

## Chapter 2

### Physically-Based Heat Release Model

To analyze and control thermoacoustic instabilities in the combustor, it is necessary to have a high-level mathematical model that captures the relevant characteristics of the system. As we indicated for the feedback structure of the system in Figure 1, the crucial element of such a model is a physically-based mathematical description of the heat release rate of the flame. As a first step in this effort, we consider a burner-stabilized, laminar premixed flame in a laboratory tube combustor. Beginning with the chemical kinetics of methane-air premixed combustion, flame dynamics are studied from the governing equations. With a set of simplified partial differential equations and proper physical constraints, the problem is converted into a two-point boundary condition problem. As an initial step, the steady-state temperature and species mass fraction profiles are obtained using the shooting method. Moreover, a finite difference method is formulated by discretizing the equations spatially in order to solve for the time-dependent solutions. Our goal is to build a physically-based heat release model that captures the relevant dynamics from the incoming mixture flow rate changes to the output heat release rate to the fluid.

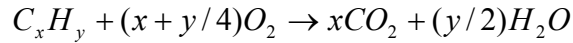
#### 2.1 Chemical Kinetics and Flame Dynamics

In this section, we will review the chemical kinetics of a laminar premixed flame. The chemical process of lean premixed methane air combustion will be approximated by a simple, one-step, global reaction mechanism with high activation energy and a proper pre-exponential factor. Starting from conservation of mass, momentum and energy, we can model the flame dynamics with a set of partial differential equations. Those equations will be solved in the following section by means of finite difference simulation. In

section 3.3.5, we will show that the modeled flame dynamics exhibits a thermo-diffusive instability at high Lewis numbers, as predicted by Margolis and others, resulting in a limit cycle in the absence of acoustic feedback [Mar80]. At low Lewis number, the linearized flame model is stable, as expected.

### 2.1.1 Simplified Chemical Kinetics of Laminar Premixed Flame

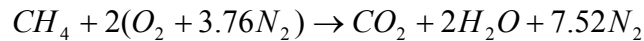
Combustion includes many chemical chain reactions and many intermediate species are involved. The hydrocarbon reaction with oxidizer includes more than 200 reaction steps [Tur96]. To model this combustion process, we use a simple global reaction mechanism as a first step. The one-step reaction mechanism of a conventional hydrocarbon fuel can be written as,



The rate of fuel consumption is usually expressed using an Arrhenius term,

$$\frac{d[C_xH_y]}{dt} = -Ae^{-E_a/R_uT} [C_xH_y]^m [O_2]^n$$

Here, we will study the premixed laminar flame with methane (CH<sub>4</sub>) as the fuel and air as oxidizer. A global reaction mechanism is proposed with high activation energy ( $E_a$ ) and a proper pre-exponential factor ( $A$ ) to approximate the complex reactions. A common assumption is that the powers of the mole concentrations of the fuel and oxidizer correspond to the mole ratio. For a premixed laminar flame, methane reacts with air in the form of,



Where  $m = 1$ ,  $n = 1$ ,  $A = 2.2 \times 10^{22} (gmol/cm^3)^{1-m-n} / s$ ,  $E_a = 40 kcal / gmol$ . This global reaction mechanism is comparable with the ChemKin result in terms of steady state temperature and fuel mass fraction profiles. (ChemKin is a combustion code for steady state solution of chemical reactions by Sandia National Laboratory.) Over 40 chemical

reactions are involved in the computation of a steady-state profile for the methane reaction using ChemKin [Kee85].

### 2.1.2 Governing Equations of Flame Dynamics

The development of our physically based model begins with the governing conservation equations of the laminar premixed flame. We assume that fuel is the limiting species, so that combustion is lean. Equivalence ratio, which is defined as the stoichiometric air-fuel ratio over the actual air-fuel ratio of the mixture, is commonly used to indicate quantitatively whether a fuel-oxidizer mixture is rich, lean or stoichiometric. Here, we study lean premixed laminar flame, and equivalence ratio  $\phi < 1$ . The following conservation equations are derived from control volume analysis of a gaseous premixed combustor [Spa56][Tur96].

Conservation of mass:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} = 0 \quad (2.1)$$

Conservation of species:

$$\frac{\partial Y_k}{\partial t} + u \frac{\partial Y_k}{\partial x} = \frac{1}{\rho} R_k M_k + \frac{1}{\rho} \frac{\partial}{\partial x} (\rho D_k \frac{\partial Y_k}{\partial x}) \quad (2.2)$$

Conservation of energy:

$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} = -\frac{1}{\rho C_p} \sum R_k M_k h_k + \frac{1}{\rho C_p} \frac{\partial}{\partial x} (\lambda \frac{\partial T}{\partial x}) + \sum_{k=1}^N \frac{C_p^{(k)}}{C_p} D_k \frac{\partial Y_k}{\partial x} \frac{\partial T}{\partial x} \quad (2.3)$$

It is simple to eliminate the continuity equation by means of streamline function,

$$\psi(x, t) = \int_0^x \rho(\bar{x}, t) d\bar{x} \quad (2.4)$$

The coordinate transformation becomes,

$$\frac{\partial}{\partial x} \rightarrow \frac{\partial \psi}{\partial x} \frac{\partial}{\partial \psi} = \rho \frac{\partial}{\partial \psi} \quad (2.5)$$

$$\frac{\partial}{\partial t} \rightarrow \frac{\partial \psi}{\partial t} \frac{\partial}{\partial \psi} + \frac{\partial}{\partial t} = (-\rho u + m_0) \frac{\partial}{\partial \psi} + \frac{\partial}{\partial t} \quad (2.6)$$

We make the additional assumptions that  $c_p$ ,  $\rho\lambda$ , and  $\rho^2D$  are constant and equal for all species. Although these assumptions could be relaxed in the future, they considerably simplify the equations. The equations can be simplified as, [Mar80]

$$\frac{\partial Y}{\partial t} + m_0 \frac{\partial Y}{\partial \psi} = \rho^2 D \frac{\partial^2 Y}{\partial \psi^2} - \rho^{-1} RM \quad (2.7)$$

$$\frac{\partial T}{\partial t} + m_0 \frac{\partial T}{\partial \psi} = \frac{\rho\lambda}{c_p} \frac{\partial^2 T}{\partial \psi^2} + \frac{RM}{\rho c_p} (h_r^o - h_p^o) \quad (2.8)$$

where  $T$  is the temperature,  $Y$  is the mass fraction of the fuel (assumed to be the limiting species) and  $R$  is the rate term in Arrhenius form,

$$R = \nu_f k \rho^{\nu_f + \nu_o} M_o^{-\nu_o} M_f^{-\nu_f} Y_o^{\nu_o} Y_f^{\nu_f} e^{-E/RT} . \quad (2.9)$$

where  $Y_f$ ,  $Y_o$  is the mass fraction of the fuel and oxidizer, and  $M_f$ ,  $M_o$  are molecular weights.  $\nu_f, \nu_o$  are the corresponding stoichiometric coefficients and  $k$  is the pre-exponential constant. One consequence is that the equations for the different mass fractions are not independent and only the fuel mass fractions must be tracked. The mass fraction for  $O_2$  is computed from the fuel mass fraction using

$$\Delta Y_{O_2} = \Delta Y_{CH_4} \frac{M_{O_2}}{M_{CH_4}} \frac{\nu_{O_2}}{\nu_{CH_4}} \quad (2.10)$$

The streamline coordinate transformation causes the input to the flame model,  $m_0 = \rho_o u_o$ , to be an explicit part of the equations. The output of the system is the rate of heat release to the fluid that is given by

$$Q_{fluid} = \int_0^{\infty} R \Delta H_{react} \rho d\psi - \rho \lambda \left. \frac{\partial T}{\partial \psi} \right|_{\psi=0} \quad (2.11)$$

where the first term represents the heat produced by reaction and the second term denotes heat loss to the burner through conduction. By solving the steady-state equations numerically, we can find the profiles  $Y^o$  and  $T^o$  at the nominal flow velocity. Physically the reaction is completely stopped at  $\psi = \infty$ , which corresponds to constant values of  $T$  and  $Y$ . It is also proper to assume that the incoming mixture is at the burner temperature. The initial mass fraction at  $\psi = 0$  is calculated according to Fick's law. The relevant boundary conditions are:

$$Y|_{-\infty} = Y|_0 - \frac{\rho^2 D}{m_0} \left. \frac{\partial Y}{\partial \psi} \right|_0 \quad (2.12)$$

$$T|_0 = T_{burner} \quad (2.13)$$

$$\left. \frac{\partial T}{\partial \psi} \right|_{\infty} = 0 \quad (2.14)$$

$$\left. \frac{\partial Y}{\partial \psi} \right|_{\infty} = 0 \quad (2.15)$$

To understand the flame dynamics, it is necessary to solve the above simplified temperature and species equations with consideration of the two-point boundary conditions.

## 2.2 Steady-State and Time-Dependent Solutions

The Flame dynamics are described by the partial differential equations (2.7-2.8) subject to the boundary conditions (2.12-2.15). To study the dynamic response of the heat release model, a steady-state, also called equilibrium solution, should be obtained as an initial step. The single step global reaction mechanism that we proposed in the previous section is used while solving the steady state and time-dependent problems. The shooting method is used to search for steady state temperature and species profiles, and the results compare favorably with ChemKin. The finite difference method is then applied to solve the partial differential equations to obtain time-dependent solutions of the flame model. With a reasonable initial guess, the simulation will eventual converge to nominal profiles as time goes on.

### 2.2.1 Shooting Method for Steady-State Profiles

To obtain the steady-state solution of the temperature and species profile, there are a couple of approaches. In steady state, time derivatives are zero. So, equations (2.7-2.8) can be expressed as,

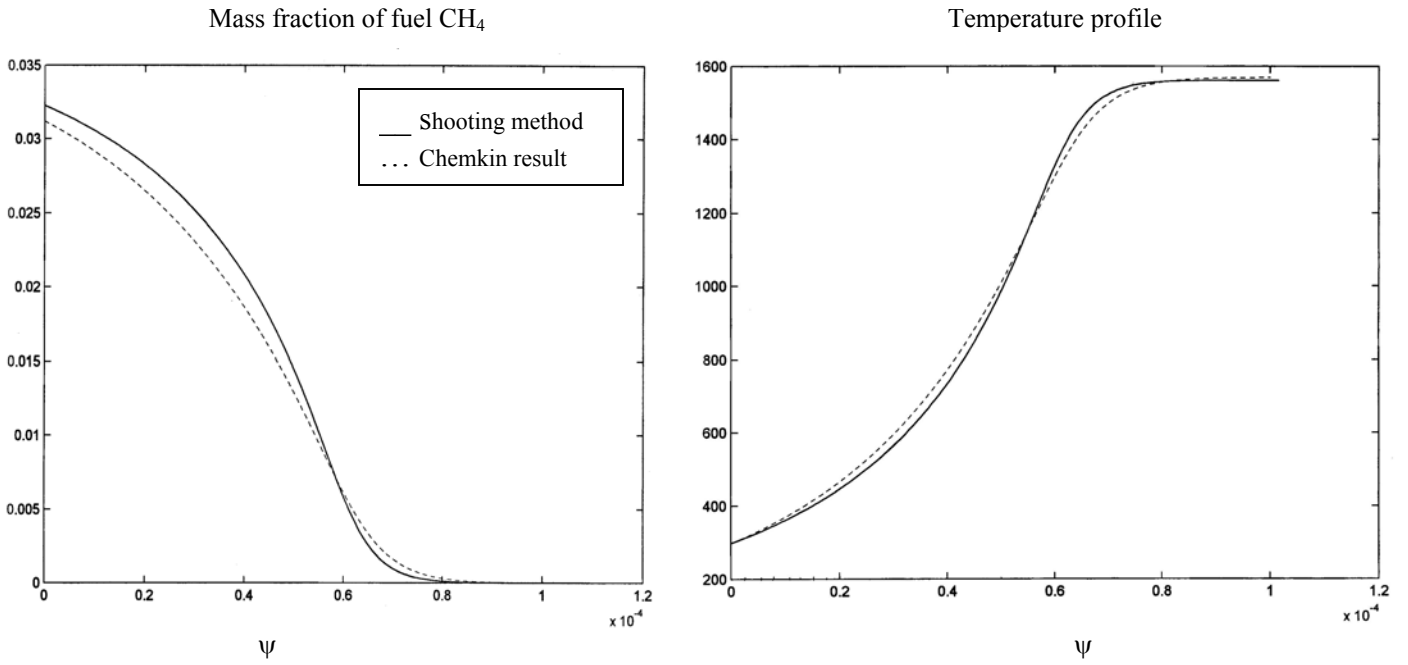
$$\frac{\partial Y}{\partial t} = m_o \frac{\partial Y}{\partial \psi} - \rho^2 D \frac{\partial^2 Y}{\partial \psi^2} + \rho^{-1} RM = F_1(u, T, Y) = 0 \quad (2.16)$$

$$\frac{\partial T}{\partial t} = m_o \frac{\partial T}{\partial \psi} - \frac{\rho \lambda}{c_p} \frac{\partial^2 T}{\partial \psi^2} - \frac{RM}{\rho c_p} (h_r^o - h_p^o) = F_2(u, T, Y) = 0 \quad (2.17)$$

Our initial approach is choosing a shooting method to solve the coupled partial differential equations.

We can easily meet the first two boundary conditions (2.12-2.13) by approximately setting the initial condition before the integration. The steady state solution has a nice property that spatial derivatives of temperature and species mass fraction approach zero at  $\psi = \infty$ . Tentatively giving some initial derivatives  $\left. \frac{\partial T}{\partial \psi} \right|_{\psi=0}$  and

$\frac{\partial Y}{\partial \psi} \Big|_{\psi=0}$ , our problem is to force two gradients at infinity to be zero. Considering the physical constraints, the temperature must increase and species be consumed in the positive spatial direction. The shooting method searches for proper initial gradients that will result in zero gradients at infinity after integration. Instead of integration towards infinity, which is not practical, the temperature and species profile is expected to be constant at the end of the combustion zoom. A sample steady-state solution is shown in Figure 2.1. The following conditions are assumed: incoming mixture flow velocity  $u_0 = 6$  cm/s, burner temperature  $T_{\text{burner}} = 300$  K, specific heat  $C_p = 1.094$  J/g-K, heat conductivity  $\lambda_0 = 2.64e-4$  J/cm-K-s, thermal diffusivity  $D_0 = 0.210$  cm<sup>2</sup>/s and Lewis number 1. Figure 2.1 also shows the comparison of the profiles with the Chemkin result. This shows the reasonableness of our method for steady state solution as well as our assumption of a single-step reaction mechanism with high activation energy that we proposed in the previous section. (ChemKin is a well-known combustion code that computes species and temperature profiles in steady-state burner-stabilized premixed laminar flames. The program accounts for finite rate chemical kinetics and molecular transport [San85].)



**Figure 2.1 Steady-state profiles for temperature and mass fraction of fuel**

### 2.2.2 Finite Difference Method for Time-Dependent Simulations

Theoretical investigations of premixed laminar flames have essentially followed two different approaches. One formulation is to seek an analytical solution of the conservation equations. By means of transformation and mathematical manipulations, it was formulated into an eigenvalue problem, and linear stability analysis was performed to study the flame dynamics [Mar79][Jou79]. Another approach is numerical simulations. This approach is more straightforward, and it can be attacked without too much knowledge of the flame speed and flame propagation. The finite difference or finite element methods are widely used to solve partial differential equations numerically if there is no straight analytical solution available.

To simulate the dynamic response of a laminar premixed flame in a finite length tube combustor, we need to solve the above governing equations with boundary conditions. We discretize the Lagrangian coordinate variable  $\psi$  into a number of equal distance locations that replaces the continuous problem domain by a finite difference



mesh or grid. The number of points  $n$  must be selected to guarantee consistence and convergence. With the consideration of the two point boundary values, the original PDE is converted into a set of  $(n - 2)$  ordinary differential equations (ODE). The ODEs re integrated to approximate the exact solution of the original PDE. First and second derivatives are obtained by “central” difference approximation: ( $h = \Delta\psi$ )

$$\frac{\partial T}{\partial x} = \frac{T_{i+1} - T_{i-1}}{2h} + O(h^2) \quad (2.18)$$

$$\frac{\partial^2 T}{\partial x^2} = \frac{T_{i+1} - 2T_i + T_{i-1}}{h^2} + O(h^2) \quad (2.19)$$

Starting the integration from the nominal steady-state solutions, we obtain the dynamic response of the system. Further grid refinement proves the consistency of the finite difference approximation

Since the flame zone is relatively small compared with the geometry of a tube combustor, we are only interested in a one-dimensional flame model that describes the local zone ( $\approx 1$  cm). The boundary condition at infinity was applied at the end of the local zone where the temperature and species profiles are steady, such that the first derivative approaches zero. The number of grid points was chosen to be sufficiently large so that truncation error is small. 82 points were used, which results in  $n - 2 = 80$  discrete points generating a system with 80 ordinary differential equations. A time step of  $10^{-4}$  seconds was used.

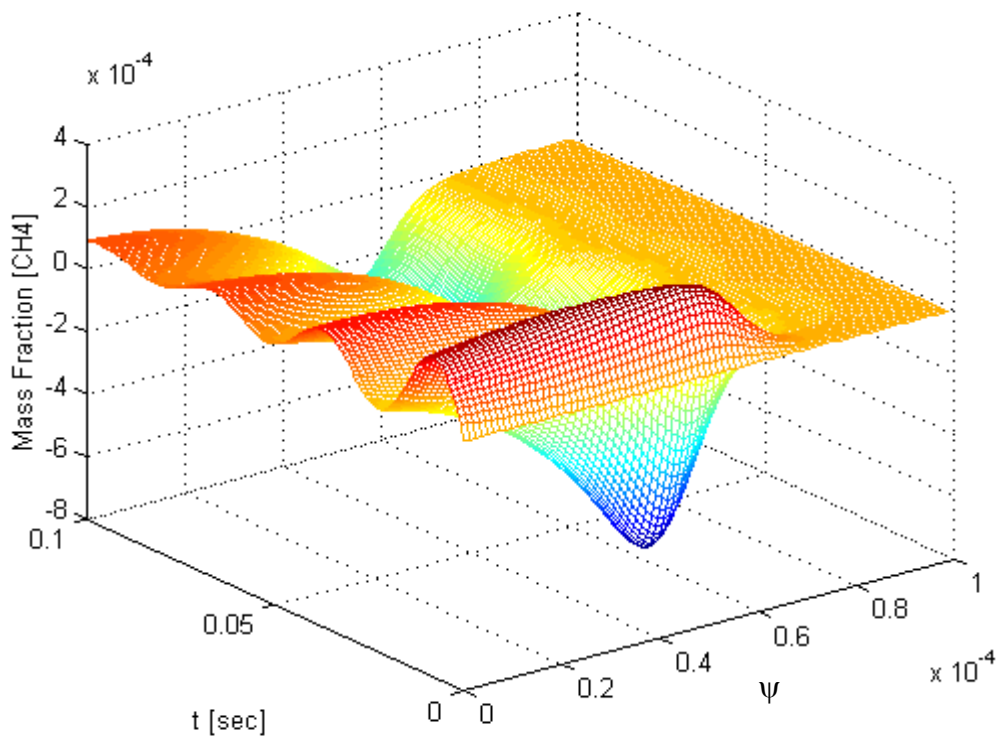
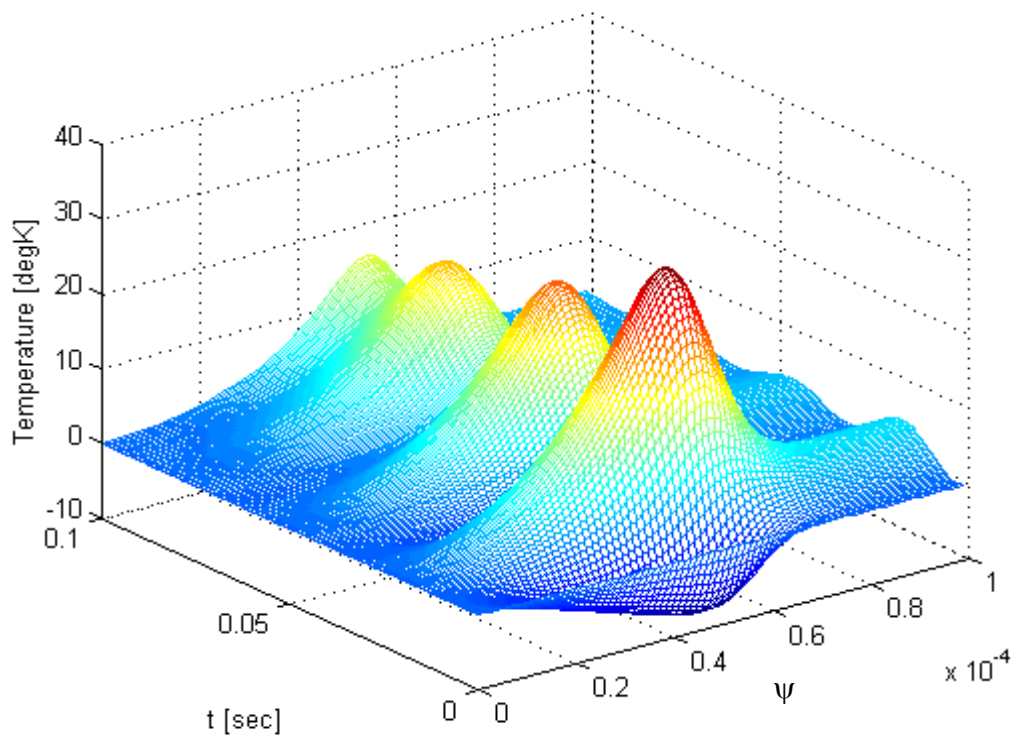
In steady state, the input velocity  $u^0$  is coupled with temperature profile  $T^0$  and species fraction  $Y^0$  by the two PDEs. At equilibrium, we have  $f_i(u^0, T^0, Y^0) = 0$  as in (2.16-17). Perturbing the incoming flow velocity above the nominal  $u = u^0 + \Delta u$ , results in perturbations of the temperature and species profiles,  $T(\Delta u, t)$  and  $Y(\Delta u, t)$ , which can be expressed as:

$$T(\Delta u, t) = T^0 + \Delta T(\Delta u, t) \quad (2.20)$$

$$Y(\Delta u, t) = Y^0 + \Delta Y(\Delta u, t) \quad (2.21)$$

With a small perturbation of the input,  $\Delta u = 0.1$ , the finite difference model simulation gives the step response of the system. Figure 2.1 shows the time-dependent variation of temperature  $\Delta T$  and mass fraction of fuel  $\Delta Y$  from the initial steady-state profiles. From the plot, we can see the temperature and species profile will stabilize at another steady state as time goes on. Another interesting thing is to compare the new steady state profiles produced by the finite difference method to the shooting method that we mentioned earlier. In practice, they matched exactly when using the same running conditions.

Various simulations can be set up for different initial conditions and different inputs. The heat release rate can be calculated from equation (6) and this is the actual output of the model. Thus, the system input of the nonlinear heat release model is variation of incoming mixture flow velocity  $u'$  and the output is heat release rate per unit area  $q'$ . This high-order simulation reproduces the dynamic response of the PDE model accurately, but requires a very high computational load. Thus, we are led to examine the question of how much the order of the model can be reduced while still capturing the relevant dynamics of the heat release system.



**Figure 2.2. Finite Difference Simulation of Temperature and Species Profile Changes**