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Group theoretical modeling of thermal explosion with reactant consumption

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ABSTRACT

Today engineering and science researchers routinely confront problems in mathematical modeling involving nonlinear differential equations. Many mathematical models formulated in terms of nonlinear differential equations can be successfully treated and solved by Lie group methods. Lie group analysis is especially valuable in investigating nonlinear differential equations, for its algorithms act as reliably as for linear cases. The aim of this article is to provide the group theoretical modeling of the symmetrical heating of an exothermally reacting medium with approximations to the body's temperature distribution similar to those made by Thomas [17] and Squire [15]. The quantitative results were found to be in a good agreement with Adler and Enig in [1], where the authors were comparing the integral curves corresponding to the critical conditions for the first-order reaction. Further development of the modeling by including the critical temperature is proposed. Overall, it is shown, in particular, that the application of Lie group analysis allows one to extend the previous analytic results for the first order reactions to *n*th order ones.

1. Introduction

The formulation of fundamental natural laws and technological problems in the form of rigorous mathematical models is frequently expressed in terms of nonlinear ordinary and partial differential equations. An appropriate method for tackling nonlinear equations is provided by Lie group analysis. Lie group analysis suggests a rigorous mathematical formulation of intuitive ideas of symmetry and provides constructive methods for solving nonlinear differential equations analytically. Familiarity with group analysis is important for constructing and investigating nonlinear mathematical models of natural and engineering problems. Differential equations, conservation laws, solutions to boundary value problems, and so forth can be derived from the group invariance principle. Some advantage of applications of Lie group analysis to modeling of spherically pulsating patterns in stratified fluid were investigated in our recent studies in Ref. [8] and modeling of mixing parameterization due to multiphase fluid–structure interaction has also been studied by using Lie group analysis in our earlier work in Ref. [7].

The emphasis in this paper will be on an application of Lie group analysis to the mathematical modeling of an exothermally reacting medium with approximations to the body's temperature distribution similar to those made by Thomas [17] and Squire [15]. As it has been proposed in Thomas [17], the absolute temperature $T(x,t)$ and the mass consumption $w(x,t)$ of reactant per unit volume per second for the symmetrical heating are related by the following system of partial differential equations:

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$$k\left(\frac{\partial^2 T}{\partial x^2}+\frac{j}{x}\frac{\partial T}{\partial x}\right)=\rho c\frac{\partial T}{\partial t}+Q\frac{\partial w}{\partial t}, \tag{1}$$

$$\frac{\partial w}{\partial t}=-\gamma w^n e^{-E/(RT)}, \tag{2}$$

where $j = 0, 1$ and 2 for a slab, cylinder and sphere, respectively, k is the thermal conductivity of the reacting material, ρ is the density, c is the specific heat, Q is the heat of reaction per unit mass of substance, γ is the frequency factor, n is the order of reaction, E is the activation energy and R is the universal gas constant (see [17] for the nomenclature). In our modeling, all the material properties are taken as constants, i.e., k, ρ, c, Q, γ, n, E and R in (1) and (2) are taken as constant values.

Following Adler and Enig [1], the initial condition for $T(x,0)$ is taken conventionally as the state when the temperature within the material is uniform and equal to that of the environment T_{in}, whereas the initial condition for the concentration $w(x,0)$ is defined as the initial concentration w_{in}. Thus, we set the initial and boundary conditions for system (1) and (2) as

$$T(x,0)=T_{\text{in}},\quad w(x,0)=w_{\text{in}},\quad \frac{\partial T(0,t)}{\partial x}=0, \tag{3}$$

where T_{in} and w_{in} are given values from experimental data and $x = 0$ is the mid-plane for a slab and the center point for a cylinder or sphere.

Thermal explosion theory is concerned with the self-heating or self-cooling phenomena which can be a result of chemical decomposition. When the reaction is exothermic, self-heating takes place, and when the reaction is endothermic, self-cooling takes place. The material in which the decomposition takes place may be a solid of given configuration or a gas contained within a vessel. The thermal properties, surface, and surroundings of a body determine its rate of heat loss. Under certain conditions the central temperature may rise to a maximum and subsequently fall below this value. If the rate of environmental cooling is insufficient to offset the rate of internal heat generation, the temperature continues to rise leading to ignition or explosion.

The exothermic reaction has been studied extensively because of the interest in the behavior of high explosives. Semenov [13] introduced the theory of thermal explosion which describes thermal ignition in a uniform temperature system. Assuming uniform temperature distribution in the solid, Semenov estimated the maximum temperature above which a steady-state solution cannot exist. Frank-Kamenetskii [2] recognized the importance of the existence of more than one solution to the Semonov problem with regarding the stability of the solution. He discussed the stability criterion as applied to the heterogeneous exothermic reactions and considered its application to the determination of the critical conditions of ignition and extinction. The theory of thermal explosion with reactant consumption has been considered by Thomas [17].

Critical properties of Semenov's model have been reanalyzed in terms of independent parameters, nondimensional activation energy, and surface heat loss in Lermant and Yip [10]. Furthermore, the analysis in [10] has been extended to the distributed temperature problem by the introduction of a correlation factor which efficiently establishes a link between the Semonov model and the Frank–Kamenetskii parameter. The results in [10] have been obtained only for the slab, so extensions to the cylinder and the sphere were left as an open issue in [10].

All previous analytical models in solving (1) and (2) were solved only for the particular case $j = 0$ [17] or the linear approximation of the exponential part in the right hand side of Eq. (2), which corresponds to a very restricted model in which $T - T_{\text{in}}$ is much less than T_{in} (the discussion of this restriction can also be found in Storey [16] and Adler and Enig [1]).

We aim to investigate the nonlinear initial boundary value problem (1)–(3) with $j = 0, 1$ and 2 from a group analysis point of view. As will be shown in the sequel of this work, group theoretical modeling provides a regular method for obtaining numerous integrable approximations to the model (1)–(3).

2. Preliminaries

This section provides a concise introduction to the calculus of Lie group analysis which represents a simplified version of the overview of basic concepts of Lie symmetry groups outlined in Ibragimov and Ibragimov [6].

Let $x = (x^1, \ldots, x^n)$ and $u = (u^1, \ldots, u^m)$ be independent and dependent variables, respectively. We will deal with one-parameter groups G of transformations of the form

$$\begin{aligned}&\bar{x}^i=\varphi^i(x,a),\quad \varphi^i|_{a=0}=x^i,\\ &\bar{u}^\alpha=\psi^\alpha(x,u,a),\quad \psi^\alpha|_{a=0}=u^\alpha,\end{aligned} \tag{4}$$

depending on a continuous parameter a. The infinitesimal transformations of the group G are written

$$\bar{x}^i\approx x^i+a\xi^i(x),\quad \bar{u}^\alpha\approx u^\alpha+a\eta^\alpha(x,u).$$

The generator (which is also sometimes called "symmetry") of the group G is the linear first-order differential operator

$$X=\xi^i(x)\frac{\partial}{\partial x^i}+\eta^\alpha(x,u)\frac{\partial}{\partial u^\alpha}. \tag{5}$$

We employ the usual convention on summation over repeated indices.

Let us consider a (linear or nonlinear) system of partial differential equations

$$F_\alpha(x, u, u_{(1)}, \ldots, u_{(s)}) = 0, \quad \alpha = 1, \ldots, m, \tag{6}$$

where $u_{(1)}, \ldots, u_{(s)}$ denote the sets of partial derivatives of the respective orders, e.g. $u_{(1)} = \{u_i^\alpha\}, u_{(2)} = \left\{u_{ij}^\alpha\right\}$ with

$$u_i^\alpha = \frac{\partial u^\alpha(x)}{\partial x^i}, \quad u_{ij}^\alpha = \frac{\partial^2 u^\alpha(x)}{\partial x^i \partial x^i}.$$

The group G is called a *symmetry group* (or admitted group) for Eq. (6) if the system (6) has the same form when it is rewritten in the new variables $\bar{x}, \ \bar{u}$:

$$F_\alpha(\bar{x}, \bar{u}, \bar{u}_{(1)}, \ldots, \bar{u}_{(s)}) = 0, \quad \alpha = 1, \ldots, m.$$

The generator of the symmetry group G is called an *admitted operator* or an *infinitesimal symmetry* for Eq. (6). The effective way of constructing the symmetry group for Eq. (6) is to solve the *determining equations*

$$X_{(s)} F_\alpha(x, u, u_{(1),\ldots,u_{(s)}})|_{(6)} = 0, \quad \alpha = 1, \ldots, m,$$

for the generator (5) of the symmetry group G, where $X_{(s)}$ is the sth prolongation for the generator X of the group G, and the notation $|_{(6)}$ means evaluated on the frame.

The admitted group G maps any solution of the system (6) into a solution of the same system. A solution that is mapped by G onto itself is known as an *invariant solution* with respect to the group G. The invariant solutions for a group with a generator X are obtained as follows. One calculates the *invariants* $J(x,u)$ of the group G by solving the first-order linear partial differential equation

$$X(J) \equiv \xi^i(x) \frac{\partial J}{\partial x^i} + \eta^\alpha(x, u) \frac{\partial J}{\partial u^\alpha} = 0,$$

or its characteristic system

$$\frac{dx^1}{\xi^1(x)} = \cdots = \frac{dx^n}{\xi^n(x)} = \frac{du^1}{\eta^1(x, u)} = \cdots = \frac{du^m}{\eta^m(x, u)}. \tag{7}$$

It is manifest from Eq. (7) that the group has $n + m - 1$ functionally independent invariants of the following form:

$$\lambda_1(x), \ldots, \lambda_{n-1}(x), \quad \Phi_1(x, u), \ldots, \Phi_m(x, u). \tag{8}$$

Then we let

$$\Phi_\alpha = \phi_\alpha(\lambda_1, \ldots, \lambda_{n-1}), \tag{9}$$

solve these equations for $u^1, \ldots, u^m$, substitute the resulting expressions for u into Eq. (6) and obtain a system of partial differential equations for the unknown functions $\phi_\alpha(\lambda_1, \ldots, \lambda_{n-1})$ depending on $n - 1$ variables.

If we will require the invariance with respect to a symmetry group with $n - 1$ linearly independent generators, then we will have only one invariant of the form $\lambda(x)$, and the system (6) will be reduced to ordinary differential equations for unknown functions $\phi_\alpha(\lambda)$.

3. Group analysis of thermal explosion

For the purposes of our work, we re-scale the model Eqs. (1) and (2) using the new variables

$$\hat{t} = \frac{k}{\rho c} t, \quad \hat{w} = \frac{Q}{\rho c} w.$$

After dropping the hat symbol, the re-scaled model (1) and (2) is equivalent to the system where all nonessential parameters equal one, and we further consider a more general system

$$T_{xx} + \frac{j}{x} T_x = T_t + w_t, \tag{10}$$

$$w_t = h(w, T), \tag{11}$$

where h is allowed to be an arbitrary function of w and T.

Note that system (10) and (11) admits the following particular solution:

$$(T, w) = \begin{cases} (T(x) = c_1 + c_2/(1-j)x^{1-j}, 0) & \text{for } j \neq 1, n \geqslant 0 \\ (T(x) = c_1 + c_2 \ln x, 0) & \text{for } j = 1, n \geqslant 0 \end{cases}. \tag{12}$$

The reckoning shows that all possible generators of the group are given by the following functionally independent operators

$$Y_1 = \frac{\partial}{\partial t}, \quad Y_2 = \frac{\partial}{\partial T}, \quad Y_3 = \frac{\partial}{\partial w}, \quad Y_4 = T\frac{\partial}{\partial T} + w\frac{\partial}{\partial w} + h\frac{\partial}{\partial h}, \tag{13}$$

$$Y_5 = 2t\frac{\partial}{\partial t} + x\frac{\partial}{\partial x} - 2h\frac{\partial}{\partial h}. \tag{14}$$

We note that the operators (13) are admitted by the equation

$$h\frac{\partial^2 h}{\partial w \partial T} - \frac{\partial h}{\partial w}\frac{\partial h}{\partial \partial T} = 0 \tag{15}$$

and, thus, they span the equivalence algebra for the system

$$T_{xx} + \frac{j}{x}T_x = T_t + w_t, \quad w_t = \phi(w)\psi(T) \tag{16}$$

for arbitrary functions ϕ and ψ.

Let us take, e.g., the following linear combination of the equivalence generators (13):

$$Y = \alpha Y_2 + Y_4 + Y_5 = 2t\frac{\partial}{\partial t} + x\frac{\partial}{\partial x} + (\alpha + T)\frac{\partial}{\partial T} + w\frac{\partial}{\partial w} - h\frac{\partial}{\partial h} \tag{17}$$

with arbitrary constant α. We take the projection Z of the operator Y to the space T, w, h as follows:

$$Z = (\alpha + T)\frac{\partial}{\partial T} + w\frac{\partial}{\partial w} - h\frac{\partial}{\partial h}, \tag{18}$$

and find its invariant equation

$$h = \varphi(T, w) \tag{19}$$

by solving the equation

$$Z[h - \varphi(T, w)]_{h=\varphi} = 0, \tag{20}$$

i.e.,

$$(\alpha + T)\frac{\partial \varphi}{\partial T} + w\frac{\partial \varphi}{\partial w} = -\varphi. \tag{21}$$

Integrating the latter linear first-order partial differential equation (21), we obtain

$$h = \frac{1}{w}F\left(\frac{w}{T + \alpha}\right). \tag{22}$$

Thus, we have the system (10) and (11) of the form

$$T_{xx} + \frac{j}{x}T_x = T_t + w_t, \tag{23}$$

$$w_t = \frac{1}{w}F\left(\frac{w}{T + \alpha}\right) \tag{24}$$

with an arbitrary function F of one variable. According to the theorem on projections (see Ibragimov and Ibragimov [6]), the system (23) and (24) has the following two symmetries:

$$X_1 = \frac{\partial}{\partial t}, \quad X_2 = 2t\frac{\partial}{\partial t} + x\frac{\partial}{\partial x} + (\alpha + T)\frac{\partial}{\partial T} + w\frac{\partial}{\partial w}. \tag{25}$$

These symmetries can be used for obtaining group-invariant solutions. Moreover, using the arbitrariness of F, we can approximate the original system (10) and (11) by Eqs. (23) and (24).

Denoting

$$\sigma = \frac{w}{T + \alpha} \tag{26}$$

and letting, e.g. $F(\sigma) = \sigma^2$, we write the system (23) and (24) as

$$T_{xx} + \frac{j}{x}T_x = T_t + w_t, \tag{27}$$

$$w_t = \frac{w}{(T + \alpha)^2}. \tag{28}$$

This is a good approximation to the system (10) and (11) for the first-order reaction ($n = 1$) and arbitrary j provided that

$$wF_2(\alpha) = w/(T+\alpha)^2 \approx -\gamma w \exp\left(-\frac{1}{T}\right) = wF_1(\gamma),$$

where we denote

$$F_1(\gamma) = -\gamma \exp\left(-\frac{1}{T}\right), \quad F_2(\alpha) = 1/(T+\alpha)^2.$$

Fig. 1 compares the approximations of the right hand side $wF_1(\gamma)$ of the nondimensionalized equation (2) to $wF_2(\alpha)$ for different values of α and the frequency factor γ versus the absolute temperature T. We observe from Fig. 1 that $\lim F_{1\gamma\to 0} = \lim F_{2\alpha\to\infty}$ for larger values of T.

Using, e.g. X_2, we obtain the *invariant solution* of (27) and (28) of the form

$$w = xf(\lambda), \quad T+\alpha = xg(\lambda), \quad \lambda = \frac{x^2}{t}. \tag{29}$$

Direct differentiation can be used to check that substitution of (29) into (27) and (28) leads to the following integro-differential equation for $g(\lambda)$:

$$[4\lambda g'' + (\lambda^2 + 6\lambda + 2j\lambda)g' + jg]g^2 = Ke^{-\int(\lambda^2 g^2(\lambda))^{-1}d\lambda}, \quad K = \text{const}. \tag{30}$$

Alternatively, $f(\lambda)$ in (29) can be expressed in terms of $g(\lambda)$ as

$$f(\lambda) = Ke^{-\int(\lambda^2 g^2(\lambda))^{-1}d\lambda}, \tag{31}$$

which allows one to reduce the nonlinear integro-differential equation (30) to the following coupled system of ordinary differential equations:

$$[4\lambda g'' + (\lambda^2 + 6\lambda + 2j\lambda)g' + jg]g^2 = -\lambda^2 f', \tag{32}$$

$$\lambda^2 f' = -\frac{f}{g^2}. \tag{33}$$

Because of the singularity of the model at $x = t = 0$, the reduction of the boundary and initial conditions (3) was based on the following simplifying assumptions and approximations:

(i) The computational domain was restricted to the set $\Omega = \{(x,t) : \delta \leqslant x \leqslant L, \varepsilon \leqslant t \leqslant T_*\}$, in which all the constants δ, ε, L and T_* are taken to be positive.

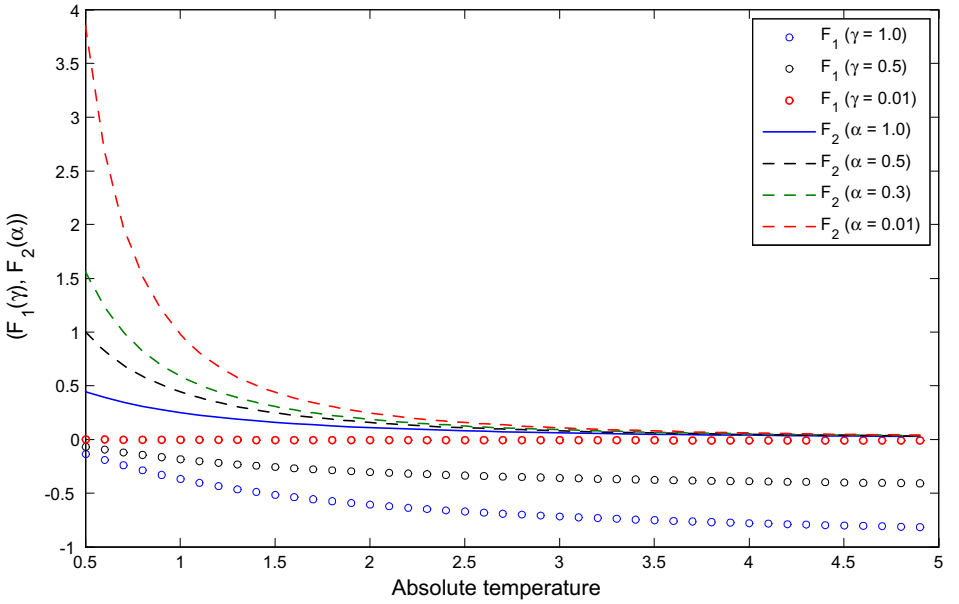

Fig. 1. Approximation of the right-hand side $wF_1(\gamma)$ by $wF_2(\alpha)$ for different values of parameters α and γ.

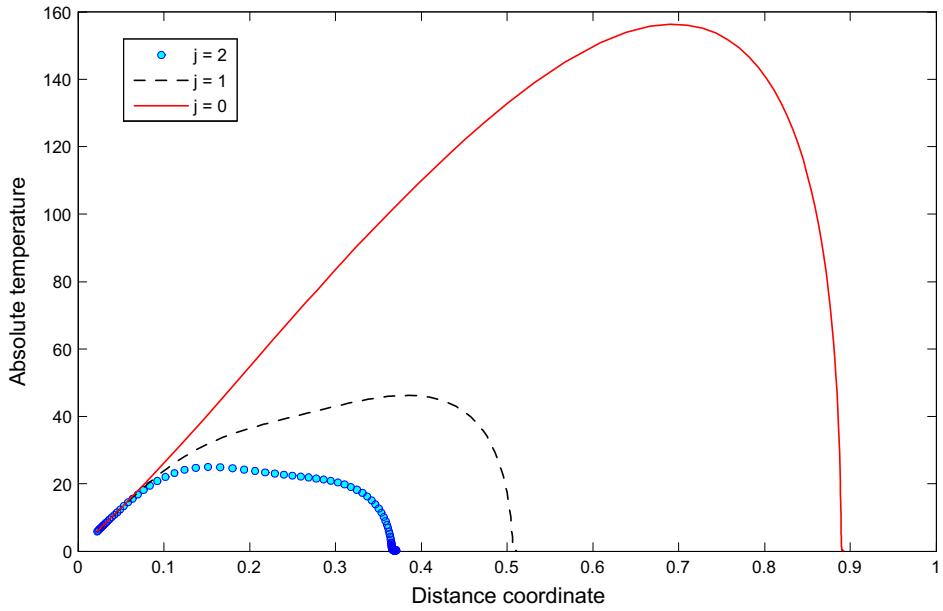

Fig. 2. Absolute temperature distribution.

(ii) The initial and boundary values for $T(x,0)$, $w(x,0)$ and $\partial T(0,t)/\partial x$ were approximated by means of the representative value x^* and t^*, such that $T(x,0) \approx T(t^*,\varepsilon) = T_B$, $w(x,0) \approx w(x^*,\varepsilon)$, and $\partial T(0,t)/\partial x \approx \partial T(\delta,t^*)/\partial x$.
(iii) Further approximations were made by $t^* = x^* = \varepsilon = \delta$.

The latter assumptions allow one to reduce the boundary and initial conditions (3) for (T,w) to the boundary conditions for the model (32) and (33) as

$$g(\delta) = \frac{T_{\text{in}}}{\delta}, \quad f(\delta) = \frac{w_{\text{in}}}{\delta}, \quad g'(\delta) = -\frac{T_{\text{in}} + \alpha}{2\delta^2}. \tag{34}$$

The latter boundary-value problem (32)–(34) has been solved numerically by using the odeint routine provided in Press et al. [12], which is based on the Runge–Kutta method with an adaptive stepsize control. The simulations were carried out using the values of parameters $\delta = 0.01$, $T_{\text{in}} = 2.465$, $\alpha = 0.3$, $w_{\text{in}} = 0.005$, $n = 1$ and $L = 1$. As a particular example, Fig. 2 is used to compare the results of numerical simulations for the absolute temperature T as a function of the distance x for $j = 0, 1$ and 2 in the original variables (x,t). The quantitative analysis presented in Fig. 2 are found to agree with the results shown in Fig. 1 in Adler and Enig in [1], where the authors were comparing the integral curves corresponding to the critical conditions for the first-order reaction. The effect of reactant consumption in non-steady explosion theory was investigated in Ref. [1] by a numerical method and an approximate analytical treatment whereas our results were presented by means of exact reduction of the analytical model and approximate boundary conditions. However, the critical conditions for the consumption $w(x,t)$ were not obtained as accurately as in an alternative analysis in Thomas [17]. As follows from our recent analysis, the latter inconsistency is caused most likely by the approximations (ii) and (iii).

The further development of the model is the topic of the current studies. The details on possible approach to the further developments and improvements are discussed in the next section. The forthcoming results will be published elsewhere.

4. Discussion

The further improvement and development of the model consists of the following two-step procedure. First, we are interested in constructing other projections of the operator Y to the space T, w and h in order to investigate other possible invariant solutions. In the frame of the present studies, the reduction of the model has been based on the choice of Z given by (18) which did not provide direct invariant solutions although it was effective in reducing the system of partial differential equations to ordinary differential equations. Our next goal is to improve the mathematical modeling by finding a such projection which will provide with the exact solution of the model directly, i.e. without a reduction. This rules out the hope to improve the results for the critical conditions for the consumption $w(x,t)$.

Our next development will consist of imposing the additional boundary condition

$$T(L,t) = T_B, \tag{35}$$

where $x = L$ is the boundary for a slab. We will also set $x = R$ for a cylinder and sphere of radius R.

In terms of simplifying assumptions (i)–(iii), the boundary condition (35) is reduced to the additional condition for the function $g(\lambda)$:

$$g(L) = \frac{T_{\text{in}} - \alpha}{L}. \tag{36}$$

As seen from (3), the problem with the imposed condition (35) is complicated significantly by the presence of a singularity in the boundary and initial conditions for T since $T(x,0)|_{x=L} \neq T(L,t)|_{t=0}$. The latter singularity arises from the following physical reason: The initial temperature is the ambient temperature assigned for the entire region. Behavior of the explosion depends on the critical temperature that is assigned at the boundary. If the boundary temperature is below the critical temperature, the temperature T will increase nonlinearly according to the exponential term until it reaches the critical temperature $T = T_*$. When T reaches (slightly below) the critical point, energy will dissipate because of the higher heat loss than generated heat. If the boundary temperature is above the critical temperature, $T(x,t) > T_*$ for $x = 0,L$, internal heat will be generated until instability will occur because the energy will be internally generated much faster than the heat lost on the boundary. Then the temperature will increase until the material is fully consumed or it reaches (a very steep temperature gradient which will be sufficient to dissipate the generated heat to reach a fictitious steady state, without depletion) the temperature assigned on the boundary.

A better understanding of a material response in terms of generalized boundary conditions could be useful in predicting the performance of materials in real use scenarios, i.e., manned space station. Material flammability, unfortunately, is not a material property, and this has led to many test methods which attempt to quantify the propensity of a material to ignite under a specified set of conditions. Generally, results are used to rank-order different materials according to results of these specific tests. A number of ASTMs and other standard methods have been proposed and utilized to make measurements of flash point, auto-ignition temperature, flammability limits, oxygen consumption index, smoke point, etc. A few attempts have been made to define ignition or flammability of gases in terms of fundamental properties. Among these are the work of Sheldon [14], who proposed a minimum heat release per unit volume of combustibles and Melhem [11], who proposed the criteria of a minimum adiabatic reaction temperature, both for gas phase reactions. However, many flammable materials naturally exist in a condensed phase: either liquid or solid. This state confounds the material response by introducing other factors such as heat diffusion, latent heat, mixing with oxidizer gas, etc. Recent literature documents attempts for predicting solid materials flammability [11,9,5], and still other literature has focused on testing procedures (see e.g., Gilman et al. [3]), the effect of gravity on material flammability and threshold oxygen concentration [4].

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