

CONVECTION, PYROLYSIS, AND DAMKÖHLER NUMBER EFFECTS ON EXTINCTION OF REVERSE SMOLDERING COMBUSTION

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In this paper, we use a one-dimensional transient model of reverse smoldering to examine possible extinction mechanisms. Experiments of Torero et al. [3] show that increased blowing rates enhanced the smoldering reaction until the propagation speed reached a maximum, after which the propagation speed diminished. Eventually, increasing the blowing rates quenched the reaction. For some range of parameters, it has been proposed in the literature that convective heat transfer from the solid to the gas, the endothermic pyrolysis reaction, and Damköhler number effects may be responsible for extinction. In this study, we use a computational model and analytical results to investigate these proposed extinction mechanisms. In contrast to many earlier models, our numerical model includes solid and gas-phase energy equations and introduces the concept of heat transfer between the phases in a quantitative way. It is therefore able to predict extinction for certain situations. We show that the most likely cause of extinction in the experiments of Torero et al. [3] is that at the higher gas velocities, the transport characteristic time is much faster than the characteristic reaction time. In addition, a criterion for extinction of smoldering in terms of a smoldering Damköhler number is developed.

Introduction

Smoldering is a slow, flameless combustion process in a porous medium. Heterogeneous chemical reactions take place at the surface of the porous combustible material. The detailed chemistry of smoldering is unknown for most materials but is typically described by two competing reacting pathways, an endothermic solid pyrolytic reaction and an exothermic heterogeneous oxidative reaction [1,2]. Both pathways form char, a high carbon material, whose oxidation rate is significantly slower than that of the fuel and whose contribution to the smoldering rate is often neglected for reverse smoldering cases [2]. Smolder propagation is supported by the heat released during the heterogeneous oxidation of the solid. This heat is transferred toward the unreacted material by conduction and radiation. The oxidizer is transported to the reaction zone by diffusion and convection.

Customarily, smoldering is classified into forward and reverse configurations. In forward smolder propagation, reaction movement is in the same direction as the airflow. In reverse smolder, the oxidizer enters the reaction zone from the opposite direction of the reaction propagation. In certain circumstances, steady-state smolder waves propagate through a solid fuel bed. In other cases, the smoldering may lead to flaming combustion or the smolder wave may extinguish. This latter process of extinguishment or extinction is the focus of this paper.

Experiments of Torero et al. [3] show that increased blowing rates enhanced the smoldering reaction until the propagation speed reached a maximum, and then the propagation speed diminished. Eventually, increasing the blowing rates quenched the reaction. It was also shown that the upper extinction limit increased by preheating the incoming air. Extinction of smolder waves has been studied by various researchers, and several causes have been proposed. In general, extinction is presumed to be determined by (1) heat loss from the solid, (2) the dominance of the endothermic pyrolysis reaction over the exothermic oxidative reaction, or (3) limiting kinetics.

The first possible extinction mechanism is heat loss from the solid. An analytical model using activation energy asymptotics was developed by Dosanjh et al. [4] to conduct a parametric investigation of reverse smoldering combustion. Schult et al. [5], Fatehi and Kaviany [6], and Aldushin et al. [7] seem to be in agreement with Dosanjh et al. [4] concerning the cause of extinction. They believe extinction occurs due to the heterogeneous nature of the process. The cold gas entering the sample absorbs heat from the solid as it moves toward the reaction site lowering the temperature of the reaction zone and causing extinction.

The possibility that pyrolysis causes extinction was proposed by Lozinski and Buckmaster [8] using a simple analytical model of reverse smolder in a porous medium. Their model included exothermic

oxidation and endothermic pyrolysis chemical reactions. The burning rate was a double-valued function of the blowing rate below some maximum blowing rate. Beyond this maximum, there were no solutions. The upper branch of the double-valued solutions was the relevant one. On it, in certain cases, the burning rate increases from zero to a maximum, and then decreases until quenching occurs at the maximum blowing rate. This behavior is the same as that was observed experimentally by Torero et al. [3].

Another possibility is that limiting kinetics may cause extinction. Williams [9] suggested that smolder will cease when the kinetic rate of oxygen consumption falls below the diffusive supply rate, that is, when kinetics become the rate-limiting step in the heat-release process. Experiments by Moussa et al. [10] for low-density fibrous cellulose cylinders in a stagnant atmosphere of varying oxygen content appear to support such a description of extinction.

Given the various postulated mechanisms for extinction that are in the literature, the goal of this paper is to analyze extinction using a computational model for smolder and then to place the results into some type of theoretical context.

Numerical Technique

In this paper, we use a one-dimensional transient model of reverse smoldering previously documented in Leach et al. [11] to examine possible extinction mechanisms. Chemistry includes fuel oxidative and pyrolytic steps. In contrast to many earlier models, local thermal nonequilibrium between the solid and gas phase is allowed. The solid- and gas-phase energy equations are coupled using a volumetric heat transfer coefficient derived from a Nusselt number correlation, which is a function of the Reynolds number and Prandtl number. It is assumed that the chemical reactions occur at the surface of the fuel and depend on the amount of oxygen at this surface. An oxygen transport model was incorporated to track the oxygen concentration at the surface and in the bulk gas. Radiative transfer was included using the diffusion approximation, which is appropriate for an optically thick system such as the one studied here.

Governing Equations

Solid-phase equations.

The governing equation in the solid is the heat equation:

$$\rho c \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left(k_s \frac{\partial T}{\partial x} + \mathbf{q}_{rad} \right) - \omega_o \Delta h_o - \omega_p \Delta h_p + hA''' (T_g - T) \quad (1)$$

where ρ is the bulk density, c is specific heat, k_s is solid conductivity, Δh_o and Δh_p are the enthalpies of

reaction for oxidation and pyrolysis, hA''' is the product of the heat transfer coefficient and the surface area per unit volume, T_g is the gas temperature, and T is the solid temperature. Note that all reactions occur on the solid.

Also, a species conservation equation can be written to govern the evolution of the char mass fraction, y_c :

$$\frac{\partial(\rho y_c)}{\partial t} = \omega_o n_{c1} + \omega_p n_{c2} \quad (2)$$

where ω_o and ω_p are the mass rates of production for oxidation and pyrolysis and n_{c1} and n_{c2} are stoichiometric coefficients.

Gas-phase equations.

The solid conversion process produces gases that flow upward through the solid pile. One-dimensional flow in the model is assumed. The gas-phase continuity equation is

$$\begin{aligned} \frac{\partial}{\partial t} (\rho_g \phi) + \frac{\partial}{\partial x} (\rho_g \phi u) \\ = \phi [\omega_p n_{g2} + \omega_o (n_{g1} - n_{O_2})] \end{aligned} \quad (3)$$

where ϕ is porosity and the subscript g is for gas.

The gas-phase energy equation is

$$\begin{aligned} \phi \rho_g c_{pg} \left(\frac{\partial T_g}{\partial t} + u \frac{\partial T_g}{\partial x} \right) = \phi k_g \frac{\partial^2 T_g}{\partial x^2} \\ + hA''' (T - T_g) \end{aligned} \quad (4)$$

where c_{pg} is the specific heat of gas.

An obvious similarity exists between heat transport between the solid and gas and mass transfer between the solid and bulk gas. Because chemical reactions occur at the surface of the fuel and depend on the amount of oxygen at this surface, it is necessary to account for this bulk gas-to-surface diffusion process. The species equation can be rewritten in terms of oxygen in the bulk gas, oxygen at the surface, and a mass transfer coefficient.

Oxygen Species in the Bulk Gas:

$$\begin{aligned} \frac{\partial}{\partial t} (\rho_g \phi_b y_{O_{2b}}) + \frac{\partial}{\partial x} (\rho_g \phi_b u_b y_{O_{2b}}) + \\ \frac{\partial}{\partial x} (\rho_g \phi_b y_{O_{2b}} V_{O_{2b}}) = -h_m A''' (y_{O_{2b}} - y_{O_{2s}}) \end{aligned} \quad (5)$$

Oxygen Species at the Surface:

$$\begin{aligned} \frac{\partial}{\partial t} (\rho_g \phi_s y_{O_{2s}}) + \frac{\partial}{\partial x} (\rho_g \phi_s u_s y_{O_{2s}}) + \\ \frac{\partial}{\partial x} (\rho_g \phi_s y_{O_{2s}} V_{O_{2s}}) = -\omega_o n_{O1} + h_m A''' (y_{O_{2b}} - y_{O_{2s}}) \end{aligned} \quad (6)$$

Here, the subscript b refers to in the bulk gas and s refers to the surface and $\phi_b + \phi_s = \phi$ where ϕ is the volume fraction of gas and $\phi_s \ll \phi_b$. We can assume that u_s , the gas velocity at the surface, is zero so that the second term in the oxygen species equation at the surface is zero. The third term in the conservation of oxygen in the condensed phase (equation 6) can be dropped because the diffusivity is much less than that in the gas phase (and has no effect on our results). V_{O_2} is the diffusional velocity of oxygen given by

$$V_{O_2} = -D_{O_2m} \frac{\partial y_{O_2}}{\partial x} \quad (7)$$

where y_{O_2} is the mass fraction of oxygen and m denotes the mixture.

Transfer Coefficients

Wakao and Kaguei [12] proposed the following correlation for the internal coefficient of heat transfer between a packed bed of spheres and the fluid blown through it:

$$Nu = \frac{h d_p}{k_g} = 2 + 1.1 Re^{0.6} Pr^{1/3} \quad (8)$$

where h is the interstitial heat transfer coefficient (per surface area of a particle); d_p is the diameter of spherical particle; k_g is the gas thermal conductivity; $Re = u \phi d_p / \nu$; ν is the gas kinematic viscosity; $Pr = \nu / \alpha$; and α is the gas thermal diffusivity. The specific interfacial gas solid surface area for a packed bed of spherical particles is

$$A'' = \frac{6(1 - \phi)}{d_p} \quad (9)$$

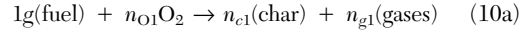
It is suspected that this heat and mass transfer model may not be precise because it is an empirical formulation obtained for piled spheres while the polyurethane foam used by Torero et al. [3] consists of thin fibers that create a low permeability/high void fraction fuel. The authors are not aware of a more appropriate model, but a discussion of the effect of the volumetric heat transfer coefficient on the smoldering characteristics is given by Leach et al. [11].

Incropera and Dewitt [13] present a heat and mass transfer analogy so that $h/h_m = \rho_g c_p Le^{(1-n)}$ where for most applications, it is reasonable to assume a value of $n = 1/3$.

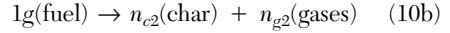
Kinetics

A three-step reaction model that allows for char formation and oxidation given by Rogers and Ohl-miller [1] is as follows:

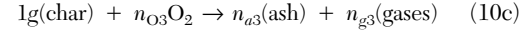
Exothermic Char Formation



Endothermic Char Formation (Pyrolysis)



Exothermic Char Oxidation



Ohlemiller and Lucca [2] noted that the contribution of the char oxidation reaction (equation 10c) to the propagation of the smolder wave can be neglected because the reaction is relatively slow and because the gas flowing over the char is partially depleted of oxygen. The smolder wave is driven by the energy released by equation 10a despite the fact that this is the less energetic process. Therefore, neglecting the second stage reaction in the model may be acceptable for the reverse smoldering case. Thus, the present model allows only for char formation. The mass rates of production are similar to those given by Kashiwagi and Nambu [14] and are of the following form:

Exothermic Char Formation Rate

$$\omega_o = (1 - y_c)^f \rho_f A_o (y_{ox})^m e^{-E_a/RT} \quad (11a)$$

Endothermic Char Formation Rate (Pyrolysis)

$$\omega_p = (1 - y_c)^g \rho_f A_p e^{-E_a/RT} \quad (11b)$$

where y_c is the char fraction, y_{ox} is the mass fraction of oxygen, A is the pre-exponential frequency factor, E_a is the activation energy, ρ_f is the density of fuel, ρ_c is the density of char, and f , m , and g are empirically determined exponents.

Boundary and Initial Conditions

The geometry is shown in Fig. 1. The left boundary is at a fixed temperature, T_w . Air flows through the right boundary into the fuel bed. The smolder front propagates from left to right.

At $x = 0$,

$$T = T_w, \quad \frac{\partial T_g}{\partial x} = 0, \quad \frac{\partial y_{O_2}}{\partial x} = 0 \quad (12)$$

At $x = l$,

$$\frac{\partial T}{\partial x} = 0, \quad T_g = T_{gin}, \quad y_{O_2} = y_{O_{2in}}, \quad u = u_{in} \quad (13)$$

At $t = 0$,

$$T = T_{\text{initial}}, \quad T_g = T_{gin}, \quad y_{O_2} = y_{O_{2in}}, \quad y_c = 0 \quad (14)$$

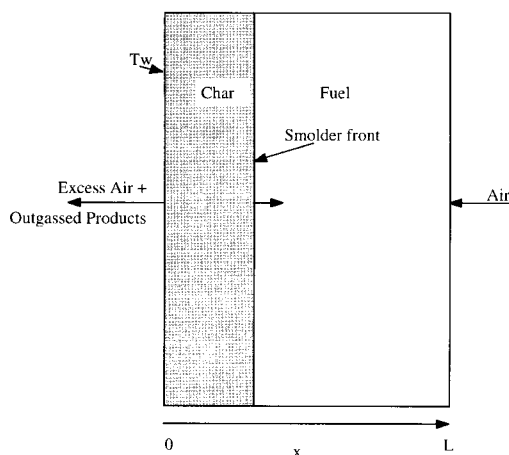


FIG. 1. Sketch of the reverse smoldering configuration with forced airflow. The left side ($x = 0$ cm) is held at 600 K. Air (23% O_2 by mass) is forced through the right side ($x = 15$ cm).

Solution Method

The solid energy, solid species, gas energy, and oxygen species equations were rearranged and discretized in space using finite-difference techniques. For this problem, the code VODE (Brown et al. [15]) is used. VODE is an ordinary differential equation integrator designed for stiff equations and is frequently used in applications involving chemical kinetics.

In this model, the pressure drop across the pile was assumed negligible. In order to clarify when this assumption is valid, the conservation of momentum equation was nondimensionalized. It was found that for high porosity, the momentum equation (i.e., the Darcy law) becomes trivial. Thus, the gas velocity is solved for directly using mass conservation.

Calculations were performed for 50 to 400 grid points for a base case to ensure grid independence of the results. Time-step selection is controlled by VODE. We tested several different error criteria (relative tolerances) to ensure that time stepping is accurate.

Possible Extinction Mechanisms

The numerical model was used to generate data over a wide range of gas velocities and oxygen concentrations. Parameters were chosen to represent the smoldering of a 15-cm porous bed of polyurethane foam. Properties are the same as those given in Leach et al. [11], with a few exceptions. The pore diameter of the fuel is 0.0064 m (Fatehi and Kaviany [16]), and the pore diameter of char is estimated to be 0.008 m. We were unable to obtain kinetic parameters for polyurethane foam and therefore used

those for cellulosic paper (Kashiwagi and Nambu [14]). However, for the material and transport property data used, these kinetic data did not produce a self-sustained smoldering front. Therefore, slightly different kinetic data are used (the frequency factor for the oxidation reaction, A_0 , is selected to be 8×10^{11} 1/s). This value was chosen to match the experimental results of Torero et al. [3] for a particular gas velocity (0.03 cm/s) and oxygen concentration (0.23) and was then unchanged for the other simulations. Particular attention was given to extinction trends and the suspected mechanisms that cause extinction. Figure 2 shows smolder velocities over a range of inlet gas velocities and inlet oxygen concentrations. As was also observed by Torero et al. [3], our numerical model shows that smolder velocities initially increase with inlet gas velocity. For the lower inlet oxygen mass fractions (0.1, 0.16, 0.23, and 0.3), extinction was obtained at increased gas velocities. It is suspected that in the higher oxygen mass fraction cases, extinction will eventually be achieved at increased flow rates, although at these high flow rates and oxygen concentrations, transition to flaming is likely. Experimental smolder velocities of Torero et al. [3] are shown for an inlet oxygen mass fraction of 0.23 over the range of inlet gas velocities. There is good agreement with these results at low inlet gas velocities. At higher gas velocities, the model predicts extinction earlier than the experiment.

Convective Heat Transfer from the Solid to the Gas

Unlike our model, previous one-dimensional models have generally failed in predicting extinction. The extinction phenomenon observed by Torero et al. [3] was predicted by our model, and we believe convective cooling of the solid to the gas passing through it plays a role in reaction extinguishment. As the heat transfer coefficient increases with increasing Reynolds number, more heat will be transferred from the solid with increasing airflow velocity. It is the solid temperature that drives the reactions. So, one possible explanation of the observed extinction is that with increasing gas velocity and heat transfer coefficient, the heat loss from the solid induces extinction.

As a test of this, we fixed the gas velocity and oxygen concentration and noted that extinction could be achieved by increasing the volumetric heat transfer coefficient. However, the levels to which the heat transfer coefficient had to be raised to promote extinction are inconsistent with increases in the heat transfer coefficient predicted by equation 8 due to the increase in the velocity.

Endothermic Pyrolytic Reaction

According to our simulations, the endothermic pyrolytic reaction (a heat sink) occurs together with

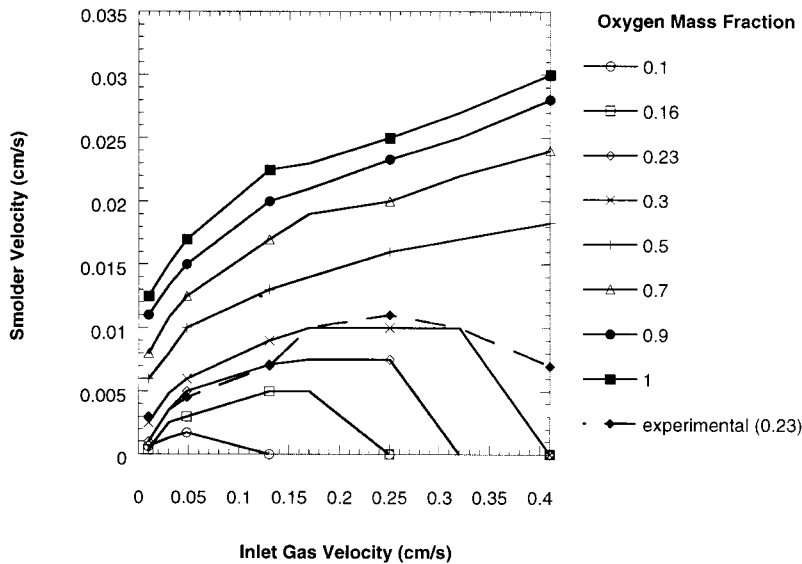


FIG. 2. Smolder velocity vs. inlet gas velocity over a wide range of oxygen concentrations. Experimental data are from Torero et al. [3].

oxidation (a heat source) in reverse smoldering. In order to determine the importance of pyrolysis in extinction, we looked at the ratio of the heat loss due to pyrolysis and the heat generated by oxidation, $(\int \omega_p \Delta h_p dx) / (\int \omega_o \Delta h_o dx)$. We discovered for our kinetics that this ratio stays relatively constant at about 0.50 when initial oxygen concentration and gas velocity were varied. While this is a significant heat loss, we do not believe it affects the extinction process because it is the same in cases that extinguish as well as those that do not.

Stoichiometry is relatively difficult to specify for smoldering systems because it depends both on the smolder rate and on the oxidative and pyrolytic rates of fuel consumption. With these restrictions, we can use the previously calculated ratio of pyrolytic to oxidative reaction rates and our computed smolder velocities to infer that our conditions are globally lean or indeterminate. For cases with very low oxygen concentration, we observed an exothermic oxidative front followed by an endothermic pyrolysis front. The oxidative front consumes all of the available oxygen leaving fuel behind the front to be endothermically pyrolyzed. This implies that it is difficult to define a unique stoichiometric condition because many conditions result in neither excess fuel nor excess oxidizer.

Limiting Kinetics

We suspect that it is possible that the kinetics may be the limiting factor in the heat-release process under certain conditions. In these situations, the gas

(oxygen) is transported through the reaction zone at a rate that does not allow time for the chemical processes to be fully completed. Not all of the oxygen has time to react with the fuel, resulting in a lower effective heat-release rate. Eventually, the reaction area is sufficiently cooled that the heat-release rate drops until reactions can no longer be sustained. In order to test Williams' [9] idea that smolder will cease when the kinetic rate of oxygen consumption falls below the diffusive supply rate (when kinetics become the rate-limiting step in the heat-release process), we held the inlet gas velocity at 0.17 cm/s and inlet oxygen mass fraction at 0.23 and varied the pre-exponential frequency factor in the oxidation kinetic equation.

It was seen that the kinetics play an important role in extinction. As seen in Table 1, when the frequency factor is decreased, a point is reached where the smolder will cease. For values less than $A_0 = 5 \times 10^{11}$ 1/s, extinction was observed. Smolder velocity increased with increasing frequency factor. Also, the oxygen concentration downstream of the reaction front decreased with increasing frequency factor. This certainly suggests that at the lower-frequency factors, the kinetics are the rate-limiting step in the heat-release process, and at the higher frequency factors, the oxygen diffusive supply rate becomes the rate-limiting step.

This is a plausible explanation for the extinction observed in the experiments of Torero et al. [3]. The kinetic dependence is also a likely explanation for the first extinction cases (Fig. 2) that we studied using our numerical model. The fact that the gas velocities that cause extinction are different for various

TABLE 1
Effects of oxidative frequency factor on smolder velocity, extinction, and final oxygen concentration

A_o (l/s)	v_{smolder} (cm/s)	Extinguish?	y_{O_2f}
5×10^{11}		yes	
7×10^{11}	0.0058	no	0.07
8×10^{11}	0.0075	no	0.055
9×10^{11}	0.0088	no	0.045
1×10^{12}	0.01	no	0.04
1.5×10^{12}	0.0163	no	0.01
2×10^{12}	0.02	no	0

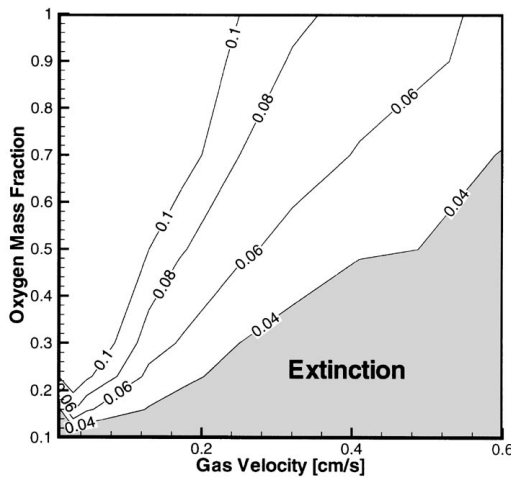


FIG. 3. The contour lines are of constant smolder velocity / (gas velocity + smolder velocity) or Damköhler numbers over a range of oxygen concentrations and inlet gas velocities. In the lower region ($Da < 0.04$), extinction is observed.

oxygen concentrations is consistent with this idea because the oxidative kinetic reaction is a function of oxygen concentration.

In the experiments of Torero et al. [3], and in our numerical studies, at the lower inlet gas velocities, the process is probably oxygen limited. Increases in gas velocity first result in increases in smolder velocity. Eventually, when the gas velocity becomes high enough, the kinetics become the limiting factor. It may be useful to think of the surface Damköhler number (the characteristic surface reaction rate divided by the characteristic diffusion rate). At low Damköhler numbers, the smolder process is limited by the surface rate reaction, and extinction will occur. At high Damköhler numbers, the oxygen supply rate becomes the rate-limiting step, and smolder velocities will decrease with decreasing oxygen supply.

Extinction Criterion

We simulated 72 different cases by varying the inlet gas velocity and the oxygen concentration. Fifteen of these conditions resulted in smolder fronts that did not propagate or extinguish. We observed that the determining criterion for extinction for all these cases was the smolder velocity nondimensionalized by the sum of the smolder and the gas velocity, $v/(u_i + v)$. This may be thought of as the Damköhler number for this problem. One might consider the smolder velocity in the numerator to be directly related to the reaction rate, while the denominator is representative of the species transport rate. This Damköhler number varied from 0 to 0.56 in the 72 cases. Extinction of the smolder front occurred when this parameter (critical Da) was between 0.025 and 0.04. Figure 3 shows the values of $v/(u_i + v)$ over a wide range of oxygen concentrations and inlet gas velocities. The shaded region contains the 15 cases where extinction occurs, and these cases represent $Da < 0.04$. Because we only examined cases for a particular gas and solid density, it is also true that extinction occurs for values less than $\dot{m}''_s/\dot{m}''_{g,i} \approx 0.7$. The robustness of this criterion was evaluated and supported by varying other physical quantities including the specific heat of the fuel. In order to most clearly examine the relevance of this parameter, we look at the conservation of energy equation using a frame of reference moving with the smolder wave (Dosanjh et al. [4]).

Integrating the conservation of energy equation over the whole domain using a single temperature model gives

$$\dot{m}'' c_{\text{eff}} (T - T_i) + (k_{\text{eff}} + k_{\text{rad}}) \frac{dT}{dx} = Q(\dot{m}''_{O_2,i} - \dot{m}''_{O_2}) \quad (15)$$

Here, Q is the effective (includes heat sink of pyrolysis reaction) heat released per gram of oxygen consumed. The mass fluxes are defined so that $\dot{m}''_s = \rho_s v$, $\dot{m}''_g = \rho_g (u + v)$, $\dot{m}''_{O_2,i} = \rho_g (u + v) y_{O_2,i}$, and $\dot{m}'' = \dot{m}''_s + \dot{m}''_g$. The effective thermal conductivity accounts for conduction heat transfer in the solid and gas phases. Radiation is incorporated using a temperature dependent conductivity. The effective specific heat is defined as

$$c_{\text{eff}} = \frac{\dot{m}''_s c_s + \dot{m}''_g c_g}{\dot{m}''_s + \dot{m}''_g} \quad (16)$$

The following boundary conditions are used:

$$\begin{aligned} x \rightarrow -\infty, \quad \dot{m}''_{O_2} &\rightarrow \dot{m}''_{O_2,i} \\ x \rightarrow +\infty, \quad \dot{m}''_{O_2} &\rightarrow \dot{m}''_{O_2,f}, \quad y_{O_2} \rightarrow y_{O_2,f}, \quad T \rightarrow T_f \end{aligned} \quad (17)$$

Using $dT/dx = 0$ at the edges of the domain it is possible to rearrange the energy equation to

$$\frac{v}{u_i + v} = \frac{Q \left[\frac{\rho_{gi} y_{O_2i} (u_i + v)}{u_i + v} - \frac{\rho_{gf} y_{O_2f} (u_f + v)}{u_i + v} \right]}{\rho_f c_{\text{eff}} (T_f - T_i)} - \frac{\rho_{gi}}{\rho_f} \quad (8)$$

Also, we can solve for the mass flux of fuel divided by the mass flux of gas:

$$\begin{aligned} \frac{\dot{m}_s''}{\dot{m}_{gi}''} &= \frac{\rho_f v}{\rho_{gi} (u_i + v)} \\ &= \frac{Q \left[y_{O_2i} - \frac{\rho_{gf} y_{O_2f} (u_f + v)}{\rho_{gi} (u_i + v)} \right]}{c_{\text{eff}} (T_f - T_i)} - 1 \quad (19) \end{aligned}$$

The foregoing quantities were evaluated in our numerical model for steady smoldering and extinction conditions. For the fuel properties and kinetics we used, these simulations showed that extinction occurs when

$$\frac{v}{u_i + v} \leq 0.04 \text{ or } \frac{\dot{m}_s''}{\dot{m}_{gi}''} = \frac{v}{u_i + v} \left(\frac{\rho_f}{\rho_{gi}} \right) \leq 0.7$$

or

$$\frac{Q \left(y_{O_2i} - \frac{\rho_{gf} y_{O_2f} (u_f + v)}{\rho_{gi} (u_i + v)} \right)}{c_{\text{eff}} (T_f - T_i)} \leq 1.7 \quad (20)$$

Dosanji et al. [4] noted a more restrictive extinction criterion; they require that extinction occurs when all of the energy released is used to heat the incoming gas. Their analysis indicates that steady smoldering is not possible when $Q y_{O_2i} / [c_{\text{eff}} (T_f - T_i)] < 1$.

Our criterion is also consistent with that of Schult et al. [5] for extinction at near stoichiometric conditions. For these conditions, they find that if each of the following parameters is varied while all the others are held fixed, extinction is expected for $y_{O_2m} < y_{O_2in}^{cr}$, $c_g > c_g^{cr}$, $Q < Q^{cr}$, $T_{in} < T_{in}^{cr}$, and $c_f \rho_f > (c_f \rho_f)^{cr}$, where the superscript *cr* refers to a critical value dependent on mathematically formulated extinction criteria.

Conclusions

Using a one-dimensional transient model of reverse smoldering, we examined possible extinction mechanisms including convection heat transfer from the solid to the gas, the endothermic pyrolysis reaction, and limiting kinetics. The numerical model introduces the concept of heat transfer between the solid and gas phase in a quantitative way.

We found that the most likely cause of extinction in the experiments of Torero et al. [3] is that at the higher gas velocities, insufficient time is allowed for the chemical processes to be completed, and the kinetics become the limiting factor in the heat-release process. A criterion for extinction of smoldering is developed in terms of a smoldering Damköhler number. This criterion is similar to but not as restrictive as that of Dosanji et al. [4]. It is also consistent with the extinction criterion for stoichiometric conditions of Schult et al. [5].

It is also worth noting that there are some interesting similarities between the findings presented in this manuscript and previously published work [17,18] in opposed flow flame spread (regarding flame spread vs. smolder spread trends, Damköhler number extinction criteria at high flow rates, and oxygen limited at low flows). These similarities might be the basis for future work on this topic.

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COMMENTS

John Buckmaster, University of Illinois at Chicago, USA.

The calculations that you report are welcome, but the line that you draw between endothermic pyrolysis effects and kinetics (Damköhler number) effects does not exist. In the absence of pyrolysis, accounting only for exothermic reaction and heat losses, the (asymptotic) flame sheet is of the classical Zeldovich form, characterized by complete depletion of at least one reactant. Proper quenching is not captured by this model. On the other hand, when endothermic pyrolysis is accounted for, the flame sheet can take a form among those that were discussed by Liñán in his seminal diffusion flame study [1]. Now reactant leakage occurs, ever more as the blowing rate is increased, and this can lead to quenching. The key conclusion of the paper by Lozinski and Buckmaster [2] is that quenching is a kinetic effect, but a kinetic effect that is only in play because of pyrolysis.

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Author's Reply. We recognize that the distinctions we make between heat transfer, pyrolysis, and kinetics are somewhat artificial. Clearly, the interplay between all the physical processes is responsible for extinction. What we hoped to find was the relative sensitivity of the extinction process to the magnitude of any of these three processes. We found that the smoldering rate was relatively insensitive to the heat-transfer coefficient for a broad range of smolder conditions. Obviously, near extinction, this sensitivity is magnified. We also found that the frequency factor of the oxidation rate strongly affected the smolder rate for some level of inlet velocities. That is, we identified a range of inlet velocities over which there was very little sensitivity to kinetics (oxygen-limited cases) and a range with much greater sensitivity to oxidative kinetics. In more recent work, we find that when the pyrolytic rates are not included in the model, the reaction rates seem to increase dramatically with increasing flow rate. Interestingly, we never saw extinction. Instead, we saw a blowup in the temperature profile as the flow rate was increased. These preliminary results appear to be consistent with analysis in Lozinski and Buckmaster.

Carlos Fernandez-Pello, University of California, Berkeley, USA. Because your results appear to indicate that

chemical kinetic effects are the primary mechanism for extinction, I wonder how important it is to include in the smolder model a nonthermal equilibrium formulation of the solid and gas phases energy equations.

Author's Reply. While the results presented in this paper indicate that chemical kinetic effects are the primary mechanism for extinction, convective and pyrolytic heat losses also appear to be important. The convective heat transfer from the solid to the gas and the pyrolytic heat sink remain relatively constant as the inlet gas velocity is increased. At the high inlet gas velocities where extinction is observed, the kinetics limit the amount of heat that is generated so that the convective and pyrolysis heat losses are sufficient to cause extinction.

Patrick J. Pagni, University of California, Berkeley, USA. For most times, between ignition and extinction, your unsteady calculations produce quasi-steady smoldering velocities. Would you please compare those results with the steady smoldering velocities given in your Ref. [4]?

Author's Reply. There are several different assumptions used in the development of the analytical model of Dosanjh et al. [4] and the present numerical model. One significant difference is that the analytical model assumes a one-step fuel decomposition rate. The numerical method has modeled smoldering combustion using a two-step mechanism (oxidation and pyrolysis). In order to account for this difference, modifications are made to the Dosanjh et al. model for comparison. Another major difference between Dosanjh et al.'s model and the numerical model is that the analytical model assumes smoldering is an oxygen-limited process. The numerical model shows that this is not necessarily the case at high gas velocities. Detailed comparison was made between the analytical results and computational results. There is relatively good agreement with the analytical model at low gas velocities where the process is indeed oxygen limited, but not such good agreement at the higher gas velocities where the process is kinetically limited. One important outcome of this comparison is that the Dosanjh et al. results can be used in describing quasi-steady smoldering in the low-velocity, oxygen-limited regimes.