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Category

Research Article

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Flame spread, Pyrolyzing materials, Crack formation, Dimensionless groups, Numerical analysis

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Cracking during flame spread over pyrolyzing solids

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Abstract

A theoretical and numerical model for the degradation of solid materials in combustion is developed. As solid materials are heated by the flame, they undergo an internal thermo- chemical breakdown process known as pyrolysis. As the pyrolysis front propagates into the sample, a charring layer is left behind which contains voids, fractures and defects. Cracks propagate to release tensile stresses accumulated when the sample is losing mass. The crack front may precede the pyrolysis front into the sample. Crack patterns and fracture behaviors vary depending on material properties and heating level and distribution. Cracks cause loss of material integrity by forming isolated loops or fragments. Cracks concentrate the stresses and reduce material ability to withstand external loads. Cracks expose uncharred materials to flame, accelerating combustion. The process is highly nonlinear: crack patterns display fractal behavior. Dimensionless groups that define the model are examined: each yields different crack patterns.

Keywords: Flame spread; Pyrolyzing materials; Crack formation; Dimensionless groups; Numerical analysis

Nomenclature

L	domain width
H	domain height
α	thermal diffusivity
T	solid temperature
ρ	solid density
ε	strain tensor
E	Young's modulus
k	thermal conductivity
γ	mass loss coefficient
ν	Poisson's ratio
l	length of heated region
q	heat flux parameter
A	pre-exponent factor
σ	stress tensor
u	displacement in x direction
v	displacement in y direction

Subscript

a	activation value
0	initial
c	critical
x, y	direction

Introduction

When solid materials like cellulose, rubber, and plastics are burned they release combustible gases via pyrolysis or evaporation of a liquid pool. The materials lose their structural integrity by charring, deforming and developing defects such as cracks, bubbles and voids. These defects enhance the combustion process by allowing oxygen to travel further into the material. They also allow pyrolysis gases to escape to the surface for subsequent combustion. For pyrolyzing materials, hot gases can force cracks to open by applying elevated hydrostatic pressures to lateral crack surfaces. The physical mechanism of crack and void formation is understood as follows: The burning sample develops cracks to relieve the tensile stress accumulated by nonuniform mass loss; when internal stresses appear in a sample not subject to external loading there exists a driving field such as temperature, moisture, or pore pressure. Sample constraints or inhomogeneity of the driving field inevitably generate tensile stresses. These crack the sample when specified limiting values are exceeded.

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Mathematical model

Our model includes heat transfer in the solid, material breakdown (pyrolysis) under high temperature, elastic deformation, and crack formation in the solid material. Here, the gas phase provides the external heat flux for the solid phase, which is the focus of our study. We consider the problem over a rectangular $L \times H$ (L is length in the x-direction, H is depth in the y-direction) domain. The temperature field $T(x, y, t)$ is described by the heat conduction equation

$$\frac{\partial T}{\partial t} = \alpha_x \frac{\partial^2 T}{\partial x^2} + \alpha_y \frac{\partial^2 T}{\partial y^2}, \tag{1}$$

where α_x and α_y are the thermal diffusivities in the x and y directions, respectively. Under a high and constant external heat flux, the solid pyrolyzes according to the following single step reaction equation

$$\frac{\partial \rho}{\partial t} = -A(\rho - \rho_c) e^{-T_a/T}, \tag{2}$$

where A is the pre-exponential factor, T_a is the activation temperature and ρ_c is the lower bound of solid density, or the char density. Because of the two-dimensional nature of the problem, the strain tensor contains only the components ε_{xx}, ε_{xy}, ε_{yx}, ε_{yy} and ε_{zz}. The stress tensor, for the state of plane stress, only consists of σ_{xx}, σ_{xy}, σ_{yx} and σ_{yy}, i.e., we use the plane stress condition, $\sigma_{zz} = 0$. When the overall strain is taken to be equal to the sum of a mechanical strain and a shrinkage strain due to loss of mass, the stress-strain relations become

$$\sigma_{ij} = \frac{E}{1+\nu}\varepsilon_{ij} + \left[\frac{E\nu}{1-\nu^2}(\varepsilon_{kk}) - \frac{E}{1-\nu}\gamma\frac{\rho-\rho_0}{\rho_0}\right]\delta_{ij} \tag{3}$$

$i = 1,2;\ j = 1,2$

where i or $j = 1,2$ represents x, y. Here E is the Young's modulus, ν is the Poisson's ratio and the coefficient γ couples material mass loss and volume reduction. The displacement fields in the x and y directions are denoted by $u(x, y, t)$ and $v(x, y, t)$, respectively. The strains in the (x, y)-plane are related to u and v by the standard relations $\varepsilon_{xx} = \partial u/\partial x$, $\varepsilon_{yy} = \partial v/\partial y$ and $\varepsilon_{xy} = (1/2)(\partial u/\partial y + \partial v/\partial x)$. The stress equations of equilibrium are $\partial\sigma_{xx}/\partial x + \partial\sigma_{xy}/\partial y = 0$ and $\partial\sigma_{xy}/\partial x + \partial\sigma_{yy}/\partial y = 0$, where we have used $\sigma_{xy} = \sigma_{yx}$. The stress tensor has three eigenvalues which represent the three principal stresses, σ_I, σ_{II} and σ_{III}. It is assumed that cracks nucleate and grow whenever the maximum principal stress σ_p, defined as $\max(\sigma_I, \sigma_{II}, \sigma_{III})$, attains a threshold value σ_c which is understood in this article as a material constant. Cracks form at locations where $\sigma_p \geq \sigma_c$.

We now write the initial and boundary conditions for the thermal-pyrolysis-stress problem. Initially, the sample has the uniform temperature $T = T_0$ which is maintained at the two sample lateral sides throughout heating. The lower surface $y = H$ is insulated so $\partial T/\partial y = 0$, while the upper surface is subjected at its surface to a constant heat flux q_0 over the central region of length l. Thus $k_y\,\partial T/\partial y = q_0$ for $|x - L/2| \leq l/2$, where k_y is the y-direction thermal conductivity. The solid density has uniform initial value $\rho = \rho_0$, which gradually decreases to its charring, or minimum value ρ_c. Regarding the imposed physical boundary conditions, the stress constraint on the lower surface is referred to as a ''roller" condition (no deflection in the y-direction, freedom of movement in the x-direction, while all three remaining sample sides are unconstrained, or traction free.

Dimensionless groups

The problem is characterized by three time scales. These scales correspond to heat conduction, heat flux, and chemical reaction. The heat conduction time scale that characterizes Eq. (1) is $t_{hc} = H^2/\alpha_y$. The heat flux time scale that characterizes the relation of thermal boundary conditions to the heat conduction equation Eq. (1) is defined as $t_{flux} = HT_0k_y/(\alpha_y q_0)$. The chemical reaction time scale characterizes the pyrolysis reaction as described by Eq. (2) and is taken as $t_{chem} = [A\exp(-T_a/T_0)]^{-1}$.

Our heat conduction- pyrolysis- elasticity problem contains sixteen constants, in which the Poisson's ratio ν and the mass loss coefficient γ are already dimensionless. The other fourteen have units composed of four basic units. Of these fourteen, q_0 and k_y only appears as a ratio, leaving thirteen constants. These constants are L, H, α_x, α_y, T_0, q_0/k_y, l, ρ_c, A, T_a, ρ_0, E, σ_c.

The four basic units can be taken as either length/time/temperature/energy or length/time/temperature/mass. By using the Buckingham π theorem, the thirteen dimensional constants are combined to form nine dimensionless π groups. We choose the following nine π groups to characterize our problem: $\Pi_1 = H/L$, $\Pi_2 = l/L$, $\Pi_3 = \alpha_y/\alpha_x$, $\Pi_4 = q_0H/(k_yT_0)$, $\Pi_5 = T_a/T_0$, $\Pi_6 = H^2Ae^{-T_a/T_0}/\alpha_y$, $\Pi_7 = \rho_c/\rho_0$, $\Pi_8 = E/[\rho_0(AH)^2]$, $\Pi_9 = \sigma_c/E$. The first two groups, Π_1 and Π_2, represent the problem geometry. The next two groups, Π_3 and Π_4, are properties of the thermal subproblem in which Π_4 equals t_{hc}/t_{flux}. The sixth group is equal to t_{hc}/t_{chem}. This group, along with Π_5, describes the relationship between the thermal and pyrolysis subproblems. The seventh group defines the extent of pyrolysis while the ninth group specifies the element removal or crack growth criterion. Group Π_8 relates material pyrolysis to the stress subproblem. Group Π_9, the ratio of the cracking stress to the elastic modulus, can also be interpreted as the crack resistance

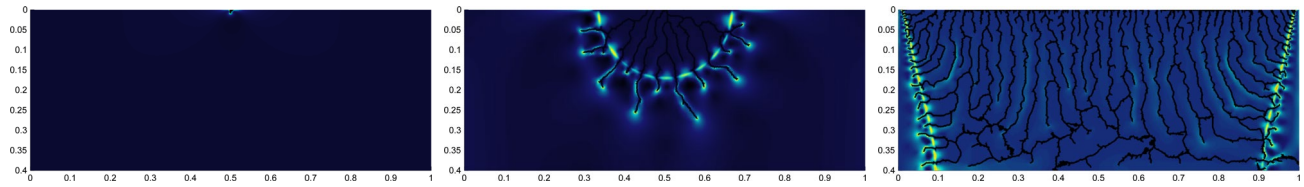

Fig. 1. Vary $\Pi_2 = l/L$. Left, $\Pi_2 = 0.01$, $\Pi_6 = 100\Pi_6^0$; Middle, $\Pi_2 = 0.1$, $\Pi_6 = \Pi_6^0$; Right, $\Pi_2 = 1.0$, $\Pi_6 = \Pi_6^0$.

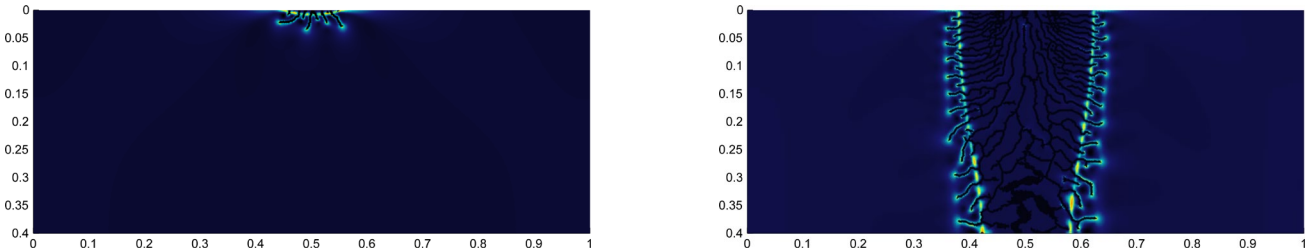

Fig. 2. Vary $\Pi_3 = \alpha_y/\alpha_x$. Left, $\Pi_3 = 0.1\Pi_3^0$; Right, $\Pi_3 = 10\Pi_3^0$.

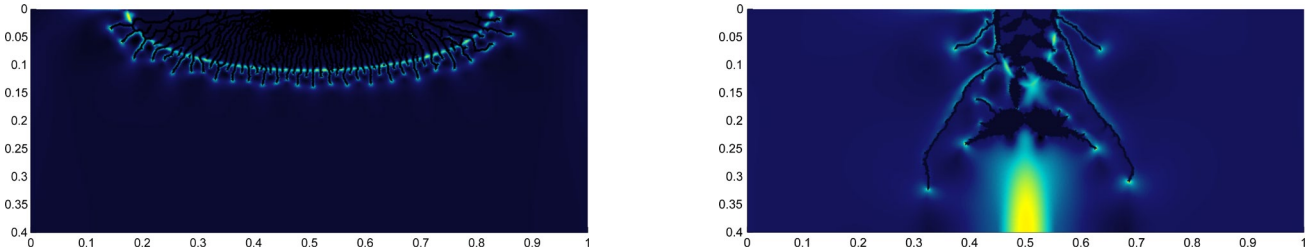

Fig. 3. Vary $\Pi_3 = \alpha_y/\alpha_x$. Left, $\Pi_3 = 0.1\Pi_3^0$ and $\Pi_6 = 10\Pi_6^0$; Right, $\Pi_3 = 10\Pi_3^0$ and $\Pi_6 = 0.1\Pi_6^0$.

parameter. When Π_9 is sufficiently large, no cracks can form.

The field of fracture mechanics often separates two distinct process, crack initiation and crack propagation. The theory of thermoelasticity suggests that materials having a high crack initiation resistance also have a high tensile strength, a high thermal diffusivity, a low Young's modulus and undergo low thermal expansion [1] during heating. During cooling, most materials contract, or shrink, just as the pyrolyzing solid in this study contracts when it loses mass. Thus, the thermal contraction coefficient in cooling is analogous to the current mass loss coefficient because both function as coefficients of the shrinkage stress.

Our problem, characterized by nine π groups, will employ characteristic units from the parameters H, t_{hc}, T_0 and ρ_0 (length, time, mass and temperature). We let $\bar{x} = x/H$, $\bar{y} = y/H$, $\tau = t/t_{hc}$, $\theta = (T - T_0)/T_0$. Then Eq. (1) can be written as: $\partial\theta/\partial\tau = (\Pi_3\partial^2\theta/\partial\bar{x}^2 + \partial^2\theta/\partial\bar{y}^2)$. The initial condition for the dimensionless temperature θ is $\theta = 0$, which is also the boundary condition at the two sides, $y = 0, L$. The boundary condition for θ on the insulated side is: $\partial\theta/\partial\bar{y} = 0$, and on the heated side is:

$$\frac{\partial\theta}{\partial\overline{y}} = \begin{cases} 0 & \text{if } \left|\overline{x} - \dfrac{1}{2\Pi_1}\right| > \dfrac{\Pi_2}{2\Pi_1} \\ \Pi_4 & \text{if } \left|\overline{x} - \dfrac{1}{2\Pi_1}\right| \le \dfrac{\Pi_2}{2\Pi_1}. \end{cases}$$

The pyrolysis equation (2) becomes

$$\frac{\partial\overline{\rho}}{\partial\tau} = -(\overline{\rho} - \Pi_7)\frac{1}{\Pi_6}e^{\Pi_5\left(\frac{\theta}{1+\theta}\right)}.$$

Finally, the stresses are non-dimensionalized with respect to Young's modulus E using $E = (\Pi_8/\Pi_6^2)\exp(2\Pi_5)\,\rho_0 H^2/t_{hc}^2$, viz. $\overline{\sigma_{xx}} = \sigma_{xx}/E$, $\overline{\sigma_{yy}} = \sigma_{yy}/E$, $\overline{\sigma_{xy}} = \sigma_{xy}/E$, $\overline{\sigma_{zz}} = \sigma_{zz}/E$, $\overline{\sigma_p} = \sigma_p/E$, where σ_p is the relevant principal stress.

Numerical results

We use thermo-mechanical properties of a rubber-like material. Also, we use $q_0/k_y = 1.2 \times 10^5$ K/m as standard values. Subsequently we vary the parameter groups with these as reference values. The sample size is taken to be 5 cm $\times$ 2 cm so $\Pi_1 = 0.4$. For rubber-like materials we use $\nu = 4.5 \times 10^{-1}$ and $\gamma = 1$. The reference values of the groups become: $\Pi_3^0 = 1.0$, $\Pi_4^0 = 4 \times 10^1$, $\Pi_5^0 = 3.15 \times 10^1$, $\Pi_6^0 = 1.0 \times 10^{-3}$, $\Pi_7^0 = 3 \times 10^{-1}$, $\Pi_8^0 = 1.8 \times 10^{-18}$, $\Pi_9^0 = 3.33 \times 10^{-2}$.

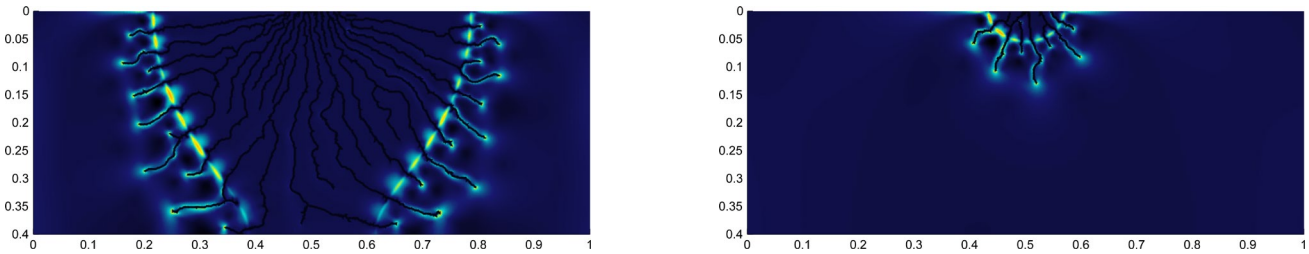

Fig. 4. Vary $\Pi_4 = q_0 H/(k_y T_0)$. Left, $\Pi_4 = 2\Pi_4^0$; Right, $\Pi_4 = 0.5\Pi_4^0$.

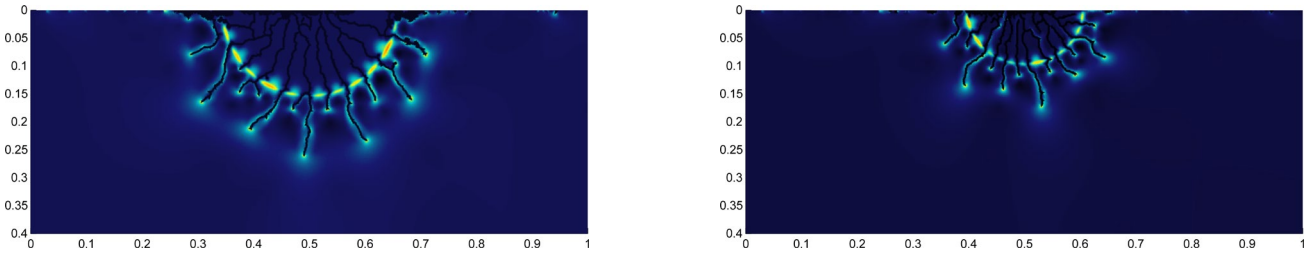

Fig. 5. Vary T_a. $\Pi_5 = T_a/T_0$, $\Pi_6 = H^2 A e^{-T_a/T_0}/\alpha_y$. Left, $\Pi_5 = 0.9\Pi_5^0$, $\Pi_6 = \Pi_6^0$; Right, $\Pi_5 = 1.1\Pi_5^0$, $\Pi_6 = \Pi_6^0$.

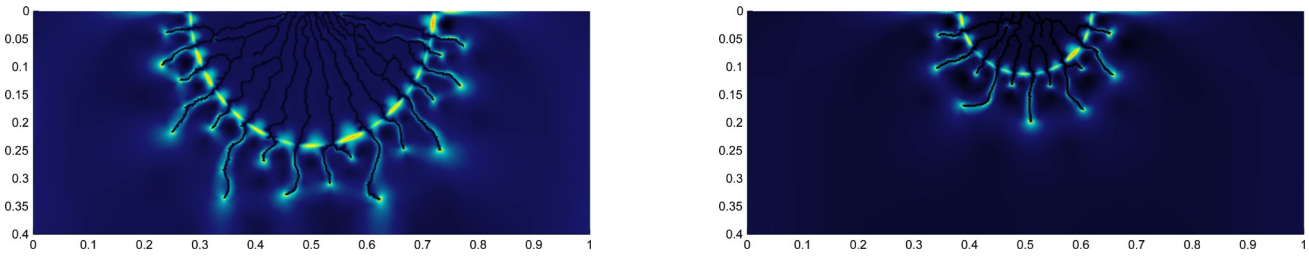

Fig. 6. Vary $\Pi_6 = H^2 A e^{-T_a/T_0}/\alpha_y$ by varying A. Left, $\Pi_6 = 10\Pi_6^0$; Right, $\Pi_6 = 0.1\Pi_6^0$.

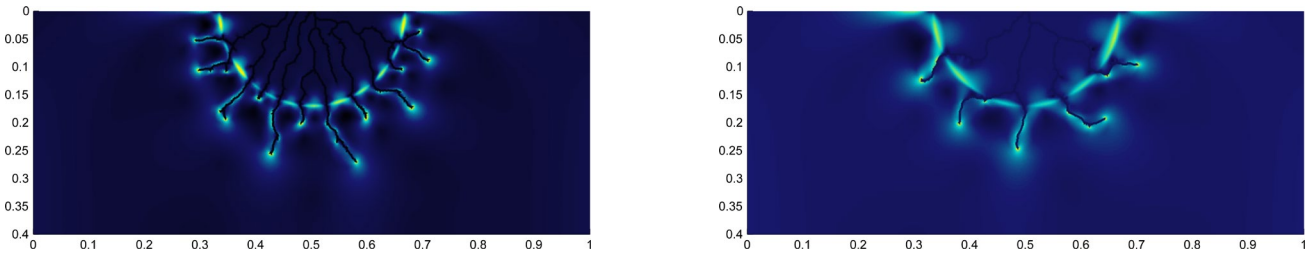

Fig. 7. Vary $\Pi_9 = \sigma_c/E$. Left, $\Pi_9 = \Pi_9^0$; Right, $\Pi_9 = 1.4\Pi_9^0$. As Π_9 increases, fewer cracks form. For very large σ_c/E no cracks will form.

All of the images below show the maximum principal stress field evaluated at the simulation time $t = 3000$ sec = 50 min. In all cases, the maximum stress is σ_I.

Vary Π_2. Group Π_2 describes the length l of the surface over which heat flux is applied. When the heat flux is centered, the cracks propagate radially (Fig. 1 middle, $\Pi_2 = 0.1$). On the other hand, a uniform heat flux over the surface causes crack growth to be vertical (Fig. 1 right, $\Pi_2 = 1.0$). When $\Pi_2 = 0.1$, the heat flux may represent a flame whose tip width is $\approx$ 5 mm. In Fig. 1 left, $\Pi_2 = 0.01$, a very small heated width, only a small slit forms at the center region of the surface, even with a very high value of $\Pi_6 = 100\Pi_6^0$ (if Π_6 were as small as the other two figures, there would be no cracks at all).

Vary $\Pi_3 = \alpha_y/\alpha_x$. As seen from Fig. 2, increasing Π_3 enhances heat transfer toward the in-depth (y) direction, leading to dramatically different crack patterns (crack growth in-depth) as well as a decrease in the crack spacing in the y-direction. On the other hand, when Π_3 is decreased, heat transfer in the horizontal (x) direction is dominant, and the cracks spread horizontally. In Fig. 2 left (right), Π_3 decreases (increases) by a factor of 10, the other π groups remaining unchanged. This corresponds to letting the thermal diffusivity in the horizontal direction α_x

increase (decrease) by a factor of 10.

Another way to change Π_3 is to change α_y, which also changes $\Pi_6 = t_{hc}/t_{chem}$. From Fig. 2 and Fig. 3, it can be seen that Π_3 determines the shape of the crack pattern: both Fig. 2 (Left) and Fig. 3 (Left) have the same Π_3. By contrast, cracks caused by a decrease in α_y or α_x lead to more cracks (Fig. 2 (Right) and Fig. 3 (Left)). Fig. 3 (Right) increases α_y by a factor of 10, keeping α_x constant.

Vary $\Pi_4 = q_0 H/(k_y T_0)$. Group Π_4 represents heat flux strength. Higher heat fluxes raise the temperature faster, enhance pyrolysis and produce more cracks, see Fig. 4.

Vary activation energy T_a. Changing T_a changes both Π_5 and Π_6. In Fig. 5 (Left), T_a is lower by 10 %, whereas in Fig. 5 (Right) it is increased by 10 % over its standard value. As expected, a lower T_a produces more damage to the sample because it pyrolyzes at a faster rate.

Vary Π_6. Group Π_6 characterizes the pyrolysis rate. As Π_6 increases, pyrolysis happens at a faster rate, and so does crack propagation as seen from Fig. 6.

Vary Π_9. Since the group Π_9 characterizes material strength, samples with higher Π_9 produce fewer cracks with larger crack spacing compared with lower strength samples, see Fig. 7.

Conclusion

This model for crack formation in a pyrolyzing elastic solid generates nine π dimensionless parameter groups. Some are related to geometry, others to heat transfer, some to material chemical breakdown, some to elastic strength parameters, and several linking or coupling these effects. For this reason, the spectrum of material response to heating can be dramatically altered. The heating length scale l appears only in the ratio $\Pi_2 = l/L$. Since the flame scale varies solely through this parameter, this model can potentially be adapted to problems that span the range between very small flames (micro-flames) and very large flames (macro-flames).

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