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Fictitious domain method for fully resolved reacting gas–solid flow simulation

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ABSTRACT

Fully resolved simulation (FRS) for gas–solid multiphase flow considers solid objects as finite sized regions in flow fields and their behaviours are predicted by solving equations in both fluid and solid regions directly. Fixed mesh numerical methods, such as fictitious domain method, are preferred in solving FRS problems and have been widely researched. However, for reacting gas–solid flows no suitable fictitious domain numerical method has been developed. This work presents a new fictitious domain finite element method for FRS of reacting particulate flows. Low Mach number reacting flow governing equations are solved sequentially on a regular background mesh. Particles are immersed in the mesh and driven by their surface forces and torques integrated on immersed interfaces. Additional treatments on energy and surface reactions are developed. Several numerical test cases validated the method and a burning carbon particles array falling simulation proved the capability for solving moving reacting particle cluster problems.

1. Introduction

Gas–solid reacting flows are significant in many industrial systems. For example, pulverised coal furnaces and circulating fluid bed reactors. With computational fluid dynamics, these flows can be predicted to improve the design and maintenance of the industrial systems. A detailed understanding of the underlying physical phenomena is crucial for modelling reacting particulate flows, and the fully resolved simulation (FRS) is needed. In FRS, solid particles are considered as immersed objects with finite size instead of point sources. The sub-grid model is no longer needed but the motion of the rigid particles must be accurately determined.

Basically, two main approaches are adopted to implement the FRS [30,8], namely body conformal mesh methods and fixed mesh techniques. In the body conformal mesh methods, a time dependent mesh is generated to accommodate the moving solid objects. Boundary conditions are imposed on the surface mesh describing the shape of particles. Representative techniques in this class include Arbitrary Lagrange Eulerian (ALE) method [12,11,13,10,28] and Space Time method [26]. The body conformal mesh methods can recover an accurate result due to the precise descriptions of particle boundaries. Besides, though most of body conformal mesh methods for particulate flows focus only on flow field and force calculations, the extension of this approach to reacting flow is straightforward because the reacting flow problems on static body conformal mesh have been widely researched and applied [19,25]. However, collisions and interactions of particles lead to rapidly

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varying complex geometries in particulate flows, and frequent re-meshing processes are needed, which cost tremendous computation time. For particulate flows with large number of particles, fixed mesh methods are preferred because of the efficiency. Reviews on immersed boundary method and fictitious domain method can be found in [8]. Most of the previous fixed mesh methods are based on incompressible Navier–Stokes equations, so only momentum interactions between the two phases are taken into account [27,29–31,24,22,21,20,3,2]. Some other works use Boussinesq approximation to solve particulate flows with heat transfer, in which the fluid properties are independent of temperature [9,5,31] and multispecies reacting simulations cannot be carried on with these methods. Dierich [4] presented a fixed mesh method to solve ice melting problem in water without chemical reactions. To our knowledge, currently there is no such fixed mesh method that is suitable to solve reacting particulate flows with surface reactions, volume reactions in fluid and varying thermal properties.

The main target of current work is to develop a new fictitious domain method, taking into account of the processing of mass transfer and chemical reactions, to solve fluid–solid reacting flows. In the current method, low Mach number governing equations of mass, momentum, energy and species are solved on a background fixed mesh by fractional step method, whilst momentum sources, energy sources and species sources are added to the equations to impose rigidly movement constraints, heat transfer constraints and surface reaction constraints on solid particles, respectively. In the spirit of non-Lagrange multiplier direct force fictitious domain method, the particles region is defined as a set of Lagrange points, which incorporate with background fixed Eulerian mesh using discrete delta functions. Thermal properties are updated every inner iteration in a time step, and volume chemical reactions are solved on each background degree of freedom. Surface chemical reactions are only calculated on the outmost Lagrange points of a particle, and the generated energy and species source terms are then projected into adjacent degree of freedoms on background mesh.

In this paper the principle and implementation issues of the method are shown in Section 2. Several test cases validating the current algorithm are illustrated in Section 3, and a reacting particle cluster problem is also in Section 3 to indicate the capability to solve complex particulate problem.

2. Numerical methods

As a fictitious domain method for reacting particulate flows, the method includes a background mesh solver, a particle solver and a strategy to link the particle variables and background mesh. Firstly, the low Mach number governing equations are discussed in Section 2.1, which is different from governing equations adopted in previous fictitious domain methods. Section 2.2 shows a fractional step, finite element discretisation formulation for the governing equations above. The strategy used to describe solid particles in the current method is then illustrated in Section 2.3, and basic interpolate formulae between particles and background mesh are also discussed. Section 2.4 shows the surface force and torque calculation, movement calculation and collision strategy of particles, which is based on classic fictitious domain methods, for instance the work of Glowinski [6] and Yu [30], with extensions to adjust large solid–fluid density ratios. Besides, energy equations, species equations and surface reaction are also treated in this paper, which is discussed in Section 2.6.

2.1. Governing equations

The governing equations of the fluid dynamics of reacting flow are the Navier–Stokes equations in compressible form. When considering a flow field in which the advection fluid speed is far less than the sound speed, a low Mach number variation of the governing equations is widely used [25,19]. The fluid region and the solid region are formulated together on a so-called “fictitious domain”, as described in Ref. [6]. The solid region obeys the rigid body’s law of motion and Fourier’s heat transfer law, and the constraints should be imposed on the Eulerian equation as source terms. On the Eulerian background perfect gas is assumed, consequently the equation of state is

$$\rho = \frac{p_0}{R_g T} \tag{1}$$

where T is the temperature, p_0 is the ambient pressure, and R_g is the local specific gas constant of mixture.

The mass conservation equation is

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{2}$$

where ρ is the density of mixture, $\mathbf{u}$ is the velocity.

The momentum equation with fictitious domain source term is

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho}\nabla p + \frac{\mu}{\rho}\nabla^2 \mathbf{u} + \frac{\mu}{\rho}\nabla[\nabla \cdot \mathbf{u}] + \frac{\nabla \mu}{\rho} \cdot [\nabla \mathbf{u} + \nabla \mathbf{u}^T] + \frac{1}{\rho}\mathbf{f} + \frac{1}{\rho}\mathbf{f}_{fic} \tag{3}$$

where p is perturbational pressure in low Mach number flow theory, which is different from ambient pressure p_0 in the equation of state (Equation (1)). This work only considers open system in calculations, so p_0 is a constant, which equals to