Numerical Analysis of a Combustion Model for Layered Media Via Mathematical Homogenization

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***Abstract*—We propose to investigate a mathematical model for combustion in a rod made of periodically alternating thin layers of two combustible materials such as those occurring in gun propellants. We apply the homogenization theory to resolve the fast oscillations of the model's coefficients across adjacent layers, and set up numerical simulations to better understand the reactions occurring in such media.**

I. Motivation

This project is motivated by Army and Navy research interest in the improvement of gun performance through the integration of layered propellants composed of new energetic materials. We study a mathematical model of combustion within an inhomogeneous rod made of thin, periodically alternating layers of two combustible materials. Direct numerical simulations through the usual finite difference/element methods face challenges due to the highly oscillatory nature of the material properties within adjacent layers. To address this issue, we turn to the mathematical theory of homogenization [3, 6] to resolve the high oscillations within the mathematical model before passing the result to computational algorithms. We conduct numerical simulations based on the mathematically homogenized model of layered combustible media in order to better understand the nature of the reaction occurring in such media.

II. Modeling Combustion in a Periodically Layered Rod

Our research focuses on modeling combustion in a periodically stratified rod consisting of two alternating combustible materials, repeating with a small period ε that make up the layers, as shown in Figure 1.

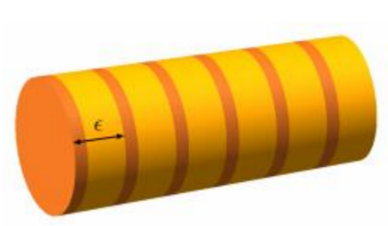


Fig. 1. Schematic of a layered rod.

The thicknesses of the layers are small compared to the length of the rod, and the two materials that make up the layers, denoted as species **A** and **B**, satisfy the following assumptions [3, 7]:

- The two species are self-contained combustibles that can ignite independently and there is no chemical reaction between them.
- There is no mass diffusion and the only mechanism that propagates the combustion is the heat conduction.

The combustion process is initiated by boundary heat addition at the left end of the rod. We study a one-dimensional model of the process, described by a system of differential equations in the following unknowns:

- $A(x,t)$: mass fraction of unreacted material **A** at location x along the rod at time t;
- $B(x,t)$: mass fraction of unreacted material **B** at location x along the rod at time t;
- $T(x,t)$: temperature at location x along the rod at time t.

We assume that the ignition temperature of the material **A** is T_A and that once it ignites, it begins releasing heat at a temperature-dependent rate $r_A(T)$, and we denote by q_A the energy content per unit mass of **A**, that is, the amount of heat released when a unit mass of A is burned completely. Similarly, we define T_B, $r_B(T)$, and q_B for material **B**. Furthermore, we denote by $\sigma_\varepsilon(x)$ the specific heat per unit volume and by $\kappa_\epsilon(x)$ the heat conduction coefficient at location x along the rod and note that these are ε-periodic functions. We assume that the outer surface of the rod is insulated, so any heat generated by combustion within the rod diffuses in the axial direction. The following system of differential equations describes the combustion process, assuming a single-step chemical reaction [3, 7]:

$$\frac{\partial A}{\partial t} = -r_A(T)A, \tag{1a}$$

$$\frac{\partial B}{\partial t} = -r_B(T)B, \tag{1b}$$

$$\sigma_\epsilon \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(\kappa_\epsilon \frac{\partial T}{\partial x}\right) - \chi_\epsilon q_A \frac{\partial A}{\partial t} - (1-\chi_\epsilon) q_B \frac{\partial B}{\partial t}, \tag{1c}$$

with $0 < x < L, t > 0$, and where L is the length of the rod and $\chi_\epsilon(x)$ is the characteristic function of the union of the intervals occupied by the material **A**. At time $t = 0$, none of the material has reacted and the temperature of the rod is known, thus we have the *initial conditions*:

$$\begin{aligned} A(x,0) &= \chi_\epsilon(x), \qquad 0 \le x \le L, \\ B(x,0) &= 1-\chi_\epsilon(x), \qquad 0 \le x \le L, \\ T(x,0) &= T_{in}(x), \qquad 0 < x < L, \end{aligned} \tag{2}$$

and, assuming the right end is insulated, the *boundary conditions*:

$$\frac{\partial T}{\partial x}(0,t) = f(t), \quad \frac{\partial T}{\partial x}(L,t) = 0, \qquad t > 0. \tag{3}$$

The main difficulty in obtaining an accurate numerical solution of the initial boundary value problem (1)–(3) is due to the highly oscillatory nature of the coefficients σ_ϵ and κ_ϵ which make a solution through classical numerical methods impractical. We turn to the mathematical theory of homogenization [4, 8] to replace the rapidly oscillating coefficients by theoretically derived averages, resulting in "homogenized" equations that we then solve using the finite difference method.

A. Homogenization of the combustion system

The combustible material under consideration consists of alternating layers of self-contained chemicals **A** and **B** which repeat periodically with a period ε. Each ε-layer consists of a sublayer of **A** of thickness $\delta\varepsilon$ and a sublayer **B** of thickness $(1-\delta)\varepsilon$, $0 < \delta < 1$. Let σ, κ, and χ be 1-periodic functions such that $\sigma_\varepsilon(x) = \sigma(x/\varepsilon)$, $\kappa_\varepsilon(x) = \kappa(x/\varepsilon)$, and $\chi_\varepsilon(x) = \chi(x/\varepsilon)$.

As is standard in homogenization theory, we consider the following expansions for the temperature T for small ε:

$$T_\varepsilon(t,x) = \sum_{k=0}^{\infty} \varepsilon^k T_k(t,x,y), \tag{4}$$

where $y = x/\varepsilon$ and T_k are 1-periodic functions in y.

Following [7], we approximate $r_A(T) \approx r_A(T_0)$ and $r_B(T) \approx r_B(T_0)$, and by substituting (4) into (1c) we obtain a sequence of equations when we collect like powers of ε. The first three equations, who are sufficient to obtain the homogenized equations, are shown here:

$$\begin{aligned} \varepsilon^{-2}: \ & \frac{\partial}{\partial y}\left(\kappa(y)\frac{\partial T_0}{\partial y}\right) = 0 \\ \varepsilon^{-1}: \ & \frac{\partial}{\partial x}\left(\kappa(y)\frac{\partial T_0}{\partial y}\right) + \frac{\partial}{\partial y}\left[\kappa(y)\left(\frac{\partial T_0}{\partial x} + \frac{\partial T_1}{\partial y}\right)\right] \\ & \qquad = 0 \\ \varepsilon^{0}: \ & \sigma(y)\frac{\partial T_0}{\partial t} = \frac{\partial}{\partial x}\left[\kappa(y)\left(\frac{\partial T_0}{\partial x} + \frac{\partial T_1}{\partial y}\right)\right] \\ & \qquad + \frac{\partial}{\partial y}\left[\kappa(y)\left(\frac{\partial T_1}{\partial x} + \frac{\partial T_2}{\partial y}\right)\right] \\ & \qquad + \chi(y) q_A r_A(T_0) A \\ & \qquad + (1-\chi(y)) q_B r_B(T_0) B. \end{aligned} \tag{5}$$

Using these equations, it can be shown that T_0 is independent of y and satisfies a heat equation with constant coefficients. We introduce the notation $\bar{T} = T_0$ and also introduce the smooth functions $\bar{A}$ and $\bar{B}$ that approximate the mass fractions A and B in the limit $\varepsilon = 0$ and note that the homogenized system is

$$\begin{aligned} \frac{\partial \bar{A}}{\partial t} &= -r_A(\bar{T})\bar{A}, \\ \frac{\partial \bar{B}}{\partial t} &= -r_B(\bar{T})\bar{B}, \\ \bar{\sigma}\frac{\partial \bar{T}}{\partial t} &= \bar{\kappa}\frac{\partial^2 \bar{T}}{\partial x^2} + \gamma_A r_A(\bar{T})\bar{A} + \gamma_B r_b(\bar{T})\bar{B}, \\ 0 < & x < L, t > 0, \end{aligned} \tag{6}$$

where $\bar{\sigma} = \int_0^1 \sigma(y)\,dy$, $\bar{\kappa} = 1/\int_0^1 1/\kappa(y)\,dy$, $\gamma_A = q_A\delta$, $\gamma_B = q_B(1-\delta)$.

We solve the system numerically with the initial conditions

$$\bar{T}(x,0) = \bar{T}_0(x), \quad \bar{A}(x,0) = 1, \quad \bar{B}(x,0) = 1, \quad 0 < x < L,$$

and the boundary conditions

$$-\bar{\kappa}\bar{T}(0,t) = F(t), \quad -\bar{\kappa}\bar{T}(L,t) = 0,$$

where $F(t)$ is the flux of heat supply that initiates the ignition. In practical applications, the heat is supplied only briefly as in $F(t) = \begin{cases} H/\tau, & 0 \le t \le \tau \\ 0, & \tau < t \end{cases}$, where $[0,\tau]$ is a small time interval and H is the total thermal energy supplied. By varying H, we obtained cases where

- Ignition does not initiate at all (insufficient heat supply);
- The ignition initiates, but dies out without propagating far into the rod (insufficient heat supply);
- The combustion completely burns one material, but leaves the other intact (moderate heat supply);
- The combustion completely burns both materials (full heat supply).

In all cases, the temperature of the rod stabilizes to a constant value since the heat flux is 0 at the right end point of the rod.

III. Numerical experiments

We used the homogenized model to conduct numerical experiments to understand how varying material properties, heat supply, and thickness of the layers affects the combustion process. We present here the results of several simulations in which we varied H to explore the relationship between the material properties and the heat supply. We take the reaction rates to be step functions

$$r_A(T) = \begin{cases} 0, & 0 \le T < T_A \\ R_A, & T \ge T_A \end{cases},$$

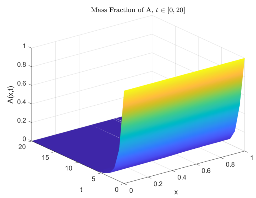
and

$$r_B(T) = \begin{cases} 0, & 0 \le T < T_B \\ R_B, & T \ge T_B \end{cases}.$$

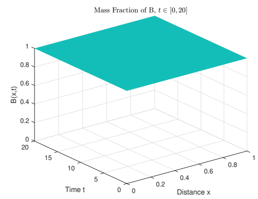
A. Example 1

To validate our expectations that if the rod does not reach the ignition temperature of material **B**, then the material **B** will not combust, we conducted the following experiment. We set $\bar{\sigma} = 1$, $\bar{\kappa} = 1$, $\gamma_A = 1.5$, $\gamma_B = 2$, the initial temperature in the rod $\bar{T}_0 = 3$, and take $T_a = 4$, $T_B = 8$, $R_A = 1$, $R_B = 2$.

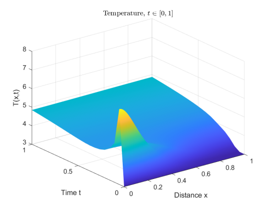
Figure 2 shows the results obtained with $H = 20$. As expected, the boundary heat addition results in a sharp temperature increase at the left side of the rod and subsequently the rod attains a uniform steady state temperature of approximately 5.5. The mass fraction of **B** remains 1 and material **A** is entirely burned.



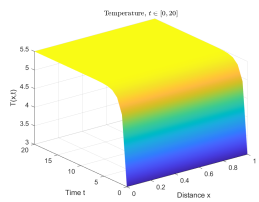
(a) Mass fraction of **A**.



(b) Mass fraction of **B**.



(c) Temperature for $0 \leq t \leq 1$.

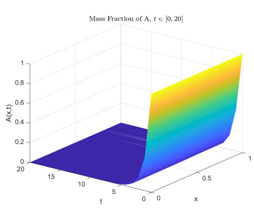


(d) Temperature for $0 \leq t \leq 20$.

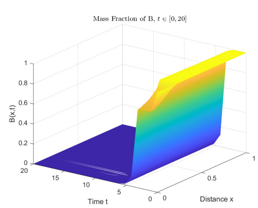
Fig. 2. Mass Fraction and Temperature for Example 1.

B. Example 2

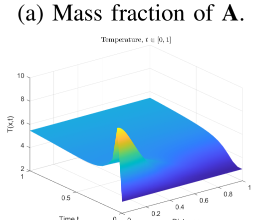
In this example we examine conditions in which **A** and **B** would both burn completely. We take $\bar{\sigma} = 1$, $\bar{\kappa} = 1$, $\gamma_A = 1.5$, $\gamma_B = 2$, $T_A = 4$, and $T_B = 6$. We took $R_A = 1$, $R_B = 2$, the initial temperature across the rod $\bar{T_0} = 3$, and $H = 30$.



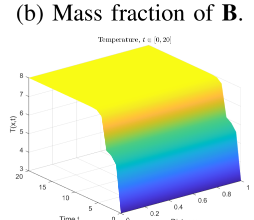
(a) Mass fraction of **A**.



(b) Mass fraction of **B**.



(c) Temperature for $0 \leq t \leq 1$.



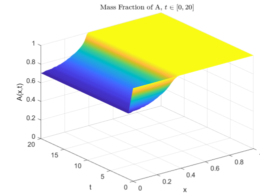
(d) Temperature for $0 \leq t \leq 20$.

Fig. 3. Mass Fraction and Temperature for Example 2.

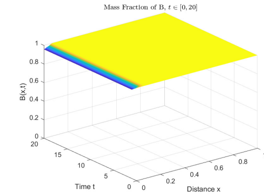
In Figure 3 we see that the temperature of the rod increases to a uniform steady state temperature of approximately 8 and **A** and **B** are both completely burned.

C. Example 3

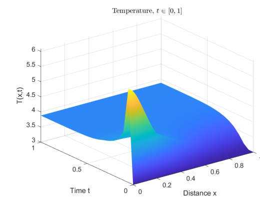
The final case we considered was one in which H is at an intermediate intensity so that both materials partially burn



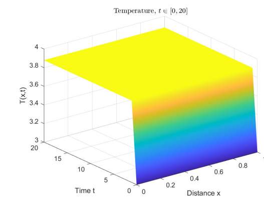
(a) Mass fraction of **A**.



(b) Mass fraction of **B**.



(c) Temperature for $0 \leq t \leq 1$.



(d) Temperature for $0 \leq t \leq 20$.

Fig. 4. Mass Fraction and Temperature for Example 3.

because the temperature of the rod falls beneath the ignition temperatures of materials **A** and **B** after combustion initiates. We take $\bar{\sigma} = 1$, $\bar{\kappa} = 1$, $\gamma_A = 1.5$, $\gamma_B = 2$, $\bar{T_0} = 3$, $T_A = 4$, $T_B = 6$, $r_A = 1$, $r_B = 2$, the initial temperature across the rod $T_0 = 3$, and $H = 15$. In Figure 4 we see that initially the temperature of the rod reaches the ignition temperatures of materials **A** and **B**, initiating combustion of both materials. Subsequently, the rod's temperature falls below the requisite ignition temperatures and the rod stops burning, ultimately attaining a uniform steady state temperature of approximately 3.88.

IV. Future Work

Future work on the topics covered in this project includes more numerical simulations of the homogenized combustion model of the periodically layered rod to more extensively determine how the various material properties, geometry, and heat source affect combustion. Another avenue would be expanding the scope of the work to three-dimensional media while assuming radial symmetry in order to keep the computational complexities manageable and at the same time realistic.

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