Thermal dilatation of solid grains: the LBM approach

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Abstract. On the way to present the detailed description of the thermal processing of fossil fuels, one has to face the task of modeling physico-chemical phenomena as complex as thermal dilatation of particles of granular bed in a hot stream of gases. The work presents main assumptions and description of modeling tool for simulate of coal grains thermal dilatations with increasing temperature. For this purpose we use the Lattice Boltzmann method with some schemes needed when the process, of coupled phenomena, in a representative element of granular media is modeled.

1. Introduction
Detailed simulation of flow thermomechanics in a complex geometry becomes achievable to perform even on desktop computers. This is due to the rapid increase of computational power and the development of numerical schemes and methods (geometrically detailed for specific phenomena) of the Computational Fluid Dynamics (CFD). Mentioned progress is desirable in particular in the case of problems where physico-chemical phenomena have to be modeled. A very demanding process to describe is the thermal processing of solid fuels where phenomena to be solved include heat and fluid flow with chemical species transport in reactive, random granular media. Great efforts have been taken to numerically model some of the phenomena. The methodology utilized in recent studies is the meso-scale simulation approach. In the case of granular media, only part of the domain is modeled taking into account the grain level with use of micro-scale results, such as chemical kinetics and transport through grain porous structure [1]. Usually the goal is to prepare the simulation case to be used in macroscale modeling. The approach is more and more often used in CFD where we need a detailed description of the process but the scale disparity (micro/macro) in industrial cases make it difficult to obtain.

Meso-scale simulations are usually performed in a selected geometry, usually called the representative element of volume (REV). The REV is chosen in the way to be much smaller than the overall size of the industrial device and much larger then size of the smallest modeled scales. With such non-trivial assumptions regarding geometry, in result some of the simple models of thermal processing of fossil fuel can be proposed. Simplifications usually concern numerical modeling in the micro scale, mentioned above, as well as in the macro scale (influence of the boundaries). Therefore, for the processes characterised by a large span of length and time scales, detailed numerical modeling of industrial scale objects is still intolerably expensive [2].

On the way to a physically sound simulation of the coking process in the meso-scale, one of the important phenomena to model is the thermal dilatation of grains. Aside of fluid flow and
heat transfer (including radiation), the list of other phenomena to be modeled contains: chemical kinetics, release of gaseous products and change of physical properties of grains. The last one includes the variations of volume: expansion (in the first stage of heating) and shrinking (in the second stage) accounting for change of shape, with implemented plasticity of the material. In both stages, the process involves also a change of topology of the solid matrix: the granular medium, through plastic deformation, becomes a porous medium.

Due to compact geometry of the granular medium (modeled with the regular lattice as a compromise between accuracy and efficiency) and a need to model physico-chemical phenomena (flow thermomechanics, species transport, plastic deformation, etc.) we choose the Lattice Boltzmann Method (LBM). LBM has received a great interest both from engineers and scientists. Thanks to its meso-scale fundamentals, the method is increasingly extended to model various phenomena; additionally, thanks to its ease of parallelization the method found application over many branches of technological problems.

Although a few papers on the modeling of fluid flow and heat transfer along with chemical species transport in granular medium have been reported [4, 3], the way for modeling thermal dilatation of grains still remains open. After implementation of the method we have to provide closure relationships and describe the process of thermal processing of fossil fuels. The paper, after introduction, contains description of the model and preliminary quantitative results regarding interface diffusion; the paper ends with a short conclusion.

2. Description of the model

2.1. LBM formulation

Here only a brief description of the method along with used schemes is mentioned. Basically, in LBM a given phenomenon is modeled by tracking the evolution of prescribed distribution functions (DF) \( f_i \) corresponding to a chosen set of discrete lattice velocities. The main advantage of LBM is the fully local character of advection and collision terms in the evolution of the DF, along with a possibly easy and effective parallelisation (see [1]). The method is usually applied on a uniform mesh and so it is often chosen to model the phenomena in domains characterised by complex geometry and random layout of elements.

The evolution of the DF in LBM over a time increment \( \delta t \) can typically be written as:

\[
\begin{align*}
  f_i(x + c_i \delta t, t + \delta t) &= f_i(x, t) + \tau^{-1} \left[ f_i^{eq}(x, t) - f_i(x, t) \right] + S_i,
\end{align*}
\]

where \( \tau \) stands for relaxation time and the equilibrium DF is usually presented in a polynomial form:

\[
  f_i^{eq} = \rho \Omega_i \left( A + B \frac{c_i \cdot u}{c^2} + C \frac{(c_i \cdot u)^2}{c^4} + D \frac{u \cdot u}{c^2} \right),
\]

The form of \( \tau \) and the coefficients of Eq. (2) depends mainly on modeled phenomenon. So in the case of heat transfer \( \tau \sim \alpha \); for the chemical species transport \( \tau \) depends on the mass diffusivity coefficient. In case of the equilibrium DF, the coefficients and exact form depend mainly on discretisation model (here D2Q9 stands for a two dimensional modeling with nine directions of DF advection). Equation (1), through the presence of source term \( (S_i) \), can be used to account for model of additional phenomena; a few to mention are influence of released chemical species on the flow field, change of internal energy due to chemical reactions, convection of the fluid, etc. Here we will not discuss in details the implementation of these as they are presented, along with a selection of results, in [3] and references therein.

In case of multiphase flow (we treat grains as non-newtonian fluid in a given range of temperatures) the model utilized here is presented in detail in [9]. The multiphase modeling can be done with use of two DF, which correspond to the evolution of pressure and phase index; in
presented paper prescribed with \( f \) and \( I \) DF, respectively. Simulation of the fluid flow is done by modifying Eq. (1) with the following terms

\[
\text{Eq. (1)}|_f + \frac{2\tau - 1}{2\tau}((c_i - u) \cdot \Gamma(u)(F_s + G) - (\Gamma(u) - \Gamma_0))\nabla \Psi(\rho)) \delta t \tag{3}
\]

\[
\text{Eq. (1)}|_I - \frac{2(\tau - 1)}{2\tau}((c_i - u) \cdot \Gamma(u)\nabla \Psi(\phi)) c_s \delta t, \tag{4}
\]

for pressure \((p)\) and index \(DF\) respectively; \(\Psi\) denotes used equation of state described below.

The surface tension and buoyancy forces are calculated from:

\[
F_s = \kappa \phi \nabla \nabla^2 \phi, \quad G = (\rho - \rho_m)g; \tag{5}
\]

where \(\phi\) is the colour index function; the magnitude \(\kappa\) of the surface tension \((\sigma)\) can be presented:

\[
\sigma = \kappa \int \left( \frac{\partial \phi}{\partial \xi} \right)^2 d\xi \simeq \frac{0.1518(a - a_c)^{1.5}}{1 + 3.385(a - a_c)^{0.5}};
\]

\(\xi\) is the local coordinate in the direction normal to the interface and \(\rho_m = (\rho_1 - \rho_2)/2\) where \(\rho_1\) and \(\rho_2\) correspond to the densities of considered fluids. In the above equation, \(a\) is a parameter describing the miscibility of the fluids; as reported in [9], if \(a > a_c\) both fluids are immiscible. The model is complemented by the Carnahan-Starling equation of state (EOS) which describes the process of separation of phases (see [9]):

\[
\Psi(\phi) = c_s^2 \phi \left[ 1 + \phi + c_s^2 - \phi^3 - 1 \right] - a\phi^2, \tag{6}
\]

where \(a\) determines the strength of molecular interactions. Critical value for Carnahan-Starling equation is \(a_c = 3.5337\) and in our simulation \(a = 4\). Then, \(\nabla \Psi(\phi)\) describes intermolecular interactions of phases and plays an important role in separating the phases.

Following [9], to calculate differential terms in Eqs. (4)–(5) we use in this work a fourth order compact scheme. \(\Gamma\) is used only for pressure and index fields so coefficients are constant:

\[
\Gamma_i(u) = \omega_i \left[ 1 + 3 \frac{e_i \cdot u}{c_s^2} + \frac{9 (e_i \cdot u)^2}{2 c_i^4} - \frac{3 u^2}{2 c_s^2} \right];
\]

Detailed formulas for macroscopic fields are presented at the end of Section 2.

The resulting density and kinematic viscosity of phases in the one-fluid formulation are calculated with use of index functions ([6]):

\[
\rho(\phi) = \rho_2 + \frac{\phi - \phi_2}{\phi_1 - \phi_2} (\rho_1 - \rho_2),
\]

for the viscosity, in [7] it is proposed to account of viscoplasticity:

\[
\nu(\phi) = \nu_1 \exp \left[ \frac{\phi - \phi_2}{\phi_1 - \phi_2} \ln \left( \frac{\nu_1}{\nu_2} \right) \right],
\]

where \(\phi_1\) and \(\phi_2\) correspond to minimum and maximum values of index functions and \(\nu_1\), \((\rho_1)\) and \(\nu_2\), \((\rho_2)\) to viscosities (densities) of fluids. Here \(\nu_2\) stands for the viscosity of coal in a plastic phase; the discussion regarding viscosity of coal in higher temperatures (thermoplastic) is presented in [10].
The developed model has to account for the evolution of temperature and chemical compounds. Most of the works presented till now (for the best knowledge of the Author) concern isothermal multiphase flow, see [6]. As the evolution of temperature field is crucial for the accurate process description, we utilize here the known scheme for Internal Energy Distribution Function (described in [2, 4]). The IEDDF scheme assumes an additional DF (prescribed usually by $g$) to be solved along with other DFs (like $f_i$, $I_i$); the evolution equation for IEDDF is very similar to Eq. (1); equilibrium Eq. (2) differs mostly in implementation (one has to pay attention to the discretisation scheme and DF direction of advection, see [2]).

In case of chemical species transport we utilize a scheme described in [8, 3]. The scheme assumes additional DF (here $\phi_k$) for every tracked chemical compound $k$. The equilibrium distribution functions account for high gradient of chemical compound concentration, this results in equilibrium terms with following modification:

$$
\phi_{0,k}^{eq} = \frac{\rho Y_k}{9} (9 - 7\psi), \quad \phi_{i=1,6,k}^{eq} = \frac{\rho Y_k}{9} (\psi + 3\epsilon_i \cdot \mathbf{u}), \quad \phi_{7,14,k}^{eq} = \frac{\rho Y_k}{72} (\psi + 3\epsilon_i \cdot \mathbf{u}),
$$

where $\psi = \rho^* / \rho$ is the ratio of a minimum density and density in a given point. The release of chemical compounds is calculated with use of the model of chemical kinetics utilized in thermal processing of fossil fuels (see [3]).

The macroscopic quantities are calculated from the following equations:

$$
p = \sum f_i - 0.5 \mathbf{u} \cdot \nabla \Psi(I) \delta t, \quad \mathbf{u} = \frac{1}{\rho c_s^2} \sum c_i f_i + \frac{1}{c_s^2} (\mathbf{F}_s + \mathbf{G}) / 2 \delta t, \quad \phi = \sum I_i, \quad \theta = \sum g_i, \quad Y_k = \sum \phi_{i,k} .
$$

The model assumes simulation of flow thermomechanics with the release of chemical compounds and plastic deformation of grains along with calculation of stresses. The work is in the development stage; an early attempt with temperature-dependent volume of grains was reported earlier. The full set of equations along with the details of the implementation can be found in [2, 4] regarding heat transfer and [8, 3] for chemical compounds evolution.

2.2. Boundary conditions

Like in our previous work, we attempt to model the coupled phenomena within a REV element being in fact a fragment of granular medium; in the present work obstacles cannot intersect the domain boundary and other obstacles surface to simplify the model of thermal dilatation. Grains at lower temperature are treated as solid obstacles and at the increasing temperature we introduce the viscoelasticity.

For the fluid flow, at the opposite walls we use periodic conditions also to simplify description at the early state of thermal dilatation of grains. At the solid boundaries of grains no-slip condition is used and half-way bounce-back scheme is implemented. For the index DF at boundaries of numerical domain we use zero flux (zero derivative) scheme. In case of heat transfer a shift-periodic boundary scheme is implemented at the two opposite walls. The condition introduces constant difference of averaged temperature between chosen points (boundaries) of the computational domain at which the scheme is implemented (for details see references in [5]). The scheme keeps a similar profile of temperature and the continuity of heat flux. At boundaries parallel to the main gradient of temperature, a simple periodic scheme is used.

Utilized boundary conditions result in forced heat transfer, whereas the fluid flow is mainly caused by free convection, thermal dilatation and the release of chemical compounds from the surface of grains. This is still not the ideal case for REV as some pressure drop is expected in the direction perpendicular to the main direction of heat transfer. Also, as the shift-periodic scheme
for heat transfer seems to be the right choice, still the difference of temperature (in function of the number of grains) is determined by our needs. Simply we want to have a maximal temperature observed in the process and temperature at which no chemical species release is started.

2.3. Thermal dilatation of grains
Dilatation of grains is mainly caused by release of gaseous products and change of viscoplasticity of the coal. To mimic this situation changes of the appropriate distribution function have to be implemented. Due to the data collected (in the volume of the grain) at every time step, the algorithm have to account (depend on) to the mean temperature of the grain (in contrast to the local temperature in the solid node) and the rate of release of the gaseous products in the current instant (recent results are presented in [3]). Still it is difficult to find a numerical dissertation or experimental results with presented empirical correlation regarding variable viscosity/geometry of fossil coal in function of temperature. Here we propose formulae that intuitively correspond to the thermo-chemical state of the coal grains with increasing temperature.

In the case of index distribution function, we modify Eq. (4) with:

\[
\text{Eq. (4)} + \Omega_i \alpha_s(\theta) [\phi_1 - \phi(i, j, k)]
\]

where the terms in bracket restrain the highest value of the index function. The \( \alpha_s \) stands for expansion function and takes the form:

\[
\alpha_s(\theta) = 0.5 + 0.5 \tanh(12\theta - 15.6)
\]

and models the release of gaseous products. This only mimics results (namely the detailed functional-group or more general one specie model, see [3]) from modeling of product release.

3. Calculation results
At first the interface behaviour is modeled for a single grain (and obstacle) with the density ratio of \( \rho_1/\rho_2 = 6 \) in the case of no forced convection. The gravity force is added (but with disabled model of buoyancy force).

As it is visible from Fig. 1, with a running simulation the interface of the obstacle undergoes strong diffusion, even for recommended value of \( a = 4.0 \) (see [7] for details).

![Figure 1](image)

Figure 1. Left: result of the Carnahan-Starling EOS, Eq. (6), in function of iteration number with used \( \kappa = 0.001 \) and \( a = 4.0 \) where the value of \( a \) is set to be larger than to \( a_c = 3.8 \); right: velocity magnitude map (grayscale) with vectors and surface nodes as points.

Although the increase of the parameter \( a \) improves the immutability of the index function, this also influences the stability of the simulation (not presented here). Thus some decrease of the time step (relaxation parameter) is necessary to hold the stable simulation.
Figure 2 presents some of qualitative results from simulation of dilatation of obstacles with increasing temperature with implemented models described above (modelling heating by infinitesimally thin wire). The smooth merging of two growing grains (no shear stress) is caused by a lack of a proper condition at the surface of disjoint obstacles.

4. Conclusion and outlook
The presented work is thought to be a brief presentation of the tool used to model the thermal dilatation of grains in reactive flow through a granular medium. In the next step of the implementation of the contact algorithm for modeling the resulting stresses between grains in contact is considered.

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