The application of the Lattice Boltzmann method to thermomechanics of granular media flow and modelling of devolatilization

Arkadiusz Grucelski, Jacek Pozorski
Institute of Fluid-Flow Machinery, Polish Academy of Sciences, Gdańsk

Introduction.   In last decades we observe a rapid growth of importance of computational fluid dynamics (CFD) tools in modelling of industrial processes on different scales. First, appropriately validated by a number of benchmarks and then implemented for the geometry and occurring phenomena, a valid tool offers the possibility to simulate behaviour of the system.

The present contribution addresses the thermomechanics of flow in granular media, aiming at improved modelling of biomass pyrolysis and coking of coal. A phenomenon of main importance is a chemical species emission from grains of biomass / coal and its further transport in the flow. Complication of the geometry coupled with fluid flow, heat transfer and chemical reactions during heating (occurring as a thermal breakage of coal molecules), make a numerical simulation of this processes a challenging issue.

As a tool we use the Lattice Boltzmann method (LBM), suitable for efficient simulations in a complex geometry. The LBM recently attracts considerable scientific interest as one of the methods to simulate coupled phenomena, also with the chemical reactions occurring in 3D flow. The present work shows a current stage of development of LBM to simulation of chemical species evolution, expanded for a 3D case. The emission of chemical species from inside of grains, or devolatilization, is maintained by a set of kinetic equations. A successfully completed simulation was obtained with the use of a weighting function for heat and mass transport, with the boundary schemes developed for density and internal energy distribution functions. Validation of the method was done for the 2D case; some qualitative and quantitative results will be shown for 3D case which is still under development.

Heat and mass transport has been validated for flow cases such as single obstacle flow and an array of circular cylinders [5] also with the temperature-affected geometry of grains [6]. The evolution of chemical species is modelled with usage of LBM scheme of di'Rienzo *et al.* [8], reporting accurate results for a combustion phenomenon. Devolatilisation of fossil carbon (from chemical point of view) can be described as thermal breakage of coal molecules; due to the complexity of the process, full and detailed analysis is impossible to achieve. Presented work shows results for a simulation of coupled di'Rienzo scheme and Functional Groups model for coal pyrolysis. The process of gas release into fluid is implemented using a positive mass flux on the surface (solid-fluid interface).

Brief description of the method.   The Lattice Boltzmann equation, discretized in time, space (by lattice), and velocity (by distinction of admissible directions) on a regular square lattice, describes the evolution of a relevant physical field in terms of its distribution function. In particular, the flow density and velocity are solved for in terms of the density distribution function f, cf. [1]; the temperature field is found from the internal energy density distribution function (IEDDF) denoted by g, cf. [2]; the evolution of chemical species k mass fraction ϕ_k is governed

by a separate distribution function, cf. [8], etc. The form of all these LB equations is similar, [1]; an exhaustive description of LBM for fluid flow is available elsewhere, cf. [1, 3, 4, 5, 7]. Here, we briefly present the form of the evolution equation for chemical species concentration:

$$\phi_{i,k}(\mathbf{r} + \mathbf{e}_i \delta t, t + \delta t) = \phi_{i,k}(\mathbf{r}, t) - \tau_k^{-1}(\phi_{i,k} - \phi_{i,k}^{eq}),$$

where $\phi_{i,k}^{eq}$ represents the equilibrium state of the distribution function of species concentration at $(\mathbf{r}, t)$ along the discrete velocity direction $\mathbf{e}_i$; in 2D, it has the following form:

$$\phi_{0,k}^{eq} = \frac{\rho Y_k}{9}(9 - 5\psi); \quad \phi_{i,k}^{eq} = \frac{\rho Y_k}{L}(\psi + 3\mathbf{e}_i \cdot \mathbf{v}), \quad \begin{cases} L = 9, & i = 1, ..., 4 \\ L = 36, & i = 5, ..., 9 \end{cases}$$

where $\mathbf{v}$ is the local fluid velocity. Relaxation time $\tau_k \sim D_k/\psi$ and $\psi = \rho^*/\rho$; here ρ^* is a minimum density in the entire domain and D_k is the diffusion coefficient for species k.

Benchmark case results. Figure 1 presents a temporal results for the concentration of a chemical species (water vapour) released from the grains during a flow through a representative element of volume of granular medium. As a result of a convection and diffusion of the released mass from the grains we observe a zone of increased concentration of the species travelling with fluid at a given temperature.
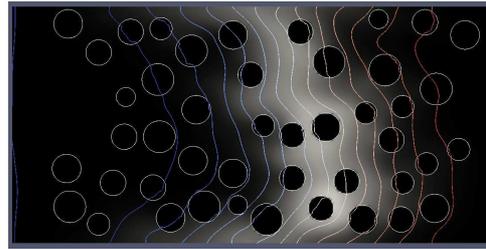
Figure 1: Isotherms and colour map of concentration profile (black – zero concentration, light shade – maximum) for water vapour released from solid grains (depicted as regular cylinders).

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