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Technical Notes

TECHNICAL NOTES are short manuscripts describing new developments or important results of a preliminary nature. These Notes cannot exceed 6 manuscript pages and 3 figures; a page of text may be substituted for a figure and vice versa. After informal review by the editors, they may be published within a few months of the date of receipt. Style requirements are the same as for regular contributions (see inside back cover).

Effect of Dual-Phase-Lag Heat Conduction on Ignition of a Solid

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Nomenclature

B = ratio of phase lags, $\frac{1}{2}(\tau_T/\tau_q)$
C = specific heat of mixture
E = activation energy
H = heat of reaction
k = thermal conductivity of mixture
q_0 = constant heat flux applied along $x = 0$
R = universal gas constant
S = volumetric rate of heat release for mixture
T = temperature of solid constituent
T_i = initial temperature
t = time
x = position
α = thermal diffusivity of mixture, $k/(\rho C)$
β = dimensionless activation energy, $E/(RT_i)$
γ = dimensionless parameter, $q_0(\alpha\tau_q)^{1/2}/(kT_i)$
δ = dimensionless heat of reaction, $2\rho\nu H(\alpha\tau_q)^{1/2}/q_0$
η = dimensionless position, $x/[2(\alpha\tau_q)^{1/2}]$
ν = preexponential factor for reaction
ξ = dimensionless time, $t/(2\tau_q)$
ρ = density of mixture
τ_q, τ_T = phase lags of heat flux and temperature gradient, respectively
φ = dimensionless temperature, $(T - T_i)k/[q_0(\alpha\tau_q)^{1/2}]$
ω = integration variable in Eq. (2)

Superscript

$*$ = value at approximate ignition time

Introduction

THIS Note shows that non-Fourier dual-phase-lag (DPL) heat conduction[1] can significantly reduce the ignition time of a solid compared to Fourier conduction. Here "ignition time" is the time needed for the solid to exhibit thermal runaway in surface temperature. Ignition is induced by subjecting the solid to an external heat flux to accelerate an internal Arrhenius reaction and rate of heat release.

Using DPL conduction may increase the accuracy of predictions for ignition and lead to other improvements not anticipated from Fourier conduction, as noted in the Conclusion. Applications[2] that may involve DPL conduction include designing rocket motors that use granular propellants and optimizing self-propagating high-temperature synthesis (SHS) for the synthesizing of ceramics from granular reactants.

Focusing for the moment, however, on nonreactive granular solids such as sand–air mixtures, we find that the conventional approach[1,3] for predicting transient temperature uses Fourier's law with locally identical temperatures for mixture constituents. Although this conventional approach is sufficiently accurate in most cases, its predictions show significant deviations from recent experiments.[1,3] For example,[1] in a block of sand with an internal heat source, the conventional approach fails to provide accurate temperature predictions near the source for a period of several seconds after heating begins. The conventional approach fails during this period because it does not account for thermal nonequilibrium between sand particles and air in the block.

In contrast to this failure, the DPL model of conduction gives accurate predictions[1] during the nonequilibrium period. Its accuracy stems from the use of different temperatures for sand particles and air along with the phase lags τ_q and τ_T of heat flux and temperature gradient, respectively. In general terms, the relative values of the lags represent deviations from Fourier's law, where, for instance, $\tau_q = 8.94$ s and $\tau_T = 4.48$ s for a block of sand.[1]

It is convenient here to interpret τ_q as representing the delay (inertia) in heat conduction that results from resistance to conduction. This delay could arise, for example, from contact resistance between sand particles. In comparison, τ_T is conveniently interpreted here as accounting for heat transfer (substructural interaction) between the particles and air. Reference 1 discusses the lags in more detail and shows that DPL predictions converge to those based on Fourier's law as sand particles and air approach local thermal equilibrium.

Turning now to reactive granular solids, we see that predictions of transient temperature also typically use the conventional approach involving Fourier's law.[4] Although experiments have not yet been performed to provide evidence of DPL conduction in these reactive solids, it is likely to occur because of structural similarities to sand.[2] However, non-Fourier behavior may have been overlooked in past experiments.[2]

For constant ρ, C, k, τ_q, and τ_T, a one-dimensional DPL heat equation[1] applicable to a reactive granular solid composed of one solid constituent and a gas (e.g., air) is

$$\tau_q \frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} + \alpha\tau_T \frac{\partial^3 T}{\partial t \partial x^2} + \frac{1}{\rho C}\left(S + \tau_q \frac{\partial S}{\partial t}\right) \qquad (1)$$

where T is the temperature of the solid constituent in the solid–gas mixture. The thermal diffusivity α should be determined under steady-state conditions to avoid biasing its value toward transient Fourier conduction or any particular model of non-Fourier conduction.

Interestingly, extended irreversible thermodynamics[5] (EIT) can provide heat equations that are analogous to DPL equations. For example, setting $S = 0$ in Eq. (1) reduces it to the EIT analog of Eq. (54) in Ref. 5.

Expression for Ignition Time

To show the effect of DPL conduction on ignition, this Note develops an expression for the approximate ignition time t^* of a semi-infinite solid occupying $x > 0$ with a uniform initial temperature. At $t = 0^+$ it is subjected to the constant heat flux q_0 along the surface $x = 0$ where ignition eventually occurs at t^*. Details of the

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solid and reaction are identical to those in Ref. 2, where ignition involves hyperbolic conduction.

The Appendix of this Note defines the physical basis for the approximate ignition time with DPL conduction and then summarizes the development of its expression, which incorporates previous work.[2,6] In dimensionless terms, the DPL approximate ignition time ξ^* is given by the implicit expression

$$\frac{1}{\pi}\left\{\int_0^{\omega_1} I_3\,\mathrm{d}\omega + \int_{\omega_1}^{\omega_2} I_4\,\mathrm{d}\omega + \int_{\omega_2}^{\infty} I_3\,\mathrm{d}\omega\right\} = \frac{1}{\gamma}\left[\frac{\beta}{\ln(\delta/2\gamma)} - 1\right] \tag{2}$$

for $B < \frac{1}{2}$, where B is a ratio of phase lags. The integrands in Eq. (2) are

$$I_3 = (1/a\omega^2)(4a - \exp(-A\xi^*/2)\{[4 + 2\omega^2(B - 1)]\sinh(a\xi^*) + 4a\cosh(a\xi^*)\}) \tag{3}$$

$$I_4 = (1/b\omega^2)(4b - \exp(-A\xi^*/2)\{[4 + 2\omega^2(B - 1)]\sin(b\xi^*) + 4b\cos(b\xi^*)\}) \tag{4}$$

where $A = (2 + B\omega^2)$, $a = (A^2 - 4\omega^2)^{1/2}/2$, and $b = (4\omega^2 - A^2)^{1/2}/2$. Further, the limits ω_1 and ω_2 in Eq. (2) are determined from

$$\omega_1, \omega_2 = \left[2(1 - B) \mp 2(1 - 2B)^{\frac{1}{2}}\right]^{\frac{1}{2}} / B \tag{5}$$

where the minus sign of $\mp$ pertains to ω_1 and the plus sign corresponds to ω_2. The integrals in Eq. (2) have to be evaluated numerically, but the limits 0, ω_1, and ω_2 are singular points. However, L'Hôpital's rule shows that $I_3 = 2\xi^*$ at $\omega = 0$. Similarly, at ω_1 and ω_2,

$$I_3 \text{ and } I_4 = (2/\omega^2)\,(2 - \exp(-A\xi^*/2)\{2 + \xi^*[2 + \omega^2(B - 1)]\}) \tag{6}$$

where ω represents ω_1 or ω_2. For $B = 0$, however, Eq. (6) pertains to only ω_1 because $\omega_1 = 1$ and $\omega_2 = \infty$ for this value of B.

Note that Ref. 1 shows $B < \frac{1}{2}$ near the source of heat in the experiments with sand cited earlier. Thus, by analogy with those experiments, $B < \frac{1}{2}$ is taken as relevant here because ignition of the semi-infinite solid is determined[2] by its transient temperature at and near the surface subjected to q_0 (the source of heat needed to induce ignition). Also, phase lags determined for sand in the experiments of Ref. 1 are used in the calculations described next because the lags have not yet been obtained for reactive solids.

Effect of DPL Conduction

This Note calculates the DPL approximate ignition time ξ^* from Eq. (2) by adopting the values of q_0 and properties for solid propellants stated in Ref. 2. These values, along with $\tau_q = 9.0$ s for sand,[1] give $\beta = 33\frac{1}{3}$, $\delta = 1.75 \times 10^8$, and $\gamma = 0.58$. For the several types of sand reported in Ref. 1, relevant values of B range from approximately 0.08 to 0.37. Here, however, B $(= \frac{1}{2}\tau_T/\tau_q)$ is treated as a parameter over the wider range of 0–$\frac{1}{2}$ by fixing τ_q at 9.0 s and varying τ_T. In particular, $B = 0$ $(\tau_T = 0)$ and $\frac{1}{2}$ $(\tau_T = \tau_q)$ correspond to the limits of hyperbolic and Fourier conduction, respectively.[6]

Values for ξ^* corresponding to $B < \frac{1}{2}$ were obtained by solving Eq. (2) with a trial-and-error method. This method guessed values of ξ^* for each B until both sides of the equation agreed to within 1%. For $B = \frac{1}{2}$ (Fourier conduction) the value of ξ^* was obtained with the same method, except that it used the approximate ignition time (not shown) corresponding to $B \geq \frac{1}{2}$. (The Appendix summarizes the development of this approximation for $B \geq \frac{1}{2}$.) For all values of B, the numerical integrations were performed as in Ref. 6. Finally, the expressions for approximate ignition time and this trial-and-error method were tested by confirming values of ξ^* calculated with approximations of ignition time obtained independently[2] for hyperbolic and Fourier conduction.

Figure 1 shows the effect of B on ξ^* for the semi-infinite solid. The dashed lines show the limiting cases of $\xi^* = 0.69$ for Fourier $(B = \frac{1}{2})$ and $\xi^* = 0.36$ for hyperbolic $(B = 0)$ conduction. The key feature of this figure is that DPL conduction can significantly reduce ignition time compared with the time obtained with Fourier's law.

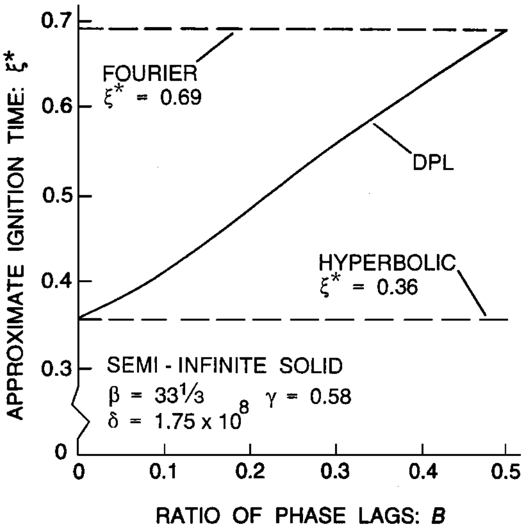

Fig. 1 Effect of phase-lag ratio B on approximate ignition time ξ^*.

In general, Fig. 1 shows that DPL ignition time decreases as B decreases from the Fourier limit of $B = \frac{1}{2}$. This decrease in ignition time occurs because, as B $(= \frac{1}{2}\tau_T/\tau_q)$ becomes smaller with constant τ_q (the case here), τ_T and its substructural effect also become smaller, corresponding to less heat transfer between solid particles and gas within the semi-infinite solid. Hence, conduction in the solid is increasingly confined to its network of particles, resulting in an increased effect of conduction delay even though τ_q is constant. In turn, this increased effect of delay causes the surface temperature of the solid to become progressively higher than the surface temperature for Fourier conduction.[6] Then this higher temperature causes faster heat release at the surface and earlier ignition compared with Fourier conduction because Arrhenius reaction rates increase exponentially with increasing temperature. The limiting case of hyperbolic conduction $(B = 0)$ shows the smallest ignition time because with $\tau_T = 0$ it corresponds to the greatest effect of conduction delay, leading to the highest surface temperature[6] and most rapid heat release.

More specifically, with $B = 0.08$, for example, and ξ^* from Fig. 1 of 0.4 and 0.69 for DPL and Fourier conduction, respectively, DPL conduction causes approximately a 40% reduction in ignition time relative to the Fourier time. In dimensional terms for this example, the DPL approximate ignition time is $t^* = 7.2$ s, whereas the Fourier time is $t^* = 12.4$ s (obtained by using $t^* = 2\tau_q\xi^*$ and $\tau_q = 9.0$ s). Furthermore, although this reduction is based on approximations, Ref. 2 shows that these types of approximations can give good estimates of reductions in ignition times.

Conclusion

The reduction in ignition time just attributed to DPL conduction raises the possibility of controlling and improving ignition in ways not anticipated from Fourier conduction. For example, it may be possible to manipulate the structure of a reactive granular solid to find values of τ_q and τ_T that maximize this reduction. Then these values would minimize the amount of energy required for ignition because the same external heat flux could be applied over a shorter period. In practical terms for space-based SHS, minimizing ignition energy could reduce the payload weight of ignition systems and the cost of lifting them into space.

In conclusion, the reduction in ignition time shown here and the potential for improvements not anticipated from Fourier conduction provide motivation to further study the effect of DPL conduction on ignition and other reactive processes involving solids.

Appendix: Development of Expression for Approximate Ignition Time

The physical basis of approximate ignition time for the semi-infinite solid with DPL conduction takes advantage of the expected behavior for its surface temperature: For small values of time after the application of q_0 along the surface $x = 0$, internal heating by reaction should be small compared with external heating by q_0 because the surface temperature and associated reaction rate are still relatively low. Thus, these small time values correspond to a period of nearly inert (nonreactive) heating dominated by q_0. During this inert period, the surface temperature is approximated by the solution to the corresponding inert DPL problem where $S = 0$. For large times, however, the surface temperature is high enough for heating by reaction to dominate and cause thermal runaway. Hence, approximate ignition time t^* is defined here as that intermediate time when rates of internal heating by reaction and external heating by q_0 become momentarily equal. The surface temperature at t^* is the corresponding approximate ignition temperature T^*.

Reference 2 develops an expression for approximate ignition time by using the physical basis of t^* just described but for hyperbolic conduction. (Reference 2 terms this hyperbolic approximation the "rough approximation.") Thus, by analogy, developing the expression for t^* with DPL conduction starts with Eq. (1A) in Ref. 2 because that equation is a convenient form for T^* of the semi-infinite solid regardless of the model chosen for conduction. Then T^* is eventually related to t^* for DPL conduction. Consequently, introducing β, δ, γ, and dimensionless DPL approximate ignition temperature φ^* into Eq. (1A) of Ref. 2 and then solving for φ^* gives

$$\varphi^* = (1/\gamma)[\beta/\ln(\delta/2\gamma) - 1] \tag{A1}$$

Equation (A1) here arises from the equivalence of external and internal heating underlying the approximate ignition time.

Completing the development for DPL conduction requires obtaining a relation between φ^* and ξ^* and then using this relation to replace φ^* by ξ^* in Eq. (A1). For this relation to be obtained, Eq. (1) from the main body of this Note is first made dimensionless by using B, φ, β, δ, and γ, along with η and ξ. In particular, $\eta = 0$ is the surface of the semi-infinite solid where ignition occurs at ξ^*. This dimensionless form of Eq. (1) replaces Eq. (3A) in Ref. 2. Next, with the use of the same reasoning as in Ref. 2, the dimensionless form of Eq. (1), with appropriate boundary and initial conditions, reduces to that describing the problem for the DPL inert heating period. Section 3.1 in Ref. 6 states this inert problem, with some differences in nomenclature from that of this Note. The solution to this inert problem for $B < \frac{1}{2}$ is given by Eq. (12) in Ref. 6. Converting that equation to the nomenclature of this Note and then setting $\eta = 0$ and $\xi = \xi^*$ in the converted equation provides the relation between φ^* and ξ^*. Then using this relation to replace φ^* in Eq. (A1) here provides the implicit expression for ξ^* when $B < \frac{1}{2}$, given as Eq. (2) in the main body of this Note. Alternatively, the expression for ξ^* when $B \geq \frac{1}{2}$ is obtained by using Eq. (11) from Ref. 6 in place of Eq. (12).

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Band Lumping Strategy for Radiation Heat Transfer Calculations Using a Narrowband Model

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Nomenclature

f = species molar fraction or the distribution function of the absorption coefficient
g = cumulative distribution function
g_i = the ith Gauss quadrature point
I_i = radiation intensity at the ith quadrature point, W/m^2 cm^{-1} sr
k = absorption coefficient, m^{-1}
k_i = absorption coefficient at the ith quadrature point, m^{-1}
L = path length, m
s = position variables along a line of sight, m
T = temperature, K
w_i = weight parameter of the ith Gauss quadrature point
$\Delta\nu$ = wave number interval of a band, cm^{-1}
ν = wave number, cm^{-1}
$\bar{\tau}$ = band-averaged gas transmissivity

Subscripts

b = blackbody
nb = narrowband
wb = wideband

I. Introduction

ACCURATE calculations of real-gas radiation are inherently difficult due to the extremely strong spectral variations of gas radiative properties. In combustion, real-gas practically means CO_2 and H_2O present in the combustion products for hydrocarbon fuels. Oversimplified gas radiation models yield large errors in the prediction of gas radiation and cannot be used as a reliable radiation submodel in an overall combustion or flame code. The exact line-by-line (LBL) calculations, however, are far too computationally intensive to be applied to problems of practical interest. Therefore, substantial research efforts have been devoted to development of accurate and efficient nongrey gas radiation models.

The statistical narrowband correlated-k (SNBCK) method represents an efficient alternative for implementing the statistical narrowband (SNB) model. The method has recently been applied to two-dimensional real-gas radiation transfer by Goutière et al.,[1] and they found that the SNBCK method yields total quantities almost identical to those of the SNB model with far less computing effort. The SNBCK method overcomes the difficulties of the SNB model because it extracts gas absorption coefficients from the SNB gas transmissivity. As a result, any radiative transfer equation (RTE) solvers, especially the efficient and accurate discrete-ordinates method (DOM), can be used. Extension of the SNBCK method to scattering problems is straightforward. The seven-point

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