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Lattice Boltzmann Modeling of Autoignition in Non-uniformly Heated Mixtures

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Abstract

Lattice Boltzmann (LB) computational model is used to simulate autoignition (thermal explosion) development in mixtures with non-uniform initial temperature conditions. The paper demonstrates LB modeling application to practically important reacting flow problem.

Complications to the classical thermal explosion problem arise in the presence of dynamical heat exchange (natural and/or forced convection), combined with non-uniform initial conditions in the reacting mixture. The present study reports critical conditions for thermal explosion in such circumstances.

Introduction

The problem of autoignition (also referred to as thermal explosion or thermal runaway) has been studied for decades in various formulations, e.g. [1-4]. Nevertheless, complications of this problem arising in the presence of dynamical heat exchange, either self-exerted by natural convection, or introduced by forced convection has been poorly investigated. Further complications arising from non-uniform initial conditions in reacting mixture have never been studied. The question of how the initial non-uniformities in the mixture temperature field affect autoignition development is of practical importance. The present paper addresses this issue in the case of natural convection conditions.

As is always the case in the theory of thermal explosion, critical conditions for autoignition are of primary interest. In the view of this, essentially an induction period of the thermal explosion is being modeled. The model predicts natural convective flows developing at this stage, associated chemical reaction and energy dissipation rates, as well as the onset of the thermal explosion (for super-critical conditions).

The conditions leading to autoignition are formulated in terms of the critical Frank-Kamenetskii parameter. Effects of convection on the critical conditions are described using ratios of the respective critical Frank-Kamenetskii parameters to the ones corresponding to no-convection conditions. Effects of non-uniform initial temperature distributions are described in terms of wavelength and amplitude of the temperature perturbation.

The parameters that are varied in simulations are flow Rayleigh numbers, as well as geometrical parameters describing initial non-uniformities in the mixture temperature field.

The Lattice Boltzmann (LB) method [5,6] is used as numerical technique in the present study. This approach becomes increasingly attractive as a fast and efficient method of solution of partial differential equations. However, application of LB method to combustion problems remains very limited, e.g. [7-10]. The present study demonstrates the potential of LB method in application to such problems. In-house CFD code LBMComb [10] is used.

Mathematical Model

Flow is considered in the Boussinesq approximation. The rationale for this assumption is that effectively only induction period of thermal explosion is considered. Separation of explosion and no-explosion regimes becomes evident before temperature variations become large enough to fail the Boussinesq approximation.

The set of governing equations is therefore as follows:

$$\frac{\partial \rho}{\partial t} + \nabla\left(\rho \vec{u}\right) = 0 \quad (1)$$

$$\frac{\partial \vec{u}}{\partial t} + \left(\vec{u}\cdot\vec{\nabla}\right)\vec{u} = -\nabla p' + \mathrm{Re}^{-1}\Delta \vec{u} - Ar\theta \vec{e}_g \quad (2)$$

$$\frac{\partial \theta}{\partial t} + \vec{u}\cdot\nabla\theta = Pe^{-1}\Delta\theta + \delta\left(1+Ar\theta\right)^{\alpha}\exp\left(\frac{\theta}{1+Ar\theta}\right) \quad (3)$$

This non-dimensional form of equations is obtained by choosing the particular length scale $\tilde{L}$, velocity scale $\sqrt{\tilde{L}\tilde{g}}$, time scale $\sqrt{\tilde{L}\tilde{g}^{-1}}$, density scale $\tilde{\rho}_0$ and pressure scale $\tilde{\rho}_0\tilde{L}\tilde{g}$. p' is pressure deviation from the background level, Re and Pe are Reynolds and Peclet numbers, respectively, $\vec{e}_g$ is a unit gravity vector.

Excess temperature is defined as $\frac{\left(\tilde{T}-\tilde{T}_0\right)}{Ar\tilde{T}_0}$ where $Ar = \frac{\tilde{R}\tilde{T}_0}{\tilde{E}}$ is Arrhenius number. The expression for the chemical source follows standard reaction rate dependence on temperature. Reactants consumption is neglected as only the induction stage of thermal explosion is considered. The Frank-Kamenetskii parameter $\delta = \frac{\tilde{Q}\tilde{B}\sqrt{\tilde{L}}\tilde{T}_0^{\alpha-1}}{\tilde{\rho}_0\tilde{c}_p\sqrt{\tilde{g}}}Ar^{-1}\exp\left(-Ar^{-1}\right)$ is defined in a slightly different manner compared to conventional. Here $\tilde{Q}$ is the heat of reaction and $\tilde{B}$ is the pre-exponential factor.

The Lattice Boltzmann equation is used here with the Bhatnagar-Gross-Krook (BGK) collision model. Accordingly, solutions of the continuum, momentum and energy equations (1-3) are approximated by the families of distribution functions $f_{i,u}$ and $f_{i,\theta}$ evolving by

$$f_{i,u}\left(\vec{x}+\vec{e}_i\Delta t, t+\Delta t\right)=$$
$$\left(1-\omega_u\right) f_{i,u}\left(\vec{x},t\right)+\omega_u f_{i,u}^{eq}\left(\vec{x},t\right)+c^{-2}\left(\left(\vec{e}-\vec{u}\right)\cdot\vec{a}\right)\Delta t \quad (4)$$

$$f_{i,\theta}\left(\vec{x}+\vec{e}_i\Delta t, t+\Delta t\right)=$$
$$\left(1-\omega_\theta\right) f_{i,\theta}\left(\vec{x},t\right)+\omega_\theta f_{i,\theta}^{eq}\left(\vec{x},t\right)+\sigma_{i,\theta}S_\theta\Delta t \quad (5)$$

on D3Q15 lattice [6]. Particular forms of distribution functions and collision frequencies $\omega_{i,\theta}$ are also given in [6]. Force and source terms $\vec{a}$ and S_θ are implemented based on their particular forms in (2,3).

Computational Parameters

Computational domain is cubic, with all the boundaries considered as solid walls with no-slip boundary condition for velocity and fixed boundary temperature $\theta=0$.

Non-uniform initial temperature distribution is taken in various forms which are specified below in the Results section.

The maximum temperature in the domain $\theta_{\max}$ allows the Rayleigh number to be defined as $Ra=\mathrm{Re}^2\,\mathrm{Pr}\,\theta_{\max}$. Results are obtained on a base grid consisting of 25x25x25 lattice cells (51x51x51 vertices). Computations performed on finer grids have produced identical results.

Thermal properties of the media are taken as those of air, Prandtl number is fixed at $\mathrm{Pr}=0.7$; $Ar=0.1$, $\alpha=0.5$.

OPENMP embedded compiler directives are used for parallelization.

The code has been validated against benchmark solutions for heat conduction, as well as for the laminar natural convection plume flow.

Results and Discussion

Principle effects of non-uniform initial conditions, combined with convective dynamics of the medium, can be clearly understood if one considers the case of isolated non-uniformities first.

Isolated Non-unifromities

Consider an initial distribution in the form of the two peaks $\theta=\theta_{\max}\left[\exp\left(-b\left|\vec{x}-\vec{x}_1\right|\right)+\exp\left(-b\left|\vec{x}-\vec{x}_2\right|\right)\right]$, where $\vec{x}_1$ and $\vec{x}_2$ are fixed locations inside the domain. The peak temperature is taken as $\theta_{\max}=6.0$

This case clearly demonstrates the effect of Rayleigh number on the development of thermal explosion. The two distinctive regimes can be observed:

1) Convection plays negligible role at small Rayleigh numbers. Consequently, locations of the peak temperatures remain nearly constant in time. Evolution of the initial temperature field is controlled by thermal conduction. This limit corresponds to high viscosity and therefore, since Prandtl number $\sim O(1)$ is fixed, to high thermal conductivity. Under the explosion limit ($\delta<\delta_{cr}$) initial clouds diffuse completely.

Above the explosion limit ($\delta>\delta_{cr}$) the temperature grows infinitely at location(s) close to initial positions of the two temperature peaks. It should be noted that slightly above the explosion limit peak temperature may grow non-monotonically, i.e. it can decrease before growing infinitely at large times.

2) The system evolution at high Rayleigh numbers is more interesting. Natural convection plays essential role in this limit, and initial clouds ascend significantly in the process of explosion development. This regime is illustrated in figures 1,2.

Below the explosion limit the initial temperature distribution dissipates and the mixture approaches thermal equilibrium.

Different scenarios are possible above the explosion limit. First of all, temperature may grow rapidly in the narrow region located between the two merging thermal clouds. This scenario is demonstrated in figure 1 and occurs if initial separation distance between the clouds d is relatively small.

In the other scenario (figure 2) the two clouds evolve initially independently, but merge later to form hot layer under the top boundary of the domain. Temperature of this layer grows infinitely. This is the case when the initial cloud separation distance is large enough.

Meaningful assessment of natural convection effect on explosion development is obtained upon comparison critical Frank-Kamenetskii parameter to the similar critical parameter at no-convection conditions. The latter is obtained when natural convection is artificially suppressed in simulations, i.e. for a quiescent medium.

The results are presented in this way in figure 3. As expected, the ratio of the critical parameters is very close to 1 at low Rayleigh numbers where convection effect is negligible. The ratio then rises monotonically with Rayleigh number. This is explained by mixing and consequently enhanced cooling of the mixture exerted by natural convection. The critical Frank-Kamenetskii parameter under convection conditions becomes therefore larger than the corresponding parameter for pure conduction process.

figure 3 also reveals the effect of initial separation distance d between the temperature peaks. Effectively, the presence of two clouds slows down the cooling rate of each one, since each cloud may come into contact with the hot surrounding, i.e. the other cloud.

For large separation distances, such interaction may only occur at late stages of induction period, and the two clouds evolve largely separately. In this case the interaction effect is weak and the curve $\frac{\delta_{cr}(Ra)}{\delta_{cr}(0)}$ approaches (in the limit $d\to\infty$) the similar curve $\frac{\delta_{cr}(Ra)}{\delta_{cr}(0)}$ for a single cloud, reported in our earlier work [10].

The interaction is most strong at short separation distances where the clouds merge quickly. The slowdown of cooling rate is expected to be more profound in this case and therefore the critical Frank-Kamenetskii parameter cannot increase significantly. This is confirmed by figure 3 (the curve $d=0.1$).

General Case

In general case, the initial non-uniform temperature distribution is taken in the form

$$\theta=\frac{\theta_{\max}}{2}\left[1+\prod_1^3\sin\left(\frac{2\pi}{\lambda}\left(x_i-\frac{1}{2}\right)-\frac{\pi}{2}\right)\right] \quad (6)$$

The problem of interest is a separation of explosive and non-explosive regimes depending on the amplitude of the initial distribution $\theta_{\max}$ and its wavelength λ.

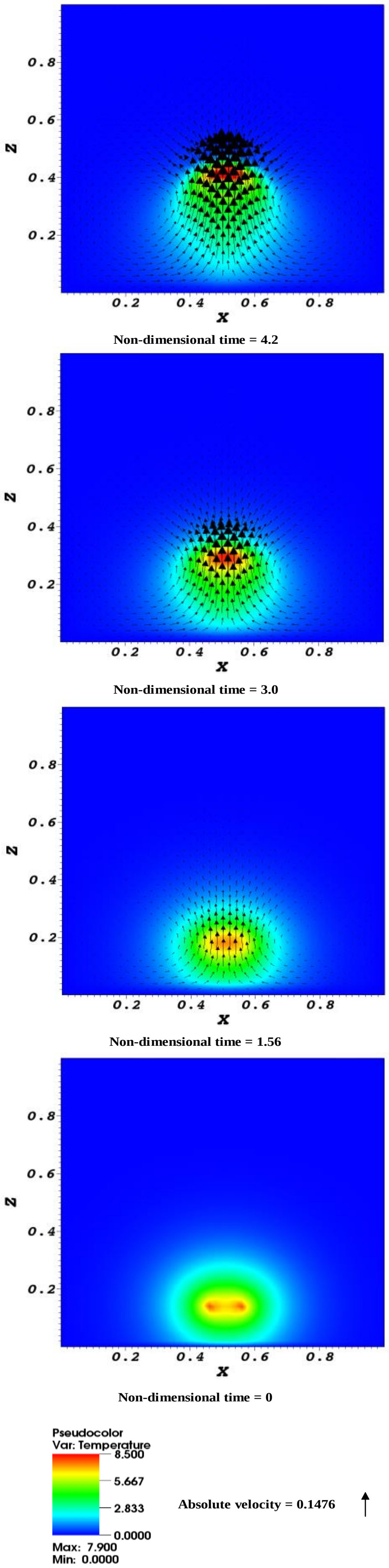

Figure 1. Thermal explosion development at $Ra = 6 \cdot 10^7$; $d = 0.1$

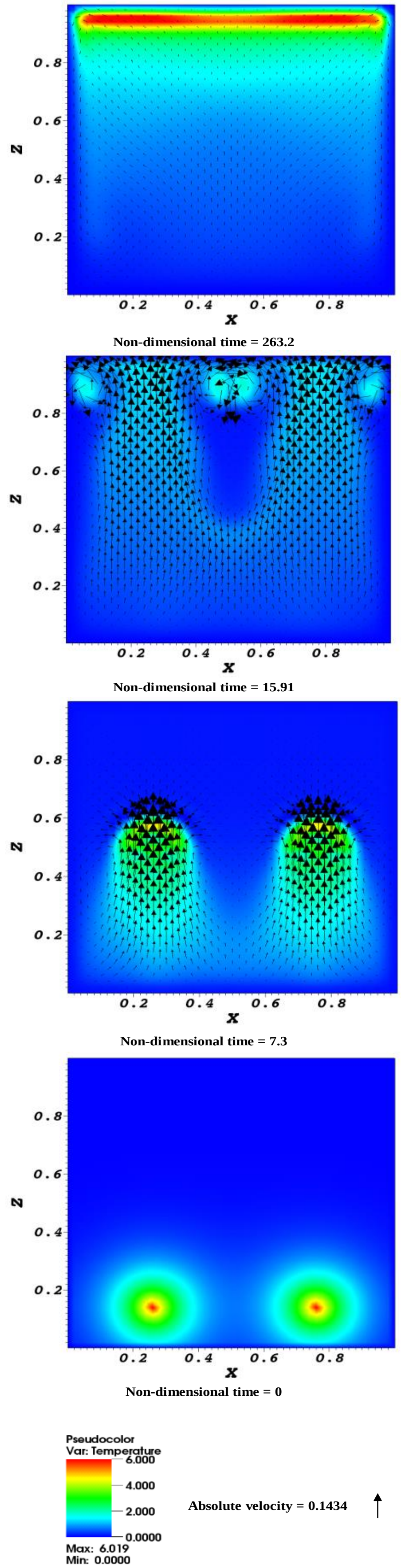

Figure 2. Thermal explosion development at $Ra = 6 \cdot 10^7$; $d = 0.5$

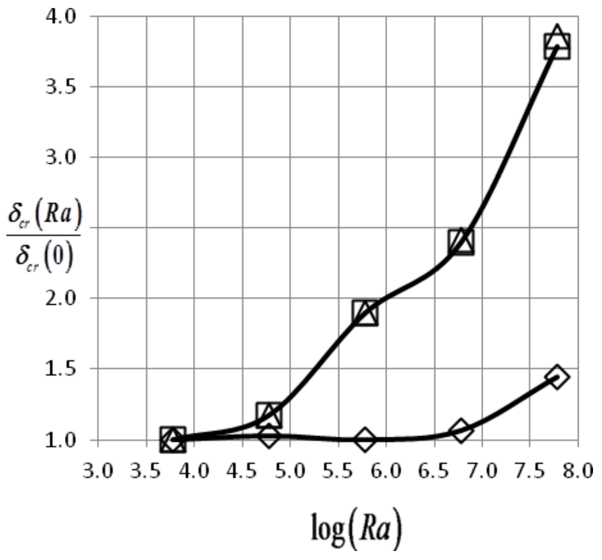

Figure 3. Critical Frank-Kamenetskii parameter ratio as a function of Rayleigh number ◇ - $d = 0.1$; □ - $d = 0.3$; ∆ - $d = 0.5$

Typical general case initial distribution is presented in figure 4.

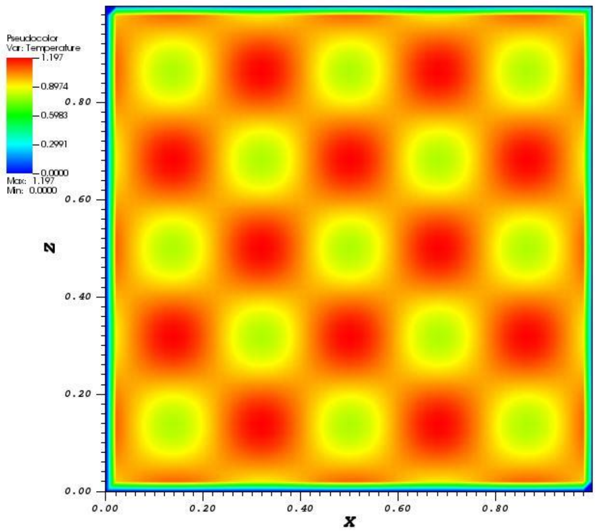

Figure 4. Initial temperature distribution for the case $\lambda = 0.35$ and $\theta_{\max} = 1$.

The parameters that play role in general case are wavelength and amplitude of the initial distribution, Rayleigh number, and subcriticality. The latter parameter measures the proximity of the system to critical conditions at *uniform* initial temperature distribution, and may be defined as $S_{cr} = (\delta_{cr} - \delta)/\delta_{cr}$ for any given system with fixed parameters where $\delta < \delta_{cr}$. Basic results for the general case are presented in figure 5. The curves consist of critical points $\left(\lambda_{cr}, \theta_{\max}^{cr}\right)$ so that the region below each curve corresponds to thermal equilibrium conditions, and the region above corresponds to thermal explosion conditions.

For a fixed $\theta_{\max}^{cr}$ points on the curves 1,2 and 3 correspond to different values of Rayleigh number Ra_1, Ra_2 and Ra_3.

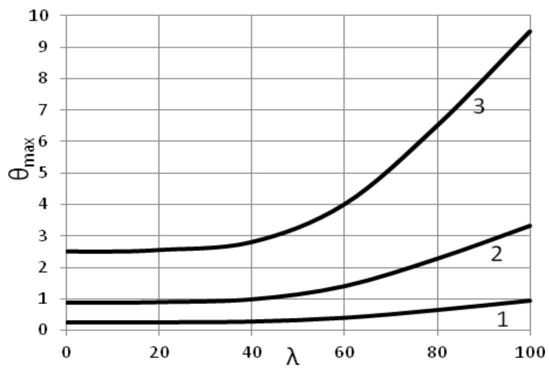

Figure 5. Critical thermal explosion conditions $\left(\lambda_{cr}, \theta_{\max}^{cr}\right)$ $Ra_3 / Ra_2 = Ra_2 / Ra_1 = 10$ (fixed $\theta_{\max}$) $S_{cr} = 0.0055$

Figure 5 demonstrates that for a fixed value of the maximum temperature $\theta_{\max}^{cr}$ the critical wavelength λ_{cr} very quickly decreases with the increase of Rayleigh number. This is consistent with the observation that convection quickly cools hot spots in the media at high Rayleigh numbers, and consequently tighter spacing between the areas of elevated temperature is required to achieve thermal explosion (i.e. critical) conditions.

Conclusions

New results on the development of thermal explosion in non-uniformly heated, convection-dominated media have been presented. It has been demonstrated that convection significantly hampers the development of thermal explosion.

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