MAXIMUM SUPERADIABATIC TEMPERATURE FOR PREMIXED FLAMES WITHIN POROUS INERT MEDIA

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Abstract. This work analyzes the superadiabatic temperature for laminar stationary lean premixed flames within porous inert media. The analysis is based on the excess enthalpy function previously defined in the literature applied to the one-dimensional volume-averaged equations. The flame structure is analyzed in three distinct length-scales, the solid-phase length-scale, the gas-phase length-scale and the reaction length-scale. Discrepancies among the characteristic lengths justify the application of asymptotic expansions to determine an approximated (analytical) solution. The excess enthalpy function formulation allows the solution of the problem including the interphase heat transfer at the gas-phase length-scale. Then, the model is valid over a large range of equivalence ratios at the lean side of the stoichiometric ratio spectrum. The results show explicitly a limit for the superadiabatic temperature for lean mixtures.

Keywords: Superadiabatic limit, Combustion in porous media

1. INTRODUCTION

The premixed combustion in inert porous media has received much attention in the last decades as a way of extending flame stability, burning fuel lean mixtures and providing radiant heating [1, 2]. The heat recirculation induced by the porous media adds to the energy released by combustion resulting in local temperatures in excess of the adiabatic flame temperature for the gas-phase, a phenomenon that has been called superadiabatic combustion [3]. This high temperature in the reaction region increases the reaction rate and allows for combustion of low heat content gas mixtures whose stoichiometric ratio lies under the flammability limit in laminar free-flames.

Some asymptotic analysis have been proposed to the problem of premixed gas combustion within inert porous media [4, 5, 6, 7, 8, 9, 10] for semi-infinite and finite length burners. All these models divide the flame in a preheating region, a thin combustion region and a pos-combustion region. Expressions for the gas and solid temperatures and flame position are obtained as a function of an imposed flame velocity.

In a previous work [11] an asymptotic solution is proposed taking advantage of the large difference between the thermal conductivity of the solid and gas phases. In this solution a two equation model for the energy conservation is used with effective properties and a diffusion approximation for the intramedium radiation. The flame structure is divided in three characteristic length scales. The two innermost length scales are the same scales defined in the classical premixed flame structure analysis. The outermost length scale is related to the heat conduction in the porous matrix. The results of the model show that the influence of the porous medium on the flame is to increase its temperature and velocity and that this influence is more pronounced for leaner mixtures, higher solid-phase thermal conductivities, lower porosities and lower fuel Lewis numbers. It is also shown that the reaction region is shorter in flames within porous media since higher flame temperatures are found. The model is valid for equivalence ratios ranging from 0.60 to 0.80. The upper bound is a result of the simplifications made in the one-step kinetic mechanism used. The lower bound is related to an interphase heat transfer parameter defined as $N \equiv \lambda_s h_v / (\rho_n s_F c_p)^2$, where λ_s is the solid-phase thermal conductivity, h_v is the volumetric heat transfer coefficient, ρ_n is the unburnt gas-phase density, s_F is the flame velocity, measured in the unburned stream, and c_p is the gas-phase heat capacity. In this work the condition $N \ll \Gamma$ is imposed, were Γ is the thermal conductivities ratio ($\Gamma = \lambda_s/\lambda_g$, where λ_g is the gas-phase thermal conductivity). With this condition the interphase heat transfer at the gas-phase and at the reaction length-scales is negligible. Then, the flame structure at the inner scales is similar to that of a free-flame. This will not hold for extremely lean mixtures where lower flame velocities are found.

In a subsequent work [12], an analysis of adiabatic stationary planar premixed flames within porous inert media is proposed for the conditions of $N \sim O(\Gamma)$ and $\varepsilon/(1 - \varepsilon) \sim O(1)$. The condition $N \sim O(\Gamma)$ is characterized by an intense interphase heat transfer and is found for extremely lean mixtures. These flames present a wide region of local thermal equilibrium between the phases and the superadiabatic effect is limited by the intense interphase heat transfer at the gas-phase length-scale. The analysis shows that the superadiabatic temperature decreases as ϕ is decreased (as the interphase heat transfer becomes more intense). Since in the previous model (for higher equivalence ratios) the superadiabatic temperature increases when ϕ is decreased, a point of maximum nondimensional superadiabatic temperature in the lean side of the equivalence ratio spectrum is expected to exist. The model also shows the existence of a flammability limit for extremely lean mixtures. This limit shows that the gas-phase temperature at the flame must reach a minimum superadiabatic temperature for the flame propagation to be possible.

The present study proposes a solution for the problem of premixed flames in inert porous media that is valid for lean mixtures with the condition $\Gamma \ge N \ge 1$. The analysis is based on the excess enthalpy function previously defined in the literature [13] applied to the one-dimensional volume-averaged equations. Approximations for the reactants and the solid-phase temperature profiles are found using the asymptotic expansion method and the dependence of the excess enthalpy function on the problem parameters is accessed. The description of the reaction region is the same as in the previous works since the interphase heat transfer in this region is still negligible.

2. Mathematical formulation

A one-dimensional two-medium model for the conservation of mass, gas-phase energy, solid-phase energy and mass of chemical species is written following Pereira et al. [11]. The mass conservation implies that $\rho_n u_n$ is constant for the one-dimensional flow with ρ_n and u_n being respectively the gas density and the gas velocity far upstream from the flame. For a steady-state stationary flame, the laminar flame speed s_F is equal to u_n . The gas-phase specific heat capacity c_p , the effective thermal conductivities (λ_g for the gas and λ_s for the solid) and the product ρD (gas-phase density times mass diffusivity) are assumed uniform along the flame. The effective thermal conductivity of the solid-phase includes the pore tortuosity and the intraphase radiation trough a radiant conductivity (Rosseland approximation). The effective thermal conductivity and mass diffusivity of the gas-phase include the pore tortuosity and the hydrodynamic dispersion effects. The gas-phase radiation and flame stretch effects are neglected. The pressure drop across the porous medium is assumed negligible compared to the total pressure and the momentum equation becomes trivial.

The fuel combustion is assumed to occur following a global one-step mechanism, represented in mass variables as

$$F + \nu O_2 \rightarrow (1 + \nu)P,$$

where ν is the mass of oxygen per mass of fuel ratio (stoichiometric).

The steady-state volume-averaged mass, energy and species conservation equations (omitting for simplicity the volumeaveraging notation) then become

$$\varepsilon \rho u = \varepsilon \rho_n s_F,\tag{1}$$

$$\varepsilon \rho_n s_F \frac{dY_F}{dx} = \varepsilon \rho D_F \frac{d^2 Y_F}{dx^2} - \varepsilon A \rho^2 Y_O Y_F T_g^a e^{-E_a/R_u T_g},\tag{2}$$

$$\varepsilon \rho_n s_F \frac{dY_O}{dx} = \varepsilon \rho D_O \frac{d^2 Y_O}{dx^2} - \varepsilon \nu A \rho^2 Y_O Y_F T_g^a e^{-E_a/R_u T_g},\tag{3}$$

$$\varepsilon \rho_n s_F c_p \frac{dT_g}{dx} = \varepsilon \lambda_g \frac{d^2 T_g}{dx^2} + \varepsilon Q A \rho^2 Y_O Y_F T_g^a \ e^{-Ea/R_u T_g} + h_v (T_s - T_g), \tag{4}$$

$$0 = (1 - \varepsilon)\lambda_s \frac{d^2 T_s}{dx^2} - h_v (T_s - T_g),$$
(5)

where ε is the volumetric porosity of the solid matrix, Y_F and Y_O are the gas-phase volume-averaged fuel and oxidant mass fractions, D_F and D_O are defined and oxidant effective mass diffusivities, T_g and T_s are the gas-phase and solidphase phasic volume-averaged temperatures, Q is the fuel mass based heat of reaction, A is the pre-exponential factor of the Arrhenius reaction rate, E_a is the activation energy, R_u is the universal gas constant and h_v is the volumetric surface-convection coefficient.

2.1 Non-dimensionalization

Defining the non-dimensional variables [14]

$$y_F \equiv \frac{Y_F}{Y_{Fn}}, \ y_O \equiv \frac{Y_O}{Y_{On}}, \ \theta \equiv \frac{c_p(T-T_n)}{Y_{Fn} \ Q} = \frac{T-T_n}{T_r - T_n} \ \text{and} \ \zeta \equiv \int_0^x \frac{\varepsilon \rho_n s_F}{(1-\varepsilon)\lambda_s/c_p} dx,$$

Eqs. (2) to (5) become

$$\frac{dy_F}{d\zeta} = \frac{1}{Le_F} \frac{d^2 y_F}{d\zeta^2} - \Gamma_e Da \ y_O y_F \exp\left[-\frac{\beta(1-\theta_g)}{1-\alpha(1-\theta_g)}\right],\tag{6}$$

$$\frac{dy_O}{d\zeta} = \frac{1}{Le_O} \frac{d^2 y_O}{d\zeta^2} - \Gamma_e \phi Da \ y_O y_F \exp\left[-\frac{\beta(1-\theta_g)}{1-\alpha(1-\theta_g)}\right],\tag{7}$$

$$\frac{d\theta_g}{d\zeta} = \frac{1}{\Gamma_e} \frac{d^2 \theta_g}{d\zeta^2} + \Gamma_e Da \ y_O y_F \exp\left[-\frac{\beta(1-\theta_g)}{1-\alpha(1-\theta_g)}\right] + N_e(\theta_s - \theta_g),\tag{8}$$

$$0 = \frac{d^2\theta_s}{d\zeta^2} - N_e(\theta_s - \theta_g),\tag{9}$$

where

$$\begin{split} \Gamma_e &\equiv \frac{(1-\varepsilon)\lambda_s}{\varepsilon\lambda_g}, \quad \phi \equiv \frac{Y_{Fn}\nu}{Y_{On}}, \quad \alpha \equiv \frac{(T_r-T_n)}{T_r}, \quad \beta \equiv \frac{E_a(T_r-T_n)}{R_u T_r^2}, \\ Le &\equiv \frac{\lambda_g}{\rho \, c_p \, D}, \quad Da \equiv \frac{A \, \rho^2 \, \lambda_g \, Y_{On} \, T_g^a \, \exp(-\beta/\alpha)}{(\rho_n^2 \, s_F^2 \, c_p)}, \\ and \quad N_e \equiv \frac{(1-\varepsilon)\lambda_s h_v}{(\varepsilon\rho_n \, s_F \, c_p)^2}. \end{split}$$

The parameter Γ_e is the effective thermal conductivities ratio, ϕ is the equivalence ratio, α is the dimensionless heat release, β is the Zel'dovich number, Le is an effective Lewis number that accounts for the thermal and species hydrodynamic dispersions, Da is the Damköhler number and N_e is the effective interphase heat transfer parameter.

2.2 Excess enthalpy formulation

The problem can be rewritten in a compact form summing up Eqs. (6) to (9)

$$\Gamma_e \frac{d}{d\zeta} \left(\theta_g + y_F\right) = \frac{d^2}{d\zeta^2} \left(\theta_g + \frac{y_F}{Le_F} + \Gamma_e \theta_s\right) \tag{10}$$

Rewriting the overall energy balance $c_p(T - T_n) = Q(Y_{Fn} - Y_F)$ in non-dimensional variables one finds $y_F + \theta_g = 1$. Then, one can define a new variable called excess enthalpy function as follows [13]

$$H = \theta_g + y_F - 1. \tag{11}$$

This function accounts for the total enthalpy of the gas, including the thermal and chemical enthalpies. Substituting Eq. (11) into Eq. (10) one finds

$$\Gamma_e \frac{dH}{d\zeta} = \frac{d^2 H}{d\zeta^2} + \left(\frac{1}{Le_F} - 1\right) \frac{d^2 y_F}{d\zeta^2} + \Gamma_e \frac{d^2 \theta_s}{d\zeta^2} \tag{12}$$

The boundary conditions for the problem are

$$\begin{split} \zeta &\to -\infty \left\{ \begin{array}{l} H = \theta_g = \theta_s = 0\\ y_F = 1\\ dH/d\zeta = d\theta_g/d\zeta = d\theta_s/d\zeta = 0 \end{array} \right. \\ \zeta &\to \zeta_f \left\{ \begin{array}{l} H = H_f\\ \theta_g = \theta_{gf}\\ \theta_s = \theta_{sf}\\ y_F = 0 \end{array} \right. \\ \zeta &\to +\infty \left\{ \begin{array}{l} \theta_g = \theta_s = 1\\ H = y_F = 0\\ dH/d\zeta = d\theta_g/d\zeta = d\theta_s/d\zeta = 0 \end{array} \right. \end{split} \end{split}$$

The H function will have a positive or negative source term depending on the signs for the diffusion-like terms involving the non-dimensional fuel mass fraction and solid-phase temperature distributions.

In the following, a solution for the excess enthalpy function is obtained.

2.3 Approximated closed form solution for the excess enthalpy function

Equation (12) is a linear non-homogeneous first order ordinary differential equation that can be solved using an integration factor $e^{-\Gamma_e \zeta}$. To perform this integration, approximations for the fuel mass fraction and solid-phase temperature are required. Theses solutions can be brought from the previous asymptotic analisys of the combustion of premixed flames in porous media [11]. In that work the following solution for the solid-phase temperature is found

$$\theta_s = \begin{cases} \theta_{sf} \ e^{r_1(\zeta - \zeta_f)}, & \text{for} \quad \zeta \le \zeta_f \\ 1 + (\theta_{sf} \ -1)e^{-r_2(\zeta - \zeta_f)}, & \text{for} \quad \zeta \ge \zeta_f \end{cases}$$
(13)

in which

$$r_1 = \frac{N_e}{2} \left[\left(1 + \frac{4}{N_e} \right)^{1/2} + 1 \right]$$

and

$$r_2 = \frac{N_e}{2} \left[\left(1 + 4/N_e \right)^{1/2} - 1 \right]$$

The solid-phase temperature at the flame, θ_{sf} , is given by

$$\theta_{sf} = \frac{r_2}{r_1 + r_2}$$

The solution for the fuel fraction profile is

$$y_F = \begin{cases} 1 - e^{Le_F \Gamma_e(\zeta - \zeta_f)}, & \text{for} \quad \zeta \le \zeta_f \\ 0, & \text{for} \quad \zeta \ge \zeta_f \end{cases}$$
(14)

The integration of (12) with the approximations for the solid-phase temperature (13) and fuel mass fraction (14) submitted to the proper boundary conditions give

$$H = \begin{cases} e^{\Gamma_e(\zeta - \zeta_f)} - e^{\Gamma_e L e_F(\zeta - \zeta_f)} + \theta_{sf} \left(\frac{r_1 \Gamma_e}{r_1 - \Gamma_e}\right) \left(e^{\Gamma_e(\zeta - \zeta_f)} - e^{r_1(\zeta - \zeta_f)}\right) + \\ (1 - \theta_{sf}) \left(\frac{r_2 \Gamma_e}{r_2 + \Gamma_e}\right) e^{\Gamma_e(\zeta - \zeta_f)}, & \text{for} \quad \zeta \le \zeta_f \\ (1 - \theta_{sf}) \left(\frac{r_2 \Gamma_e}{r_2 + \Gamma_e}\right) e^{-r_2(\zeta - \zeta_f)}, & \text{for} \quad \zeta \ge \zeta_f \end{cases}$$
(15)

From (11) the solution of the gas-phase temperature is

$$\theta_{g} = \begin{cases} e^{\Gamma_{e}(\zeta-\zeta_{f})} + \theta_{sf}\left(\frac{r_{1}\Gamma_{e}}{r_{1}-\Gamma_{e}}\right)\left(e^{\Gamma_{e}(\zeta-\zeta_{f})} - e^{r_{1}(\zeta-\zeta_{f})}\right) + (1-\theta_{sf})\left(\frac{r_{2}\Gamma_{e}}{r_{2}+\Gamma_{e}}\right)e^{\Gamma_{e}(\zeta-\zeta_{f})}, & \text{for} \quad \zeta \leq \zeta_{f} \\ 1 + (1-\theta_{sf})\left(\frac{r_{2}\Gamma_{e}}{r_{2}+\Gamma_{e}}\right)e^{-r_{2}(\zeta-\zeta_{f})}, & \text{for} \quad \zeta \geq \zeta_{f} \end{cases}$$

$$(16)$$

The gas-phase temperature at the flame is obtained imposing $\zeta = 0$ in Eq. (16) and gives

$$\theta_{gf} = 1 + (1 - \theta_{sf}) \left(\frac{r_2 \Gamma_e}{r_2 + \Gamma_e} \right). \tag{17}$$

The gas-phase temperature profile given by Eq. (16) is valid over the solid- and gas-phase length-scales.

2.4 Inner zone: reaction region $O(\delta\Gamma^{-1})$

In a region of the order of $\delta\Gamma^{-1}$ around the flame, the variables present a variation of the order of δ . The solution follows the same steps already discussed in the previous works [11, 12].

The expression relating the flame velocity with the problem parameters is

$$s_{F}^{2} = \frac{2A\rho_{f}^{2}\lambda_{g}Y_{On}T_{gf}^{a} \exp(-\beta/\alpha)}{(\rho_{n}^{2} c_{p})} \left[\delta^{2}Le_{F}(1-\phi)\right] \times \\ \exp\left\{\frac{-\beta(1-\theta_{gf}^{(*)})}{1-\alpha(1-\theta_{gf}^{(*)})} + mn\right\},$$
(18)

in which

$$\delta = \frac{\left[1 + \alpha(\theta_{gf}^{(*)} - 1)\right]^2}{\beta}.$$

In Eq. 18 the parameter n is a displacement in the coordinate axis in order to match the solution in the reaction lengthscale l_R with the solution in the gas-phase length-scale l_G . The parameter m represents the ratio of the thermal flux downstream from the flame to the total heat release. Liñán [15] proposed an approximate expression for the numerical solution of the problem in the reaction region relating theses two parameters as follows

$$mn = 1.344m - 4m^2(1-m)/(1-2m) +$$

 $3m^3 - ln(1-4m^2).$ for $-0.2 < m < 0.5$ (19)

The value of m can be determined from the gas-phase temperature profile Eq. (16) resulting in

$$m = \frac{r_1 r_2^2}{(r_2 + \Gamma_e)(r_1 + r_2)} \tag{20}$$

As already pointed in the previous work, in combustion within a porous-medium the value of m is bounded by $0 \le m \le 0.5$. The limit m = 0 corresponds to a freely propagating flame where there is no excess enthalpy. Thus, the excess of enthalpy requires m > 0. The limit m = 0.5 corresponds to a situation in which the heat loss downstream from the flame is equal to the heat loss upstream and under this condition the flame is not stable, i.e. there is extinction.

3. DISCUSSION

The reaction rate parameters were adjusted to give a reasonable agreement with measured laminar flame speeds for free flames [16] with equivalence ratios ranging from 0.5 to 0.6. The heat of reaction was adjusted to reproduce the adiabatic flame temperature for $\Phi = 0.5$. The gas-phase properties were approximated by the air properties evaluated at 1000 K. The volumetric heat transfer coefficient h_v is modeled following Fu et al. [17] which uses a volumetric Nusselt number $Nu_v = C'Re^{m'}$, where $Nu_v = h_v d_m^2/\lambda_g$ and Re is the Reynolds number, $Re = \rho_n s_F d_m/\mu_n$. The mean pore diameter is modeled as $d_m = \sqrt{4\varepsilon/\pi}/(39.37\varphi)$, which is a uniform pore distribution model, where φ is the linear pore density given in pores per inch (ppi). Transport and geometric properties of the solid-phase are typical of porous burners. [18, 19]. Table **??** shows the parameters and properties used in the calculations and some results obtained for $\phi = 0.5$, $\Gamma_e = 15$, $\varepsilon = 0.8$, $\varphi = 50ppi$ and $Le_F = 1$.

Table 1. Properties and parameters used in the calculations and a few results for $\phi = 0.5$, $\Gamma_e = 15$, $\varepsilon = 0.8$, $\varphi = 50ppi$ and $Le_F = 1$.

Properties and Parameters			Results		
R_u	8.314	$J(mol K)^{-1}$	λ_s	4.041	$W(m K)^{-1}$
E_a	1.2×10^5	$J \text{ mol}^{-1}$	h_v	1.30×10^5	$W (m^3 K)^{-1}$
A	1.0×10^{10}	$m^{3}(kg s)^{-1}$	T_r	1479	K
a	0		T_{gf}	1944	K
Q	4.759×10^{7}	$ m J~kg^{-1}$	T_{sf}	1145	K
c_p	1141	$J(kg K)^{-1}$	s_F	31.21	${ m cm~s^{-1}}$
λ_g	0.06735	$W(m K)^{-1}$	N_e	2.97	
ρ_n	1.185	${ m kg}~{ m m}^{-3}$	α	0.80	
T_n	298	K	β	7.79	
C'	0.146		Da_f	1.86	
m'	0.83		m	0.04	
ε	0.8		n	1.34	
ϕ	0.5		δ	0.22	
φ	50	ppi	θ_{gf}	1.39	
Γ_e	15				
Le_F	1				

Figure 1 shows the flame structure for the condition described in Table 1. This condition was not covered by the previous models and represents a situation where the interphase heat transfer parameter N_e assumes an intermediate vale

between 1 and Γ_e . The solid- and gas-phase temperatures far from the flame are close due to the intense interphase heat transfer, but thermal nonequilibrium is still considerable at this large scale. The maximum gas-phase temperature exceeds the adiabatic limit in 40%.



Figure 1. Flame structure for the condition described in Table ??.

Figure 2 shows the gas-phase temperature at the flame as a function of the equivalence ratio. It is possible to see that the superadiabatic effect has a maximum around $\phi = 0.27$. This was already pointed out in a previous work [12] and can be understood considering two limiting cases. For $N_e \rightarrow 0$ the two equations for the conservation of energy are decoupled and the flame structure has the same structure of a free-flame. The solid-phase plays no role in the solution and superadiabatic temperatures are not possible. For $N_e \rightarrow \infty$ the two phases are in local thermal equilibrium and the problem reduces to a one-equation model, i.e. a free-flame like structure for a homogeneous medium with effective properties and again superadiabatic temperatures are not possible. For intermediate values of N_e thermal non-equilibrium between the phases and superadiabatic temperatures are found and a point of maximum nondimensional superadiabatic temperature must exist.

For higher equivalence ratios the excess temperature decreases with ϕ in accordance with the model developed for $N_e \sim O(1)$ [11]. For lower equivalence ratios the excess temperature increases with ϕ in accordance with the model developed for $N_e \sim O(\Gamma_e)$ [12]. This inversion happens because as ϕ is decreased lower flame velocities are found, resulting in a extended time for heat transfer between the phases. For higher flame velocities (higher ϕ) gas and solid phases have less time of contact at the thin region around the flame defined by the gas-phase length-scale. Then, in this condition, the interphase heat transfer is negligible at this length-scale. For lower flame velocities (lower ϕ) there is more time of contact between the phases and the interphase heat transfer becomes increasingly more important. This intense interphase heat transfer leads to local thermal equilibrium in a large region around the flame and limits the superadiabatic effect. The model also shows that the flame propagation is not possible for $\phi < 0.241$. This flammability limit was already found and discussed in a previous work [12].



Figure 2. gas-phase temperature at the flame as a function of the equivalence ratio

4. CONCLUSIONS

In the present work an analytical model for premixed flames within porous inert media, valid for a large range of equivalence rations, is shown. This model extends the results of previous works to the region where intermediate values of an interphase heat transfer parameter are found. This region shows a limit for the superadiabatic temperature of the gas-phase. This limit is related to the intense interphase heat transfer at the flame for lower equivalence ratios. The model also shows a flammability limit for the premixed combustion within porous inert media.

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