

IGNITION AND SUBSEQUENT FLAME SPREAD OVER A THIN

CELLULOSIC MATERIAL

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Introduction

Both ignition and flame spread on solid fuels are processes that not only are of considerable scientific interest but that also have important fire safety applications. Both types of processes, ignition and flame spread, are complicated by strong coupling between chemical reactions and transport processes, not only in the gas phase but also in the condensed phase. In most previous studies, ignition and flame spread were studied separately with the result that there has been little understanding of the transition from ignition to flame spread. In fire safety applications this transition is crucial to determine whether a fire will be limited to a localized, temporary burn or will transition into a growth mode with a potential to become a large fire. In order to understand this transition, the transient mechanisms of ignition and subsequent flame spread must be studied. However, there have been no definitive experimental or modeling studies, because of the complexity of the flow motion generated by buoyancy near the heated sample surface. One must solve the full Navier-Stokes equations over an extended region to represent accurately the highly unstable buoyant plume and entrainment of surrounding gas from far away. In order to avoid the complicated nature of the starting plume problem under normal gravity, previous detailed radiative ignition models were assumed to be one-dimensional (ref.1) or were applied at a stagnation point (ref.2). Thus, these models cannot be extended to include the transition to flame spread. The mismatch between experimental and calculated geometries means that theories cannot be compared directly with experimental results in normal gravity.

To overcome the above difficulty, theoretical results obtained without buoyancy can be directly compared with experimental data measured in a microgravity environment. Thus, the objective of this study is to develop a theoretical model for ignition and the transition to flame spread and to make predictions using the thermal and chemical characteristics of a cellulosic material which are measured in normal gravity. The model should take advantage of the microgravity environment as much as possible in the gas phase instead of modifying a conventional normal-gravity approach. A thermally-thin cellulosic sheet is considered as the sample fuel, which might ignite and exhibit significant flame spread during test times available in NASA's drop towers or in the space shuttle, without requiring a pilot flame. This last situation eliminates many complicating parameters such as pilot flame location, temperature, and size (ref.3).

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2. Theoretical Model

2.1 Gas Phase Model

The absence of gravity (microgravity is approximated to be zero gravity) removes the buoyancy-induced vorticity generation mechanism. The small scale of the planned experiment, together with the slow external flow (less than 10 cm/s), simulating the ventilation flow level in a spacecraft, implies a low Reynolds number flow domain. When surface pyrolysis is present, the thermally-induced surface blowing velocity must be taken into account, even at low Reynolds numbers. Both these concepts can be accommodated by assuming the velocity field to be a potential flow. The only loss is the no-slip boundary condition which is already relaxed in the classical Oseen approximation to low Reynolds number phenomena. This approximation is adopted and is implicit in the analysis. The conservation equations of mass, energy and species in the gas phase under low Mach number combustion and heat transfer conditions can be written as:

$$\begin{aligned} \frac{D\rho}{Dt} + \rho \nabla \cdot \vec{v} &= 0, & \rho \frac{D \int_0^T c_p dT}{Dt} - \nabla \cdot (k \nabla T) &= \Delta H \dot{m}_f + \dot{q}_R \\ \rho \frac{DY_{ox}}{Dt} - \nabla \cdot (\rho D \nabla Y_{ox}) &= -v \dot{m}_f, & \rho \frac{DY_f}{Dt} - \nabla \cdot (\rho D \nabla Y_f) &= -\dot{m}_f \end{aligned} \quad (1)$$

We assume that the reaction is represented by a global one step Arrhenius reaction and its kinetic constants are selected. Equations (1) are supplemented by an equation of state, taken in a form appropriate for low-Mach-number flows. Now multiply the first of Eqs. (1) by enthalpy, h , and add it to the second. The result is:

$$\rho h_\infty \nabla \cdot \vec{v} - \nabla \cdot (k \nabla T) = \Delta H \dot{m}_f + \dot{q}_R \quad (2)$$

Equation (2) is the fundamental equation for determining the velocity field \vec{v} . Since \vec{v} is a vector field it can be decomposed into the gradient of a potential ϕ and a solenoidal field \vec{u} .

$$\vec{v} = \nabla \phi + \vec{u}, \quad \nabla \cdot \vec{u} = 0 \quad (3)$$

Substitution of Eq. (3) into Eq. (2) yields:

$$\nabla^2 \phi = \frac{1}{\rho_\infty h_\infty} (\Delta H \dot{m}_f + \dot{q}_R + \nabla^2 \psi), \quad \psi = \int_{T_\infty}^T k(T) dT \quad (4)$$

Note that the third term on the right hand side of the first equation of Eq. (4) can be eliminated by introducing a particular solution ϕ_P as:

$$\phi_P = \frac{\psi}{\rho_\infty h_\infty} \quad (5)$$

Moreover, it is convenient to introduce another particular potential ϕ_{p_∞} representing the effects of the external wind velocity u_∞ . Then, introducing a remainder potential Φ , ϕ may be expressed in the

$$\phi = \phi_p + \phi_{p_{\infty}} + \Phi, \quad \nabla^2 \Phi = \frac{\Delta H \dot{m}_f + \dot{q}_R}{\rho_{\infty} h_{\infty}} \quad (6)$$

mf

Equations (5) and (6) relate the potential field to the temperature distributions in the gas phase. In the calculation the sample is irradiated and auto-ignited at the center by continuous thermal radiant flux with a Gaussian distribution. Far from the surface, ϕ , T and Y_i must decay to their ambient initial values. T and Y_i decay exponentially to their ambient values. However, the potential field decays slowly away from the heated region. Thus, putting ϕ or its gradient equal to zero at the computational boundary would introduce unacceptable error into the calculation. These errors are avoided by using the analytical solution to Eq.(6) subject to the boundary condition at the sample surface to generate accurate values for ϕ on the computational boundary (ref.4). Then, Eqs.(1) are solved by a time-splitting algorithm.

2.2 Condensed Phase Model

It is assumed that the condensed phase is a thermally thin sheet of cellulosic material, and uniform in composition through its depth. The thermal degradation of the cellulosic sheet is described by two global thermal degradation reactions and a char oxidation reaction (ref.5). They are; (1) endothermic global pyrolysis reaction which degrades the cellulosic sheet to gases and a char, (2) weakly exothermic global thermal oxidative reaction which degrades the cellulose sheet to gases and a char, (3) highly exothermic global char oxidation reaction which degrades the char to gases and ash. Here, it is assumed that the reactivity of the char with oxygen formed from the above two reactions with oxygen is the same. In the above global reactions combustible gases represent hydrocarbons and CO and non-combustible gases represent CO₂ and H₂O. Here, it is assumed that the combustible gases formed from each reaction above are the same. Although these reactions are crudely approximated compared to the actual, extremely complex degradation reactions, their accuracy is comparable to the global one-step gas phase oxidation reaction for the combustible gases, which is used for the gas phase reaction in this study.

The reaction rate of each reaction above, RR_i , is approximately expressed by the following Arrhenius-type equations:

$$\begin{aligned} (1) \quad RR_p &= A_p (\rho_s Y_f / \rho_{s0})^{np} \exp(-E_p / RT) \\ (2) \quad RR_{ox} &= A_{ox} (\rho Y_{ox} / \rho_{0,ox})^{nox} (\rho_s Y_f / \rho_{s0})^{nf,ox} \exp(-E_{ox} / RT) \\ (3) \quad RR_{char} &= A_{char} (\rho Y_{ox} / \rho_{0,char})^{no2,char} (\rho_s Y_{char} / \rho_{s0})^{nchar} \exp(-E_{char} / RT) \end{aligned}$$

Values for the above kinetic parameters together with the heats of reaction, ΔH_i , for a black cellulosic paper have been measured; the details are given in Ref.5.

The equations for the condensed phase are given as follows.

Conservation of solid mass:

$$\partial(\rho_s / \rho_{s0}) / \partial t = -(1 - v_{char,p}) RR_p - (1 - v_{char,ox}) RR_{ox} - (1 - v_{ash,char}) RR_{char} \quad (7)$$

$$\text{Conservation of initial cellulosic material:} \quad \partial(\rho_s Y_f / \rho_{s0}) / \partial t = -RR_p - RR_{ox} \quad (8)$$

Conservation of char:

$$\partial(\rho_s Y_c / \rho_{s0}) / \partial t = v_{char,p} RR_p + v_{char,ox} RR_{ox} - RR_{char} \quad (9)$$

Conservation of energy:

$$\delta \cdot \partial(\rho_s c_s T) / \partial t = \left(-\Delta H_p RR_p - \Delta H_{ox} RR_{ox} - \Delta H_{char} RR_{char} \right) \rho_s \delta + \frac{(1-r) \dot{q}_{ex} - \epsilon \sigma (T_s^4 - T_0^4)}{k} + k \partial T(r, 0, t) / \partial z \quad (10)$$

where δ is the half-thickness of the paper. The mass flux of evolved combustible gases from the surface is given by the following expression:

$$\dot{m}_s = [(1-v_{char,p}) RR_p + (1-v_{char,ox}) RR_{ox} + (1-v_{ash,char}) RR_{char}] \rho_s \delta \quad (11)$$

The cellulosic material used in the present study is a 0.38×10^{-4} m thick sheet.

3. Results and Discussion

Four different cases are being studied: (1) heat transfer with the degradation of the paper sheet irradiated by the external radiation at the center of the paper in an axisymmetric configuration, no gas phase reaction; no external flow, (2) ignition and subsequent flame spread in an axisymmetric configuration; no external flow, (3) heat transfer with a slow external flow in a three-dimensional configuration, and (4) ignition and subsequent flame spread with a slow external flow in a three-dimensional configuration. Since the results in the first case were published in ref.4, they are not discussed here due to space limitations.

3.1 Quiescent axisymmetric configuration

A maximum external radiant flux of 5 W/cm^2 (continuously on during computation) at 21%, 30% and 50% oxygen concentrations was used in the calculation. The results indicate that ignition is observed for 21% and 30% oxygen concentrations but the transition to flame spread does not occur. However, in 50% oxygen the transition is achieved as shown in Fig.1 which plots the gas phase temperature distribution at 1.0s after initiation of the external radiation. Each temperature isotherm line is a 100°K interval starting from 350°K . There are two high temperature regions; one is behind the flame front and the other is at the center where the external radiation continuously irradiates the sample. The results at later time show that there are two separate flames; the primary flame propagates radially outward, while the secondary flame stays at the center and becomes gradually weaker and disappears. Eventually one ring-like flame appears to continue its spread radially outward. The distribution of velocity vectors at the same time is shown in Figs.2. The large expansion flow motion near the flame front is clearly seen in Fig.2. The large mass addition near the center is caused by the continuously applied external radiation. Since the sample was nearly completely converted to char at the center, little mass is added there. The distribution of oxygen and fuel concentration indicates that the flame near the traveling front is a premixed flame followed by a diffusion flame behind the flame front. The energy balance at the sample surface at 1.0s is shown in Fig.3, where Q_{ex} is the external radiant flux, Q_{rad} is the re-radiation loss, Q_{rr} is the net heat balance of the three solid degradation reactions and Q_{fcon} is the convective/conductive heat transfer from the gas phase to the sample. A high energy feedback rate of nearly 6 W/cm^2 is calculated as opposed to the nearly 1 W/cm^2 for the 21% oxygen concentration case at 1.6s after initiation of the external radiation as shown in Fig.4. This difference in energy feedback rate is mainly caused by differences in flame temperature (about 1400°K for 21% vs 2000°K for 50%) and also in the location of the peak gas phase reaction rate (closer to the sample surface in 50% oxygen concentration).

The previous experiment in a quiescent microgravity environment showed that the flame spread limit is about 20% oxygen for a light paper towel (Kimwipes paper) (ref.6). Thus, unsuccessful transition to flame spread in 21% and 30% oxygen predicted in this study does not agree with successful transition observed in the experimental work. Also, the predicted flame spread rate in 50% oxygen concentration is about 19 cm/s which is roughly five times faster than the experimentally-measured rate using the drop tower (ref.6). In the calculation the only uncertainty is the kinetic constants for the gas phase oxidation reaction. Since

there are no data available on the degradation products of the paper, the accuracy of the selected values is questionable. Since there are significant differences between the experimental setup and the calculation, for example, a two-dimensional experimental configuration vs. an axisymmetric calculation and piloted ignition in the experiment vs. auto-ignition, no attempt is made to adjust the kinetic constants of the gas phase reaction to match with the experimental data. These constants will be measured in the future.

3.2 Three-dimensional Calculation

Although preliminary results on ignition in the three dimensional configuration with a slow external flow have been obtained, more time is needed to determine their accuracy and correctness. It is hoped that the results will be presented at the meeting. Here, the results for the three dimensional heat transfer problem are briefly discussed. In this problem either a thermally thin or thick non-reactive condensed material is irradiated by continuously applied external radiation with a Gaussian flux distribution. Typical examples of the distributions of velocity vectors relative to the ambient flow and temperature contours in the gas phase for a thermally thick non-reactive material are shown in Figs. 5 at 8s after the initiation of an external radiant flux of 4 W/cm^2 with an external velocity of 2 cm/s (from left to right). The left corner figure in Figs. 5 represents the front view (looking in the downstream direction) distribution. The top rectangular figure represents the side view of the distribution and the lower rectangular figure represents the top view of the distribution. The distribution of velocity vectors represent the flow motion generated by heat addition from the irradiated surface. This flow is smaller than the external flow of 2 cm/s . Its center is located at a short distance upstream from the center of the external irradiation ($x=0$). This indicates that the steepest temperature gradient occurs at the upstream location due to downward pushing of the heated layer by the ambient flow. At a short distance downstream from $x=0$, there is a sink of flow due to the steep temperature gradient due to heat loss from the hot gas stream to the cold surface. Since the temperature gradient drives the flow, the flow generated by the external radiation is limited to a region near the irradiated surface area at an early time.

4. Future plans

1. Complete development of the three-dimensional ignition and flame spread code.
2. Conduct parametric study to determine which parameters affect ignition, the transition, and flame spread.
3. Measure global gas phase oxidation reaction rate for the degradation products of the paper.
4. Modify the codes to include piloted-ignition.

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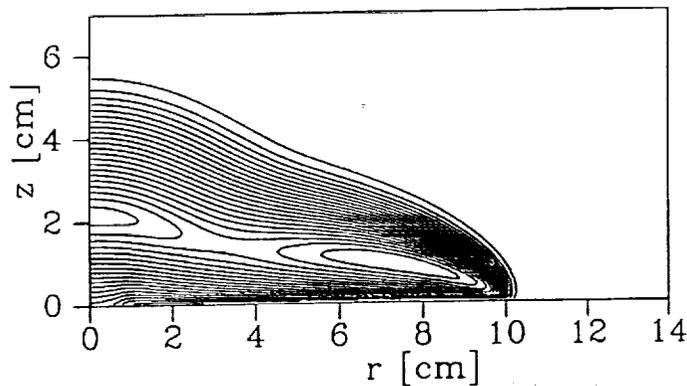


Fig. 1 Temperature contour in the gas phase

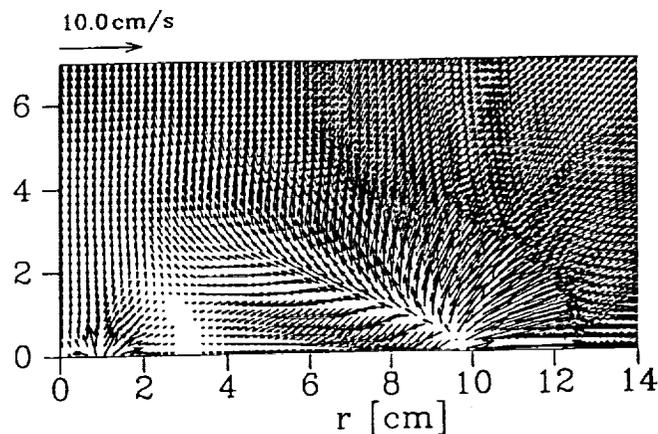


Fig. 2 Velocity vector

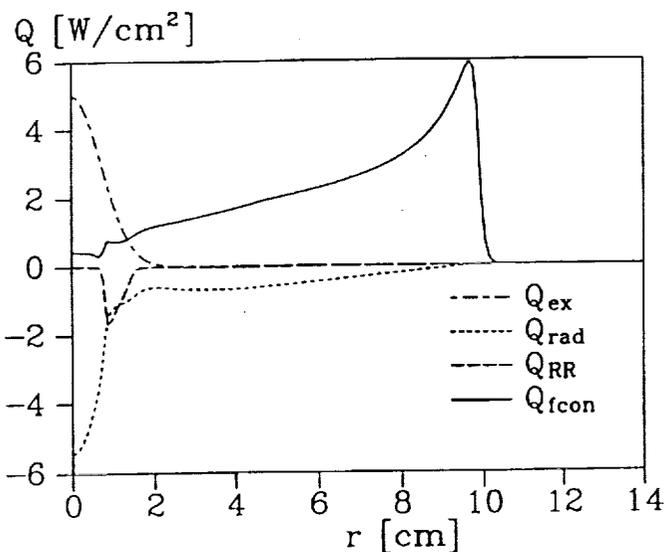


Fig. 3 Energy balance at the surface
50% oxygen

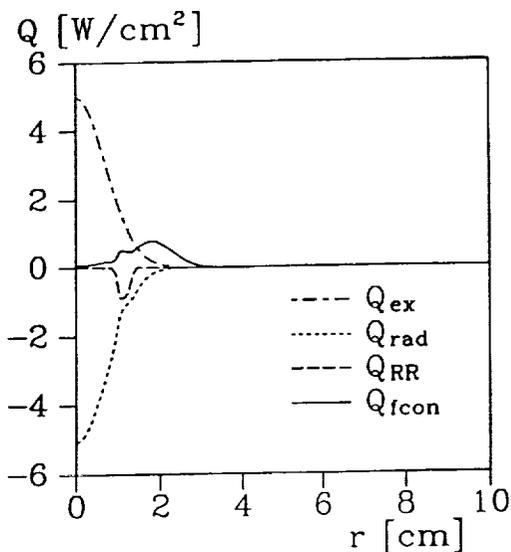


Fig. 4 Energy balance at the surface in air

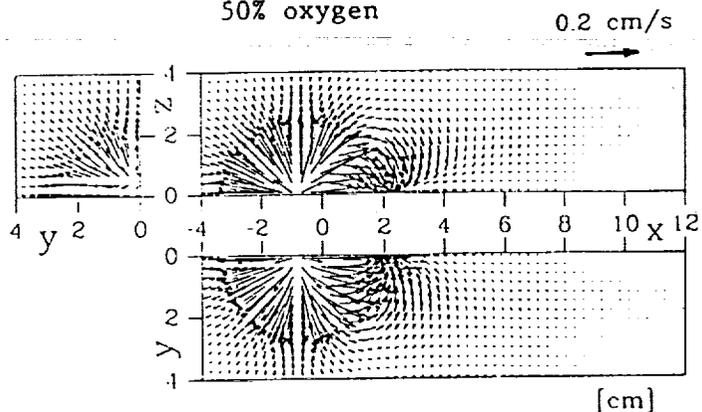
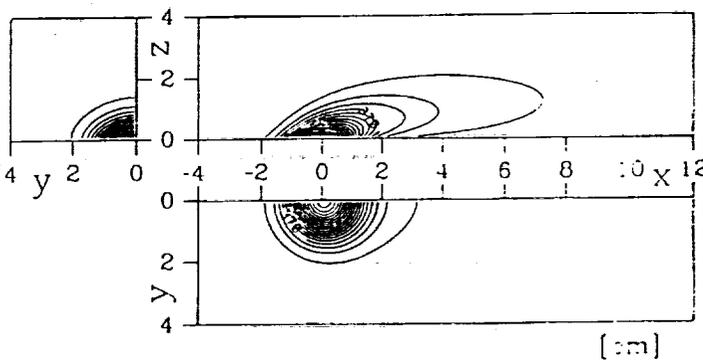


Fig. 5 Velocity vector in 3D flow



Temperature contour in 3D flow

COMMENTS

Question (David Schiller, U.C. Irvine): I have two questions regarding your numerical technique:

(1) In your paper, you state that you use a time-splitting algorithm to solve the governing equations. I have tried using different time steps for transport and chemical kinetics in my model of flame spread over liquid fuel pools. I have found that significant errors are introduced if the solution of the chemical kinetic and transport conditions are decoupled in this manner. Will you please describe your time-splitting algorithm in more detail and also tell me what you've done (if anything) to show that your time-splitting algorithm is "time step independent" and/or gives the same results as you would get if no time-splitting was used?

(2) It appears ignition occurs very close to the solid fuel surface. Is your solution grid independent? How fine a mesh was required in the gas just above the fuel surface (I use Δy_g of about 50 microns at the gas/liquid interface in my problem. Do you incorporate a partially or fully adaptive grid scheme to provide fine resolution near the flame leading edge as the flame propagates?

Answer: The algorithm employed in the computations is not time-split in the sense suggested in the question. It is a member of a class analyzed by Wichman (1). Basically, for a single-step reaction model of the kind used in many combustion studies (including this one) the reaction is almost always either much slower than or much faster than the local diffusion-convection balance. Under these circumstances, it is possible to show analytically that the species and energy equations can be advanced by splitting the time step in the following way: first the species in each computational cell are allowed to react as if the system were spatially homogeneous for the duration of the time step. The resulting temperature and species distributions are then initial conditions for the diffusion-convection problem, which is solved implicitly for the same time step. A stiff ODE solver is used for the first part of the calculation. The solver may require many internal steps to calculate the homogeneous reaction. The error is first order in the time-step if the reaction time is comparable to or greater than the diffusion-convection time and is smaller than this by a factor of the time-scale ratio when the reaction is fast. These statements are true for any scheme which is itself stable for the convection-diffusion problem.

The scheme has been tested by numerically computing solutions to the three-dimensional time-dependent heat transfer problem with an Oseen flow in the same geometry that has also been solved exactly analytically. The computer temperatures agree with the analytical results to better than 1/2 percent for the grid used. The ODE solver is a package with its own internal error controls, with a tolerance that can be set by the user. We require convergence in temperature to less than 0.5 degrees Kelvin in our computations. No adaptive grid schemes is employed. The gas phase grid is one millimeter on a side and a time step of 4×10^{-4} seconds is employed. This is certainly sufficient to put the flame in approximately the right place, although details of the flame structure might be lost. However, if fine structure in the flame leading edge is wanted, a considerably more sophisticated reaction scheme is also required. Such a study in the context of a three-dimensional transient problem is well beyond the current state-of-the-art.

**ORIGINAL PAGE IS
OF POOR QUALITY**

Question (Subrata Bhattacharjee, San Diego State): (1) How do you justify the flow being potential as well as creeping?

(2) In the absence of imposed convection, could the gas phase (combustion product) radiation cause significant flame cooling?

Answer: The velocity field that is used to evaluate the convection term in the diffusion-convection balance at low Reynolds numbers is a potential flow in almost all of the existing fluid flow, heat transfer, and combustion literature. As a simple example, the "Oseen flow" of any quantity at low Reynolds number is the leading order approximation to the solution for that quantity everywhere for a constant property fluid. The flow field that is used in the convection terms is a uniform flow which is trivially a potential flow. The approximation is correct even when the quantity being convected is the fluid vorticity! Indeed, this is exactly how the classical low Reynolds number drag, heat transfer, and combustion results are obtained. The actual velocity fields are far more complex, but additional detail is not needed if only the quantities that satisfy the Oseen equations are required. For further explanation and additional references see Kushida, et. al. (2).

The major role of radiation is in cooling the condensed phase surface. Its importance in the gas phase is unclear, in part because the precise nature of the gaseous combustion products is not yet well understood. We intend to investigate this further in the future.

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