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Numerical method based-cellular automata for heat transfer with application to the self-ignition of energetic materials

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1 Introduction

Energetic materials have many applications in both civil and military fields. They allow, under certain conditions, to deliver a large amount of energy by reduction-oxidation reactions. However, modeling their combustion is not an easy task due to the heterogeneity of their composition. This heterogeneity is particularly strong in the case of pyrotechnic compositions because they are granular mixtures of one or more pairs of compressed oxidant / reducing agent. Each grain will then have different physical properties. This type of field is very difficult to model with conventional methods because of the discontinuity of thermal properties. Thus, having a numerical tool to predict the combustion in pyrotechnic materials is of practical interest for saving time and money (cost of making experiments).

To do so, cellular automata (CA) simulation is judged to be promising for predicting the combustion of heterogeneous pyrotechnic materials. CA are discrete mathematical models capable of performing local computations [1]. The cells have states that change iteratively over time by respecting simple and identical rules. The local behaviors over time in each cell is based on the state of the cell itself and the state of their neighborhood. CA were invented in the 1950s by John Von Neumann [2] and Stanislaw Ulam [3] during their research on self-reproducing automata. Since their invention, CA have been used in different fields[4][5]. Few works on CA are found in the literature proposing to use it to model heat transfers coupled with chemical reactions[6][7]. However, to our knowledge, there is no reports dealing with energetic materials.

Accordingly, this study presents the development of a numerical model based on CA approach which simulate the combustion in a section of axisymmetric cylinder of energetic materials using simple rules. The prediction performance of the developed model was compared with experimental and analytical results found in the literature.

2 Numerical methodology

The purpose of the CA model presented here is to simulate the thermal diffusion within an axisymmetric cylinder of pyrotechnic materials. The different steps necessary to simulate the combustion of a pyrotechnic material via CA are presented as follows.

2.1 Domain discretization and CA states

The first step of CA model is the discretization of the domain. In this study, the studied domain is a section of an axisymmetric cylinder which is discretized into 2D regular grid of $m \times n$ squares (m and n are the number of cells in the r and z directions respectively). The cells have a dimension of $e \times e$. Each cell represents a grain of one of the material compositions that make up the cylinder. The physical properties associated with each cell are therefore different and depend on the nature of the material of the cell. The four states of CA cells are material type, temperature, liquid titer (for phase changes) and product concentration (for reactions). The neighborhood used is that of Von Neumann with a neighborhood radius of 1 and is represented in Figure 1. The temperature of the cells will evolve at each time step from a transition rule based on the resolution of the heat equation. The new temperature of a cell at generation $t + \Delta t$ will depend on its temperature and those of its neighborhood at generation t . This rule is detailed in the following section.

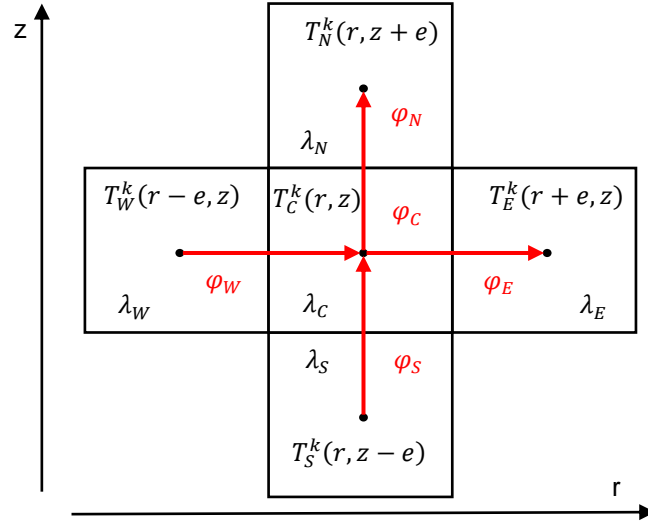


Figure 1. Representation of the discretization of the space.

2.2 Diffusion in the cellular automaton

The equation of heat transfer without source term is as follows:

$$\rho C_p \frac{\partial T}{\partial t} = \text{div}(\varphi) \quad (1)$$

Where ρ is the density of the material, C_p is the specific heat of the material and φ is the heat flux.

The next temperature iteration $T_{C_{inert}}^{k+1}$ at the center of cell C (without taking account the chemical reaction) is calculated as follows:

$$T_{C_{inert}}^{k+1} = T_C^k + \frac{\Delta t}{e \cdot \rho_C \cdot C_{pC}} (\varphi_S - \varphi_N + \varphi_W - \varphi_E) \quad (2)$$

Where k is the time iteration and $t = k \times \Delta t$.

To calculate the fluxes between the central cell C and the neighboring cells i , the surface thermal resistances are used:

$$\varphi = \frac{\Delta T}{R} \quad (3)$$

Where R is the thermal resistance.

These resistances will depend on the conductivity λ_C of the central cell C , the conductivity λ_i of the neighboring cell as well as the direction of the flux. Calculating the thermal resistance between the center of two cells a and b is equivalent to calculate resistance between the center of the cell a and the interface between the two cells, next the resistance between the interface and the center of cell b . Then to put these two resistances in series.

In the z direction, φ_N and φ_S are calculated as follows:

$$\varphi_N = \frac{T_C^k - T_N^k}{e \left(\frac{1}{\lambda_C} + \frac{1}{\lambda_N} \right)} \quad (4)$$

$$\varphi_S = \frac{T_S^k - T_C^k}{e \left(\frac{1}{\lambda_S} + \frac{1}{\lambda_C} \right)} \quad (5)$$

In the r direction, φ_W and φ_E are calculated as follows:

$$\varphi_E = \frac{T_C^k - T_E^k}{er_C \left(\frac{\log \left(\frac{r_C}{r_{E/C}} \right)}{\lambda_C} + \frac{\log \left(\frac{r_{E/C}}{r_E} \right)}{\lambda_E} \right)} \quad (6)$$

$$\varphi_W = \frac{T_W^k - T_C^k}{er_C \left(\frac{\log \left(\frac{r_W/C}{r_W} \right)}{\lambda_W} + \frac{\log \left(\frac{r_C}{r_{W/C}} \right)}{\lambda_C} \right)} \quad (7)$$

Where r_i is the coordinate of cell i along the r direction and r_{ij} is the coordinate of the interface between cell j and cell i along the r direction. Since an explicit method is used in this study, the stability of the method can only be achieved by respecting the following criteria:

$$Fo = \frac{\max(\alpha_i)\Delta t}{e^2} < \frac{1}{2} \quad (8)$$

Where $\max(\alpha_i)$ is the maximum of the diffusivity $\alpha_i = \frac{\lambda_i}{\rho_i c_{p_i}}$ among the materials and their different phases (since material properties change with phase and temperature). Fo is the Fourier number. In this study, Fo is taken equal to 0.2.

2.3 Chemical reaction model

The chemical reaction rules used in this study are presented in this section. Every cell that has at least one adjacent reacting neighbour (for example, a reductant cell has at least one air cell or oxidant cell) will start its conversion to its oxidized or reduced counterpart and generate heat. The chemical reaction speed is modeled using equation (9):

$$\frac{d\alpha}{dt} = (1 - \alpha)^n Z e^{\frac{-Ea}{RgT}} \quad (9)$$

Where α is the conversion of the product, Z is the pre-exponential factor in s^{-1} , Ea is the activation energy in Joules, Rg is the ideal gas constant and n is the reaction order.

The temperature resulting from the reaction is calculated using the method of Zinn and Mader [8].

$$T_C^{k+1} = T_{C_{inert}}^{k+1} + \frac{QZ\Delta t}{C_{p_C}} e^{\frac{-Ea}{RgT_C^k}} (1 - \alpha_C^{k+1})^n \quad (10)$$

Where Q is the heat of decomposition ($J.kg^{-1}$)

3 Results and discussions

To validate and analyze the performance of the developed model, its results have been compared to experimental and analytical case studies found in the literature.

3.1 First case study

This first case study relates to the work of Roux et al. [9]. In their works, Roux et al. propose an experimental method for determining the thermal diffusivity of pyrotechnic compositions (iron/sulfur mixture). Indeed, they introduced a cylindrical sample into heated tube furnace which upper and lower walls are insulated in the first step of heating and then they took a temporal reading of the temperature at the wall (T_w) and at the center of the composition (T_c) shown in Figure 2b. The wall is heated increasingly from 18 to 35°C. The cylinder has a height of 70 mm and a radius of 7 mm.

To represents the experimental sample, it is assumed that the grains of sulfur, iron, and the pores (here air) are of identical size (one cell). The CA grid (50×500) is randomly filled by respecting the volume proportions of the sample used in Roux et al. [9] experiments. The thermal properties of the used materials are those at 20°C but can be variable. A small part of the used grid is presented in Figure 2a to better visualize the random spatial distribution of the different composition of the studied material (Sulfur, iron, and air).

The comparison between the calculated temperature profile at the center of the composition over time and the experimental one is presented in Figure 2b.

It can be observed that the two temperature profiles (experimental and CA) coincide. This result shows that the developed CA model can correctly simulate the heat transfers within a cylinder composed of a stack of random grains of energetic materials with different thermal properties.

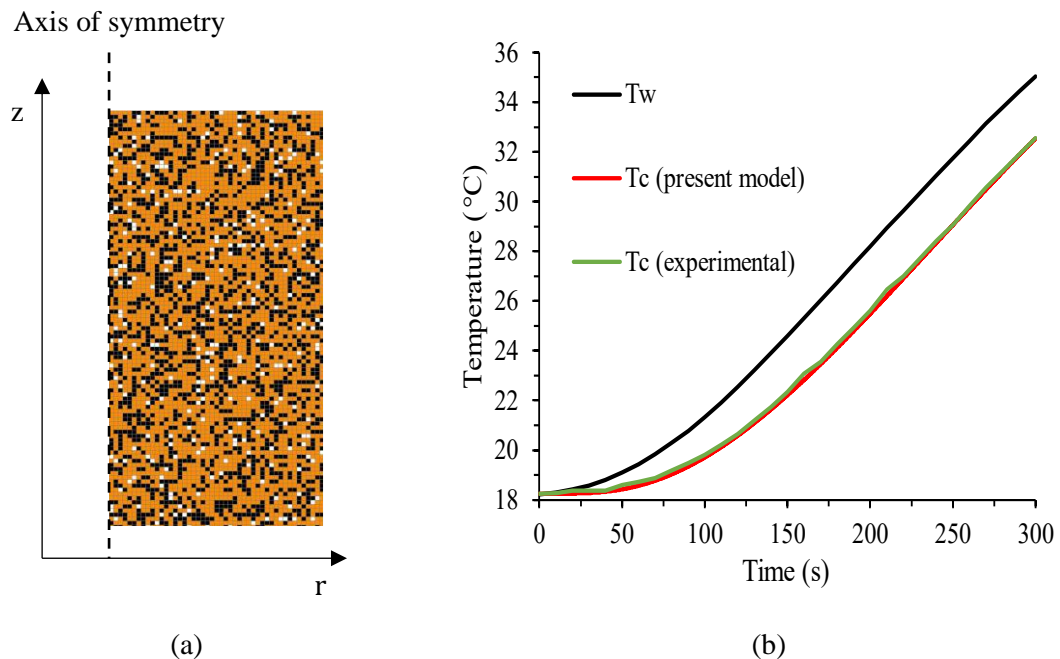


Figure 2. (a) Part of the spatial distribution of the different composition of the studied material (colors white, orange, and black represent air, sulfur, and iron respectively), (b) Experimental and numerical temperature profiles at the center and at the wall of the studied cylindrical sample.

3.2 Second study case

In this section, the results of CA model are compared to the results of the quasi-stationary theory of the Frank-Kamenetskii thermal explosion [10]. The goal of this comparison is to validate the chemical reaction rules used in the developed CA model. According to the works of Gillard [11] the critical temperature (temperature from which the self-ignition phenomenon is observed) for a cylinder with a

radius of 7 mm and height of 7 mm composed of the iron/sulfur mixture (same mixture is used in Roux et al. [9]) is determined analytically ($T_{\text{crit}} = 244.43^\circ\text{C}$).

To determine the critical temperature using the CA model, it would be necessary to use infinite simulation times. However, this being impossible, a simulation time of 1200 s was chosen. This duration seems to be a good compromise between calculation time and precision. The CA grid has 20×20 square cells. The kinetics parameters of the reaction are: $n = 1$, $E_a = 168000 \text{ J}$, $Z = 10^{13} \text{ s}^{-1}$ and $Q = 10^6 \text{ J.kg}^{-1}$ [11].

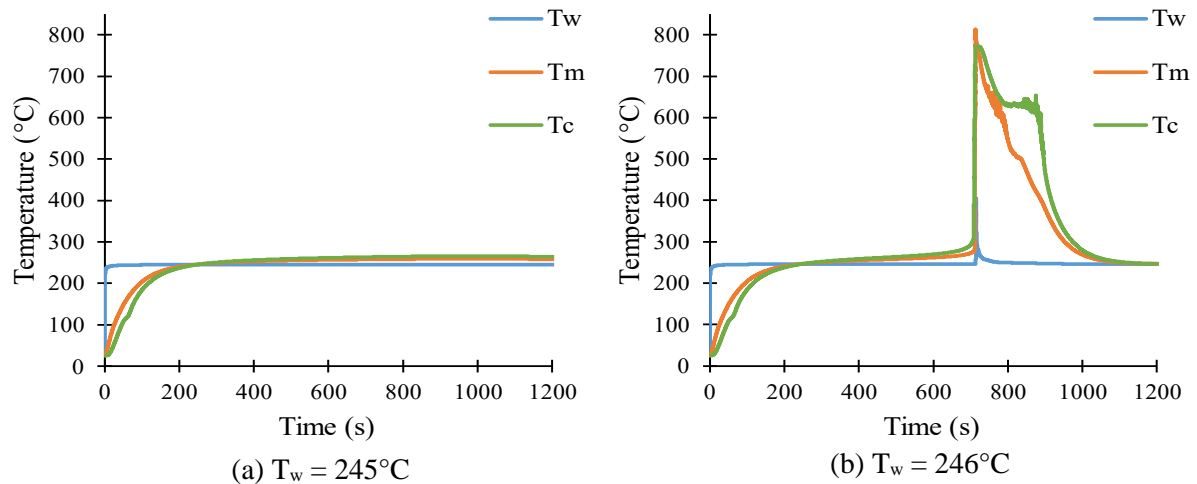


Figure 3. Temperature profile of the CA for different heating temperatures (T_w).

Figure 3 shows the simulated temperature profiles at the center of the cylinder (T_c) and in the middle of the cylindrical radius (T_m) using the developed model for different heating temperatures of the wall (T_w). It can be observed that there is no auto-ignition for a heating temperature of 245°C (Figure 3a). The simulated critical temperature using the developed model is found between 245°C and 246°C . This critical heating temperature fitted well with experiments provided by Roux [9] and is also consistent with Frank-Kamenetskii [10] critical parameter $\delta_c = 2.0$ for the iron/sulfur studied cylinder.

It can be observed that the maximum temperature is reached in the center of the cylinder. This is due to the explosion that took place in the center of the cylinder. In this study, the developed model gives realistic predictions even if the stochastic grain stacking, as represented in Figure 2a, change locally. The only condition to be respected is to keep the same global proportion of reducer, oxidizer and internal porosity initially filled up with air.

4 Conclusion

A numerical model based on CA has been used to predict the combustion in heterogeneous pyrotechnic materials. The validation showed excellent performance of this numerical model. This study is a contribution to the growing evidence of the benefits of CA in measurement Science.

The next step will now be to apply the model developed in this work with cells of hexagonal form. The influence of the distribution and size of the grains will be studied. The influence of the distribution and size of the grains will be studied to . Then, it will be very useful to add to the developed model other physical phenomena like the permeation.

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