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IGNITION FOR A GASEOUS THERMAL REACTION

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1. The ignition model for a reactive gas. The ignition period of a thermal event for a perfect compressible reactive gas as derived by D. Kassoy and J. Poland [3] can be described by the following model

(1) $\theta_t - \Delta\theta = \delta e^{\theta} + \frac{\gamma - 1}{\gamma} \frac{1}{\text{vol } \Omega} \int_{\Omega} \theta_t(y,t)dy$

(2) $\theta(x,0) = \theta_o(x) \quad , x \in \Omega \; ; \quad \theta(x,t) = 0 \quad , x \in \partial\Omega \; , \; t > 0$

where $\Omega \subset \mathbb{R}^n$ is a bounded open container, $\theta(x,t)$ is the temperature perturbation of the gas, δ is the Frank-Kamenetski parameter, $\gamma \geq 1$ is the gas constant, and $\theta_o(x)$ is the initial temperature perturbation.

For a reactive gas in a bounded container, the associated thermal event can be violent or mild. In the former case when explosion occurs, the event is supercritical or explosive. In the latter case when there is no dramatic event, the reactive event is subcritical. The questions we wish to answer are the following. 1) Can we describe the time-history of $\theta(x,t)$? 2) Can we distinguish between explosive and nonexplosive events as the parameters δ and γ vary ?

2. Results for a solid fuel. For a solid fuel in a bounded container, the above questions were answered in [1]. Formally when $\gamma = 1$ IBVP (1)-(2) reduces to the classical ignition model for a solid fuel.

(3) $\theta_t - \Delta\theta = \delta e^{\theta}$

(2) $\theta(x,0) = 0 \quad , \quad x \in \Omega, \quad \theta(x,t) = 0 \quad , x \in \partial\Omega \quad , t > 0$

The associated steady state problem is:

(4) $-\Delta\phi = \delta e^{\phi} \qquad , x \in \Omega$

(5) $\phi(x) = 0 \qquad\quad , x \in \partial\Omega$

We now summarize the results for IBVP (3)-(2) and BVP (4)-(5).

A] Given any bounded domain $\Omega \subset \mathbb{R}^n$, there exists $\delta_{FK} > 0$ such that:

a) for $0 < \delta < \delta_{FK}$, BVP (4)-(5) has at least one positive solution, and
b) for $\delta > \delta_{FK}$, no solution exists. The classical definition of criticality is based on this number δ_{FK} . Another question arises. What does δ_{FK} have to do with IBVP (3)-(2) ? B] For any $\delta > 0$, IBVP (3)-(2) has a unique solution $\theta(x,t)$ on $\bar{\Omega} \times [0,t^*)$, $t^* > 1/\delta$, with $0 \leq \theta(x,t) \leq \ln(1-\delta t)^{-1}$,

$(x,t) \in \bar{\Omega} \times [0, 1/\delta)$. C] For any $\delta \in (0, \delta_{FK}]$, IBVP (3)-(2) has a unique solution $\theta(x,t)$ on $\bar{\Omega} \times [0,\infty)$ with $0 \le \theta(x,t) \le \psi(x)$ where ψ is the minimal solution of BVP (4)-(5). D] For $\delta > \delta_{FK}$, IBVP (3)-(2) has a unique solution $\theta(x,t)$ on $\bar{\Omega} \times [0,t^*)$, $1/\delta \le t \le \infty$, with $\sup_{x \in \bar{\Omega}} \theta(x,t) \to \infty$ as $t \to t^*_-$. Thus for $\delta > \delta_{FK}$ the temperature θ becomes unbounded as $t \to t^*_-$ and thermal runaway occurs at t^*. Can we determine t^*? E] Let θ be the solution of IBVP (3)-(2) on $\Omega \times [0,T)$. Let $\xi(t)$ satisfy

(6) $\xi' = \delta e^{\xi} - \lambda_1 \xi$, $\xi(0) = 0$ on $[0,T)$ where λ_1 is the first eigenvalue of:

(7) $-\Delta\phi = \lambda\phi$, $x \in \Omega$

(8) $\phi(x) = 0$, $x \in \partial\Omega$

Then $\sup_{x \in \bar{\Omega}} \theta(x,t) \ge \xi(t)$ on $[0,T)$. F] The solution $\xi(t)$ of IVP(6) exists on $[0,T)$ for any $\delta > 0$ where

(9) $$T = \int_0^{\infty} \frac{dz}{\delta e^{z} - \lambda_1 z},$$

$T < \infty$ if and only if $\delta > \lambda_1/e \equiv \delta^*$, and $\lim_{t \to T^-} \xi(t) = +\infty$ if $\delta > \delta^*$.

G] Let $\delta > \delta^*$. Then the solution $\theta(x,t)$ of IBVP (3)-(2) exists on $\Omega \times [0,t^*)$ with

(10) $$1/\delta \le t^* \le T \equiv \int_0^{\infty} \frac{dz}{\delta e^{z} - \lambda_1 z} < \infty$$

and $\lim_{t \to t^{*-}} [\sup \theta(x,t)] = +\infty$. Thus, for $\delta > \delta^* \equiv \frac{\lambda_1}{e} > \delta_{FK}$, the thermal event for a solid fuel is explosive since $\theta(x,t)$ becomes unbounded at t^* and t^* can be estimated by the inequality (10).

3. **Results for a reactive gas.** The implicit integro-partial differential equation (1) is certainly more complicated than the ignition model (3) for a solid fuel. This complication is due to the gas motion caused by the phenomena of thermal expansion which leads to the integral term involving the time deviative of the temperature perturbation. The results of this section are joint with A. Bressan and will appear in detail in [2]. The first step in dealing with IBVP (1)-(2) is to put the problem in a more tractable equivalent form.

Theorem 1. IBVP (1)-(2) is equivalent to IBVP (11)-(2) and to IBVP (12)-(2) where

(11) $$\theta_t - \Delta\theta = \delta e^{\theta} + \frac{\gamma-1}{\text{vol}\,\Omega} \int_{\Omega} [\Delta\theta + \delta e^{\theta}]\, dy$$

and

(12) $$\theta_t - [\Delta\theta + \frac{\gamma-1}{\text{vol}\,\Omega} \int_{\partial\Omega} \frac{\partial\theta}{\partial\nu}\, d\sigma] = \delta e^{\theta} + \frac{\gamma-1}{\text{vol}\,\Omega}\, \delta \int_{\Omega} e^{\theta}\, dy$$

where ν is the exterior normal to $\partial\Omega$ and $d\sigma$ is the element of surface area on $\partial\Omega$. The equivalent forms follow by integrating (1) over Ω to get (11). (12) follows by the divergence theorem. The next two theorems are obtained using semigroup theory and invariance results for an abstract perturbation of a linear problem associated with the linear part of (12).

Theorem 2. For any $\delta > 0$, $\gamma \geq 1$, and any $\theta_0 \in L^2(\Omega)$, $\sup_{x\in\Omega} \theta_0(x) < \infty$, IBVP (1)-(2) has a unique solution $\theta(x,t)$ on $\Omega \times [0,\sigma)$, $\sigma > 0$, where either $\sigma < +\infty$ and $\lim_{t\to\sigma^-}[\sup \theta(x,t)] = +\infty$.

Let $\Omega = B \equiv \{x: \| x \| < 1\} \subset \mathbb{R}^n$ and set $\theta_0(x) \equiv 0$.

Theorem 3. For $\delta > 0$, $\gamma \geq 1$, the solution $\theta(x,t)$ of IBVP (1)-(2) is nonnegative, radially symmetric, and nondecreasing on $[0,\sigma)$.

As for a solid fuel, we can mathematically distinguish between explosive and nonexplosive events by considering the following comparison equations:

(13) $\varphi_t - \Delta\varphi = \delta e^{\varphi} + \frac{\gamma-1}{\text{vol}\,\Omega}\,\delta\int_\Omega e^{\varphi}dy$

(3) $\chi_t - \Delta\chi = \delta e^{\chi}$

(4) $-\Delta\chi = \delta e^{\chi}$

Theorem 4. For $\delta > 0$, $\gamma \geq 1$, the solution $\theta(x,t)$ of IBVP (1)-(2) satisfies $\chi(x,t) \leq \theta(x,t) \leq \varphi(x,t)$ for all $x\in\Omega$ and all $t \geq 0$ on their common interval of existence where χ is the solution of IBVP (3)-(2) and φ is the solution of IBVP (13)-(2).

Since for $B \subset \mathbb{R}^n$, $\delta > \delta^* = \lambda_1/e > \delta_{FK}$, the solution χ of IBVP (3)-(2) blows up in finite time t^*, we have that $\sigma < t^*$ for $\delta > \delta^*$ and $\theta(x,t)$ blows up as $t \to \sigma_-$. Physically, this means that the temperature for an ideal gas is always greater than that for a solid in identical bounded containers and hence a gas explodes sooner than a solid fuel. Finally, we have

Theorem 5. If χ is any solution of BVP (4)-(5) then $\theta(x,t) \leq \chi(x)$ on $\Omega \times [0,\infty)$ where θ is the solution of IBVP (1)-(2).

References

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