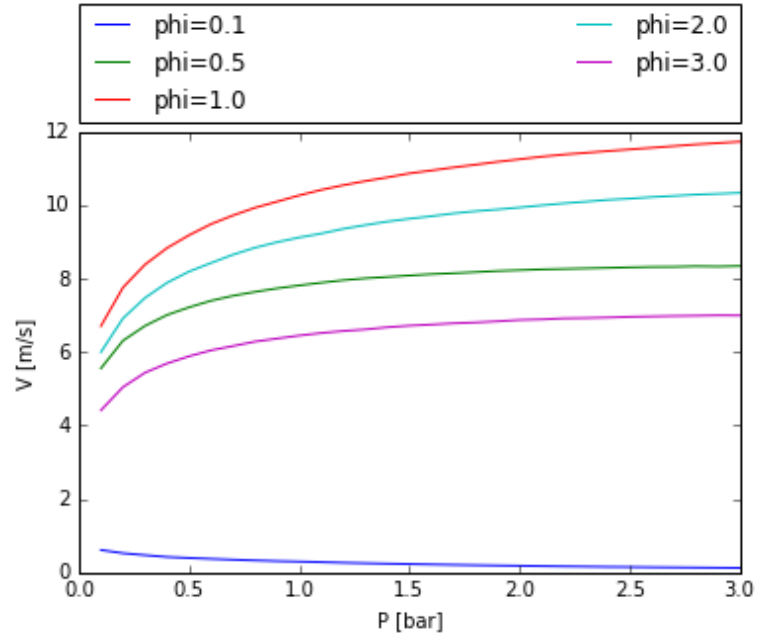


Figure 3: Laminar flame speed vs pressure and air-fuel equivalence ratio.
 $p = 1 \text{ bar}$

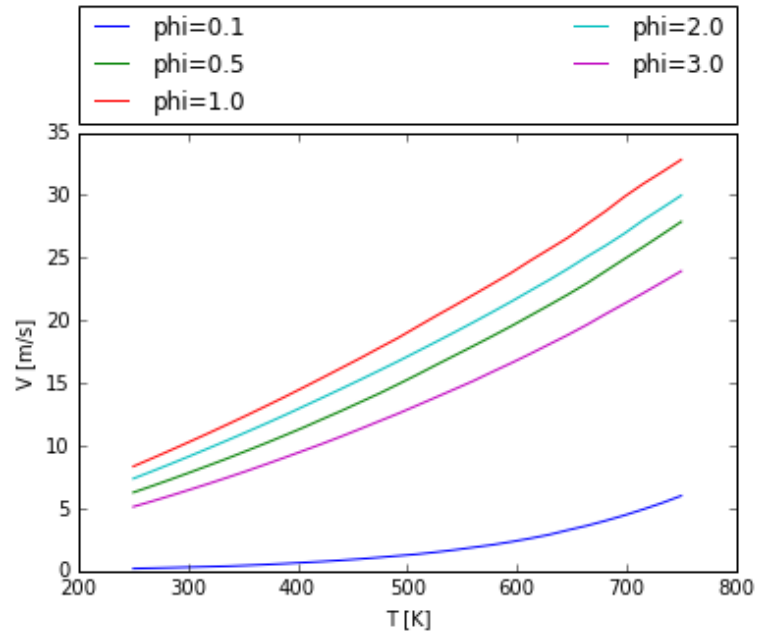


Figure 4: Laminar flame speed vs temperature and air-fuel equivalence ratio.
 $T = 300K$

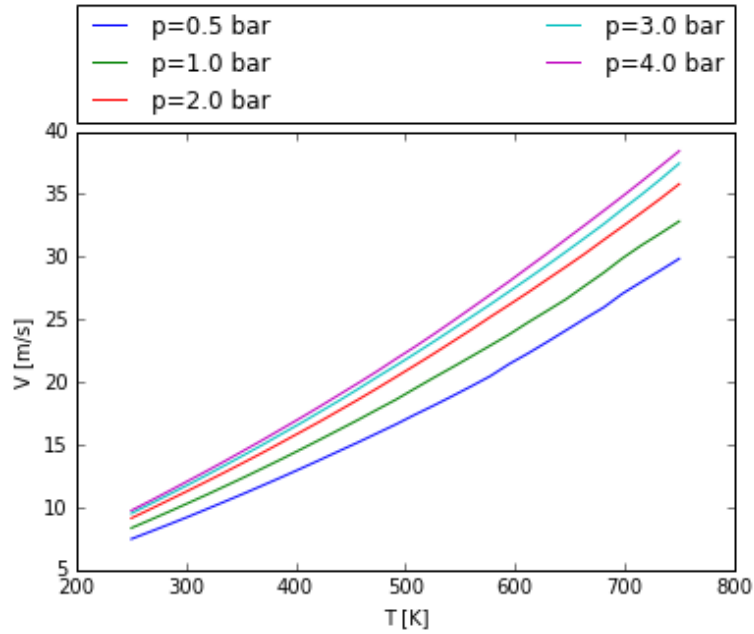


Figure 5: Laminar flame speed vs temperature and pressure. $\phi = 1$

4 Summary

As it can be seen, the strongest factor affecting the flame propagation speed is the temperature, with pressure being less influential. As expected, the maximum speeds occur at the equivalence ratio equal to 1, corresponding to the stoichiometric mixture. An interesting phenomenon happens for a very lean mixture ($\phi = 0.1$), where the flame speed gets lower with growing pressure.

5 References

- [1] Kee, Coltrin, Glarborg: Chemically Reacting Flow. Wiley-Interscience, 2003
- [2] www.cantera.org