

Article

## Burning Speed and Entropy Production Calculation of a Transient Expanding Spherical Laminar Flame Using a Thermodynamic Model

Kian Eisazadeh-Far <sup>†,\*</sup>, Ali Moghaddas, Faranak Rahim and Hameed Metghalchi

Department of Mechanical and Industrial Engineering, Northeastern University, Boston, Massachusetts, MA 02115, USA; E-Mails: moghaddas.a@neu.edu (A.M.); Faranak.Rahim@honeywell.com (F.R.); Metghalchi@coe.neu.edu (H.M.)

<sup>†</sup> Current address: Department of Aerospace and Mechanical Engineering, University of Southern California, Los Angeles, CA 90089, USA.

\* Author to whom correspondence should be addressed; E-Mail: eisazade@usc.edu.

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**Abstract:** A thermodynamic model has been developed to calculate burning speed and entropy production of transient expanding spherical laminar flame in an enclosed vessel. The model also predicts the particle trajectories of both unburned and burned gases in the vessel. The input to this model is the dynamic pressure rise due to combustion process. The unburned gases are divided into three regions: The core unburned gases which are compressed isentropically, the vessel walls and electrodes boundary layer gases, and gases in the preheat zone of the flames. The burned gases are in many shells having the same pressure but different temperatures. The model also includes radiation losses from the burned gases to vessel walls. Entropy production due to irreversibility has been calculated by applying entropy balance to the gas mixtures. Burning speed of premixed *n*-decane air mixture has been reported for temperatures and pressures along an isentrope.

**Keywords:** thermodynamic model; laminar burning speed; premixed flame; entropy production in a flame

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## 1. Introduction

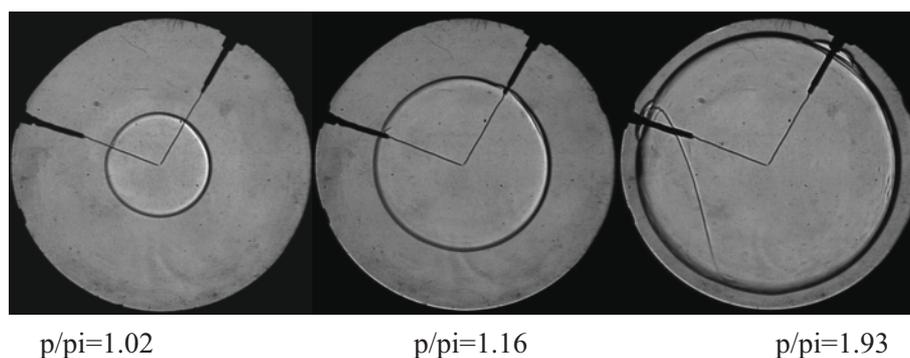
The definition of a flame needs more detailed clarification which is due to the manner of fuel/oxidizer mixing. In some combustors fuel and oxidizer are initially separated spatially. This means that the mixing process is slow before chemical reactions and mixing processes occur in chemical reaction sheet. This mixture and the consequent flame is *non-premixed* or *diffusion*. If fuel and oxidizer are mixed and initiation of chemical reactions is achieved in a combustible mixture, the consequent flame is *premixed*. In a premixed flame reactants enter the flame through the preheat zone and in a thin layer, which is called reaction zone, chemical reactions take place and combustion products leave the flame. At each zone the balancing factors are different, for example in preheat zone the convection of reactants are balanced by energy and mass diffusion from the reaction zone and in reaction zone the reaction source term is balanced with energy and mass diffusion to preheat zone. In premixed flames, an external energy source is usually required to initiate the flame. It can be a spark, high energy laser, surface plasma, hot spots, etc. No matter what the source of ignition is, a self-sustaining wave of an exothermic reaction propagates throughout the combustible mixture. Propagation speed of premixed flame is strongly a function of burning rate of the mixture which is called *laminar burning speed* in combustion community. The term of laminar emphasizes that the flame should be absolutely smooth and the propagation of the wave is only derived by chemical reactions and transport phenomena. Laminar burning speed is a function of temperature, pressure and composition of the mixture. At a given temperature, pressure and fixed composition of mixture, there is a unique value of laminar burning speed which is a property of the mixture. More details about the theory of flame and its formation and propagation can be found in [1–2].

Laminar burning speed of fuel/air mixtures are required both in theoretical and practical studies. It is needed to validate chemical kinetics mechanisms of combustion of fuel air mixtures. It is also needed in turbulent flame speed correlations in burners and internal combustion engines. There are several techniques for the measurement of laminar burning speed which can be found in [3–11]. In this paper we report a thermodynamic model to calculate burning speed of fuel/air mixtures. The model also calculates entropy production due to chemical reaction and predicts the location of gas particles in the vessel.

## 2. Theoretical Model

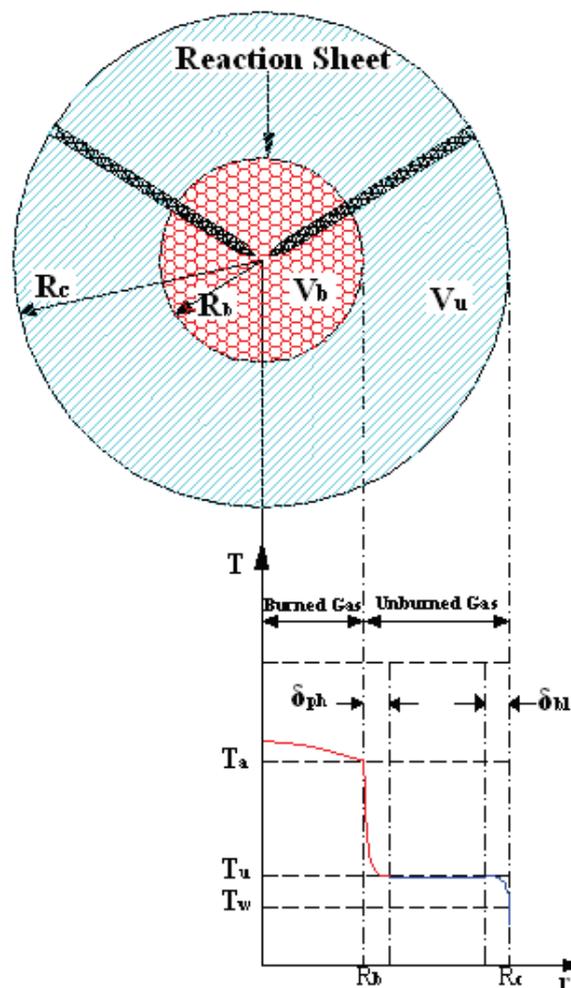
Figure 1 shows the snapshots of a transient expanding spherical laminar flame in an enclosed vessel.

**Figure 1.** Snapshots of a typical propagating spherical flame.



The thermodynamic model which has been developed uses the dynamic pressure rise of the combustion process to calculate burning speed of the fuel air mixture. The details of experimental facilities and systems to do the measurements can be found in previous publications [12–15]. In this model, it is assumed that gases in the combustion chamber can be divided into burned and unburned regions separated by a pre-heat and a reaction zones as shown schematically in Figure 2. It is further assumed that: the burned and unburned gases are ideal, the burned gas is in chemical equilibrium, the unburned gas composition is frozen, the pressure throughout the chamber is uniform, compression of both burned and unburned gases is isentropic. For the conditions of interest in the present work, all these assumptions have been validated by numerous experiments in constant volume chambers and internal combustion engines carried out over the past several decades [1].

**Figure 2.** Schematic of different zones and their corresponding temperatures in the thermodynamics model.



2.1. Burned Gas Mass Fraction, Temperature and other Thermodynamic Properties

For spherical flames, the temperature distribution of the gases in the combustion chamber and the burned gas mass fraction can be determined from the measured pressure using the equations for conservation of volume and energy together with the ideal gas equation of state:

$$pv = RT \tag{1}$$

where  $p$  is the pressure,  $v$  is the specific volume,  $R$  is the specific gas constant and  $T$  is the temperature.

The mass conservation equation is:

$$m = m_b + m_u = p_i(V_c - V_e)/RT_i \tag{2}$$

where  $m$  is the mass of gas in the combustion chamber,  $m_b$  is the burned gas mass,  $m_u$  is the unburned gas mass,  $V_c$  is the volume of the combustion chamber,  $V_e$  is the electrode volume, and the subscript  $i$  denotes initial conditions.

The total volume of the gas in the combustion chamber is:

$$V_c - V_e = V_b + V_u \tag{3}$$

where:

$$V_b = \int_0^{m_b} v dm = \int_0^{m_b} v_{bs} dm - V_{eb} \tag{4}$$

$V_b$  is the volume of the burned gas,  $v_{bs}$  is the specific volume of isentropically compressed burned gas:

$$V_{eb} = \int_0^{m_b} (v_{bs} - v) dm \tag{5}$$

$V_{eb}$  is the displacement volume of the electrode boundary layers:

$$V_u = \int_{m_b}^m v dm = m(1 - x_b)v_{us} - V_{wb} - V_{ph} \tag{6}$$

$V_u$  is the volume of the unburned gas,  $x_b = m_b/m$  is the burned gas mass fraction,  $v_{ub}$  is the specific volume of isentropically compressed unburned gas:

$$V_{wb} = \int_{wb} (v_{us} - v) dm \tag{7}$$

$V_{wb}$  is the displacement volume of the wall boundary layer:

$$V_{ph} = \int_{ph} (v_{us} - v) dm \tag{8}$$

$V_{ph}$  is the displacement volume of the preheat zone ahead of the reaction layer.

The energy conservation equation is:

$$E - Q_w - Q_e - Q_r = E_b + E_u \tag{9}$$

where  $E$  is the initial energy of the unburned gas,  $Q_w$  is the conduction heat loss to the wall,  $Q_e$  is the conduction heat loss to the electrodes,  $Q_r$  is the heat loss due to radiation from the burned gas:

$$E_b = \int_0^{m_b} e dm = \int_0^{m_b} e_{bs} dm - E_{eb} \tag{10}$$

$E_b$  is the energy of the burned gas,  $e_{bs}$  is the specific energy of isentropically compressed burned gas:

$$E_{eb} = \int_0^{m_b} (e_{bs} - e) dm \tag{11}$$

$E_{eb}$  is the energy defect of the electrode boundary layer:

$$E_u = \int_{m_b}^m e dm = m(1 - x_b)e_{us} - E_{wb} - E_{ph} \tag{12}$$

$E_u$  is the energy of the unburned gas,  $e_{us}$  is the specific energy of isentropically compressed unburned gas:

$$E_{wb} = \int_{wb} (e_{us} - e) dm \tag{13}$$

$E_{wb}$  is the energy defect of the wall boundary:

$$E_{ph} = \int_{ph} (e_{us} - e) dm \tag{14}$$

$E_{ph}$  is the energy defect of the preheat layer.

Using the perfect gas relation:

$$e - h_f = pv/(\gamma - 1) \tag{15}$$

where  $h_f$  is the specific enthalpy of formation of the gas at zero degrees Kelvin and  $\gamma = c_p/c_v$  is the ratio of the constant pressure and constant volume specific heats, and assuming constant specific heats for the gases in the boundary layers and the preheat zone, the integrals in Equations (11), (13) and (14) may be evaluated approximately to give:

$$E_{eb} = p \int_{eb} (v_{bs} - v) dm / (\gamma_b - 1) = pV_{eb} / (\gamma_b - 1) \tag{16}$$

$$E_{wb} = p \int_{wb} (v_{us} - v) dm / (\gamma_u - 1) = pV_{wb} / (\gamma_u - 1) \tag{17}$$

$$E_{ph} = p \int_{ph} (v_{us} - v) dm / (\gamma_u - 1) = pV_{ph} / (\gamma_u - 1) \tag{18}$$

A relationship between the wall heat transfer and the displacement volume for a gas subject to a time dependent pressure has been derived by Keck [16]. In the case of rapidly increasing pressure such as that occurring during constant volume combustion, the terms representing compression work on the boundary layer may be neglected and resulting equations are:

$$Q_e = pV_{eb} / (\gamma_b - 1) = E_{eb} \tag{19}$$

$$Q_w = pV_{wb} / (\gamma_u - 1) = E_{wb} \tag{20}$$

in which we have used Equations (16) and (17). Note that, to this approximation, the heat loss to the wall exactly equals the energy defect in the boundary layer. Substituting the relation  $dm = \rho dV$  into Equations (5), (7) and (8) we obtain:

$$V_{eb} = 2\pi r_e r_b \delta_{eb} \tag{21}$$

$$V_{wb} = 4\pi r_c^2 \delta_{wb} \tag{22}$$

$$V_{ph} = 4\pi r_b^2 \delta_{ph} \tag{23}$$

where  $r_e$  is the radius of the electrodes,  $r_b$  is the radius of the burned gas,  $r_c$  is the radius of the combustion chamber:

$$\delta_{eb} = \int_0^{r_b} \int_0^\infty (\rho(r, \eta) / \rho_{bs} - 1) d\eta dr / r_b \tag{24}$$

$\delta_{eb}$  is the displacement thickness of the electrode boundary layer in which  $\eta$  is the radial distance from the electrode:

$$\delta_{wb} = \int_{wb} (\rho(r) / \rho_{us} - 1) dr \tag{25}$$

$\delta_{wb}$  is the displacement thickness of the wall boundary layer, and:

$$\delta_{ph} = \int_{ph} (\rho(r) / \rho_{us} - 1) dr \tag{26}$$

$\delta_{ph}$  is the displacement thickness of the preheat zone. Using the approximation:

$$\int_{eb} (\rho(\eta, r) / \rho_{bs} - 1) d\eta = (\alpha_b (r_b - r) / \dot{r}_b)^{1/2} (T_b / T_w - 1) \tag{27}$$

Equation (24) can be integrated over  $r$  to give:

$$\delta_{eb} = (2/3)(\alpha_b r_b / \dot{r}_b)^{1/2} (T_b / T_w - 1) \tag{28}$$

where  $\alpha_b$  is the thermal diffusivity of the burned gas,  $T_w$  is the wall temperature, and  $T_b$  is the burned gas temperature.

The wall boundary layer displacement thickness can be calculated using the expression derived by Keck [16]:

$$\delta_{wb} = \left(\frac{\alpha_u \tau}{\pi}\right)^{1/2} z^{-1/\gamma} \int_0^z (z' - z'^{1/\gamma}) \left(\int_{z'}^z z'' dz''\right)^{-1/2} dz' \tag{29}$$

where  $\alpha_u$  is the thermal diffusivity of the unburned gas,  $\tau$  is a characteristic burning time,  $y = t/\tau$  is the dimensionless time, and  $z = p/p_i$  is the dimensionless pressure. For combustion in closed chambers, the dimensionless pressure can be approximated by:

$$z = 1 + y^3 \tag{30}$$

Substituting this expression in Equation (29) we obtain:

$$\delta_{wb} \approx (\alpha_u t / \pi)^{1/2} (p_i / p)^{1/2} \left( (p / p_i)^{(1-1/\gamma_u)} - 1 \right) \tag{31}$$

The displacement thickness of the preheat zone has been evaluated assuming an exponential temperature profile:

$$T / T_u \approx 1 + (T_b / T_u - 1) \exp(-\alpha_u (r - r_b) / \dot{r}_b) = \rho_{us} / \rho(r) \tag{32}$$

Substituting Equation (32) into Equation (26) we obtain:

$$\delta_{ph} = - \int_{ph} ((T_b / T_u - 1)^{-1} \exp(r - r_b) \dot{r}_b / \alpha_u + 1)^{-1} (r / r_b)^2 dr \tag{33}$$

$r \gg \alpha_u / \dot{r}_b$ , Equation (33) can be integrated approximately to give:

$$\delta_{ph} \approx -(\alpha_u / \dot{r}_b)(T_b / T_u - 1) \ln(T_b / T_u) \tag{34}$$

Note that the displacement thickness of the preheat zone is negative while those of the thermal boundary layers are positive.

The radiation heat loss from the burned gas was calculated using:

$$Q_r = \int_0^t \dot{Q}_r dt \tag{35}$$

where:

$$\dot{Q}_r = \alpha_p V_b \sigma T_b^4 \tag{36}$$

is the radiation rate,  $\alpha_p$  is the Planck mean absorption coefficient and  $\sigma$  is the Stefan-Boltzman constant. Finally combining Equations (3), (4) and (6) gives:

$$\int_0^{x_b} (v_{bs} - v_{us}) dx = v_i - v_{us} + (V_{eb} + V_{wb} + V_{ph}) / m \tag{37}$$

and combining Equations (9), (10), (12) and (18)–(20) gives:

$$\int_0^{x_b} (e_{bs} - e_{us}) dx = e_i - e_{us} + (pV_{ph} / (\gamma_u - 1) + pV_{eb} / (\gamma_b - 1) + pV_{wb} / (\gamma_u - 1) - Q_r) / m \tag{38}$$

where  $v_i = (V_c - V_e) / m$  and  $e_i = E_i / m$  are the initial specific volume and energy of the unburned gas in the chamber.

Equations (37) and (38) contain the three unknowns  $p$ ,  $x_b(p)$ , and  $T_b(x_b)$ . Given pressure,  $p(t)$ , as a function of time, they can be solved numerically using the method of shells to obtain the burned mass fraction,  $x_b(t)$ , as a function of time and the radial temperature distribution  $T(r, t)$ . The mass burning rate,  $\dot{m}_b = m \dot{x}_b$ , can be obtained by numerical differentiation of  $x_b(t)$ . The thermodynamic properties of the burned and unburned used in the calculations were obtained from the JANAF Tables [17].

Total entropy production throughout the process is:

$$\mathcal{S}_{prod} = \mathcal{S}_t - \mathcal{S}_0 - \int (\frac{\dot{Q}_w}{T_w} + \frac{\dot{Q}_e}{T_e} + \frac{\dot{Q}_r}{T_w}) dt \tag{39}$$

$\mathcal{S}_{prod}$  is the entropy produced during the combustion process,  $\mathcal{S}_t$  is the total entropy at  $t$ ,  $\mathcal{S}_0$  is the initial entropy,  $T_w$  is the wall temperature and  $T_e$  is the electrode temperature.

### 2.2. Burning Speed and Flame Speed

For closed flames, the burning speed may be defined:

$$S_b = \dot{m}_b / \rho_u A_b \tag{40}$$

where  $A_b$  is the area of a sphere having a volume equal to that of the burned gas. This expression is valid for smooth, cracked, or wrinkled flames of any shape. For smooth spherical flames:

$$\dot{m}_b = \dot{\rho}_b V_b + \rho_b A_b \dot{r}_b \tag{41}$$

where  $\rho_b$  is the average value of the burned gas density.

Differentiating the mass balance equation:

$$m_b = m - \rho_u V_u = m - (\rho_u / \rho_b) \rho_b (V_c - V_e - V_b) \tag{42}$$

with respect to time and neglecting the small contribution from the derivative of  $\rho_u/\rho_b$ , we obtain:

$$\dot{m}_b = (\rho_u / \rho_b)(\rho_b A_b \dot{r}_b - (V_c - V_e - V_b)\dot{\rho}_b) \tag{43}$$

where:

$$A_b = 4\pi r_b^2 - 2\pi r_e^2 \tag{44}$$

is area of the reaction zone,  $r_e$  is the electrode radius and  $r_b$  is given by the equation:

$$V_b = (4/3)\pi r_b^3 - 2\pi r_e^2 r_b \tag{45}$$

Using Equation (41) to eliminate  $\dot{\rho}_b$  in Equation (43), gives:

$$S_f = \dot{r}_b = S_b(\rho_u / \rho_b - y_b(\rho_u / \rho_b - 1)) \tag{46}$$

where  $S_f$  is the flame speed and  $y_b = V_b/(V_c - V_e)$  is the burned gas volume fraction. Note that for  $y_b = 0$ ,  $S_f = (\rho_u/\rho_b)S_b$  and for  $y_b = 1$ ,  $S_f = S_b$ .

### 2.3. Particle Trajectories

Assuming that unburned gas is compressed isentropically, the unburned gas particle trajectories can be calculated using the following equations:

$$\frac{V_{ut}}{V_{u0}} = \frac{r_c^3 - r_{ug}^3}{r_c^3 - r_{g0}^3} = \left(\frac{P_0}{P}\right)^{\frac{1}{\gamma_u}} \tag{47}$$

where  $V_{ut}$  is the volume of the unburned gas at time  $t$ ,  $V_{u0}$  is the volume of unburned gas at time zero,  $r_{ug}$  is the location of an unburned gas particle at time  $t$ ,  $r_{g0}$  is the location of an unburned gas particle at time zero, and  $P_0$  is the initial pressure of the mixture. Equation (47) can be rewritten as:

$$\frac{r_{ug}}{r_c} = \left[ 1 - \left( 1 - \left( \frac{r_{g0}}{r_c} \right)^3 \right) \left( \frac{P_0}{P} \right)^{\frac{1}{\gamma_u}} \right]^{\frac{1}{3}} \tag{48}$$

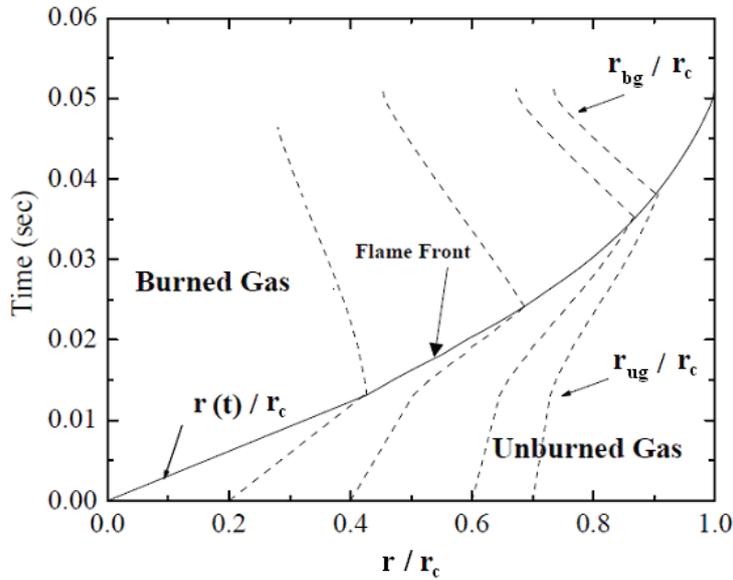
After the particles is burned it would be pushed back towards the center, because of the compression and it will asymptotically go to its original location. The burned gas particles trajectories can be calculated using the following equations, using the isentropic compression relation:

$$P_b V_b^{\gamma_b} = P V_{bg}^{\gamma_b} \tag{49}$$

$$\frac{V_{bg}}{V_{bt}} = \left( \frac{r_{bg}}{r_{bt}} \right)^3 \tag{50}$$

where  $V_{bg}$  is the volume of the burned gas at time  $t$ ,  $V_{bt}$  is the volume of burned gas at the time the gas particle burned,  $P_b$  is the pressure of the mixture at the time the particle burned,  $r_{bg}$  is the location of a burned gas particle at time  $t$  and  $r_{bt}$  is the location of a burned gas particle at the time it burned. Figure 3 shows trajectories of unburned gases throughout the process. It can be seen that unburned gas is pushed toward vessel walls before flame catches up. It then goes back toward its original location by being compressed after combustion.

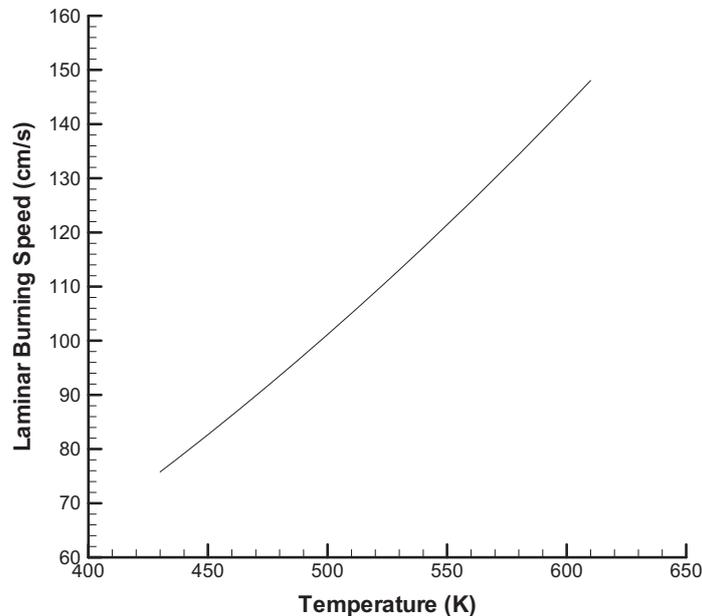
**Figure 3.** Gas particles and flame front trajectories.



### 3. Results and Discussion

Figure 4 shows the laminar burning speeds of stoichiometric *n*-decane-air mixture versus temperature at atmospheric pressure.

**Figure 4.** Laminar burning speed ( $S_b$ ) curves for stoichiometric *n*-decane/air mixtures as a function of temperature,  $P = 1$  atm.



It can be observed that increasing the temperature, increases the laminar burning speed. The reason for this is the activation of chemical reactions by temperature. Figure 5 shows the comparison of results with other researchers. It can be seen that the data are in good agreement with other results. This figure also shows the laminar burning speed at higher temperature (600 K) and again presents that the laminar burning speed is strongly dependent on temperature.

**Figure 5.** Laminar burning speeds of *n*-decane/air mixture and its comparison with other researchers [18,19].

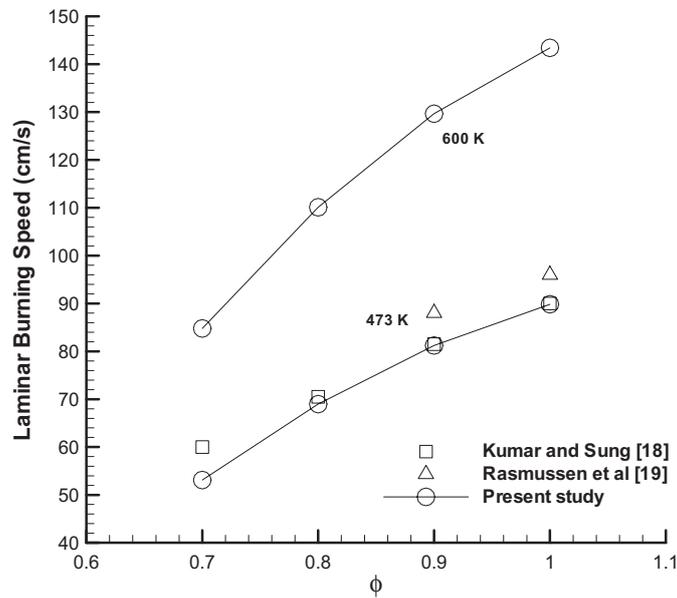
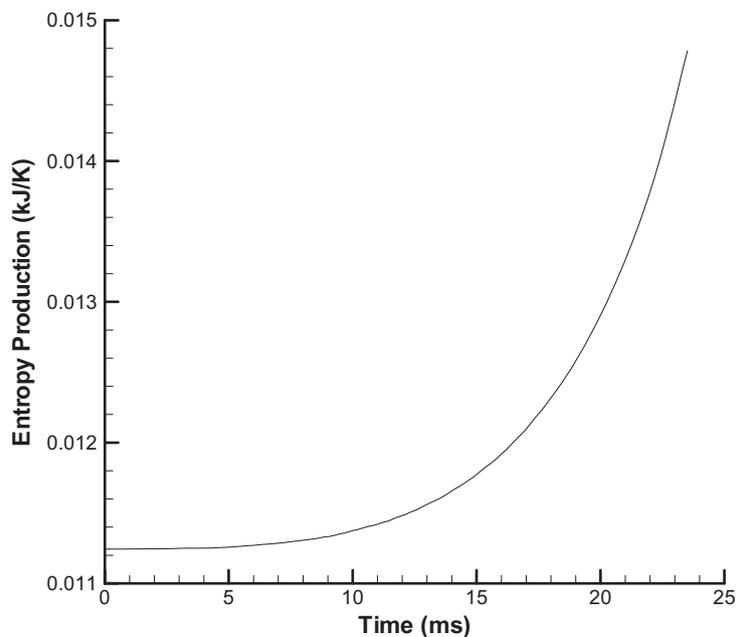


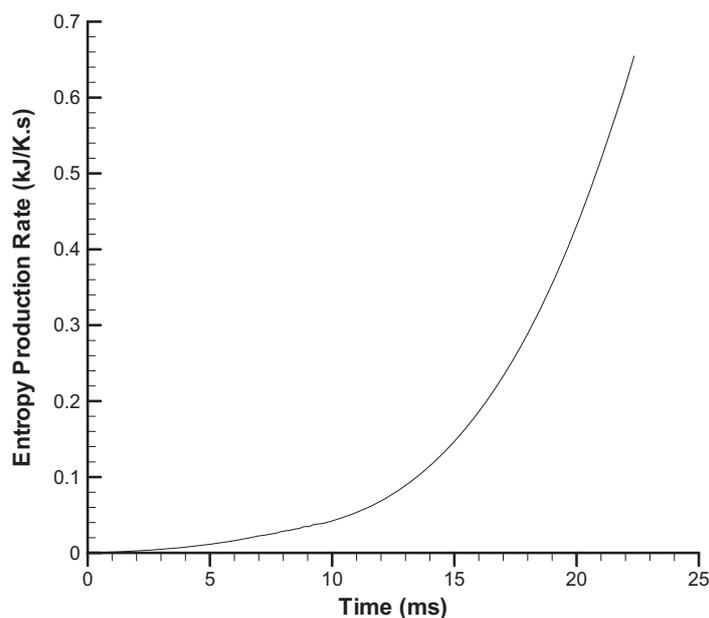
Figure 6 presents the entropy produced throughout the combustion process for the stoichiometric *n*-decane air mixtures.

**Figure 6.** Entropy production as a function of time for stoichiometric *n*-decane/air mixture at  $P_i = 1$  atm,  $T_i = 420$  K.



This figure demonstrates that entropy increases during the combustion process dramatically. This figure proves that combustion process is extremely irreversible due to chemical reactions. Another source of irreversibility is the mass transport phenomenon within the flame which is a major source of entropy generation at premixed flames [20]. Figure 7 shows that the rate of entropy production increases as the flame propagates.

**Figure 7.** Entropy production rate for stoichiometric *n*-decane/air mixture at  $P_i = 1$  atm,  $T_i = 420$  K.



#### 4. Summary and Conclusions

A complicated thermodynamic model to calculate laminar burning speeds and entropy production of a premixed spherical laminar flame is presented. Laminar burning speeds of *n*-decane/air mixtures were calculated from the dynamic pressure rise of a combustion process and it was observed laminar burning speed increases as temperature of the unburned mixture rises. The results of calculated values were compared with other published data and were in excellent agreement. Total entropy production and the rate of entropy production were also calculated. It was observed that combustion process is a highly irreversible process. Particle trajectories of the gas mixture in the vessel were also determined.

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