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# Direct numerical simulation of solid–liquid–gas three-phase flow: Fluid–solid interaction

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ABSTRACT

A direct numerical simulation (DNS) model for three-phase flow (solid, liquid, and gas) with the main purpose of analysing wet granulation processes is presented in this paper. In the present model, liquid–gas two-phase flow is solved by the constrained interpolation profile (CIP) method developed by Yabe et al. (2001) [1], and the interaction between fluid phases and solid particle phase is taken into account by using the immersed boundary (IB) method developed by Kajishima et al. (2001) [2]. The surface tension as well as the wetting are modelled by using the continuous surface force (CSF) model suggested by Brackbill et al. (1992) [3], and the dynamic contact angle is represented by Fukai's (1995) [4] approach, which selectively uses advancing and receding contact angles depending on the movement of fluid interfaces on a solid surface. The accuracy of the model is examined in terms of (i) the drag force exerted on a single particle, (ii) the drag force exerted on a regular particle array, (iii) the surface tension force, and (iv) the wetting. A number of test simulations have been carried out with different numerical cell sizes, and the results are compared with the reported experimental work and theoretical values.



## 1. Introduction

Wet granulation is a complex process of forming powder particle assemblies by the adherence of a liquid binder so as to improve handling and physical properties of the powder. Wet granulation takes place as a result of the combination of three processes, that is, "wetting and nucleation", "consolidation and growth", and "breakage and attrition" [5]. Since the wetting and nucleation process influences the flow dynamics during granulation and influences the quality of the final product, this process has been intensively studied by experiments in both the microscopic and macroscopic scale. The former includes the dynamics of a liquid bridge formed between a pair of particles [6–8], and the latter includes droplet penetration into a powder bed [9–11].

Numerical simulation of the wetting and nucleation process is a challenging issue since it is categorised into the complicated multi-phase flow of solid, liquid, and gas with sharp interfaces existing. Here, "a sharp interface" indicates a sudden transition of the phase. In numerical simulations of the liquid–gas two-phase flow, a curvilinear coordinate is sometimes used to describe the detailed flow-structure [12,13]. However, a curvilinear coordinate cannot handle mixing or breakup of fluids. Alternatively, a fixed Cartesian grid is used with some multi-fluid solvers. The most commonly used solvers are the volume of fluid (VOF) [14,15], level set [16,17], front tracking [18,19], marker particle [20], and constrained interpolation profile (CIP) [1,21]. Each of these has its respective advantages and disadvantages, which are well summarised in [14].

A fixed Cartesian grid has also drawn attention for the investigation of the interfacial relationship between fluid phases and solid phase due to an easy implementation and low computational expense. The momentum exchange between fluid phases and solid phase can be considered by the interaction force incorporated into the dynamics of both phases, and there are several interaction force model proposed: the feedback-forcing method [22], direct-forcing method [23], combination of the feedback-forcing and direct-forcing [24], and body force type [2]. These methods are collectively called Immersed Boundary (IB) method.

The most frequently used surface tension model with a fixed grid seems to be the continuous surface force (CSF) model proposed by Brackbill et al. [3], and it has been proven very successful in simulating free-interface flow [14,25]. In the case of simulating small droplet behaviour, however, it was pointed out by Scardovelli and Zaleski [26] that the CSF model, as well as other conventional models and Lattice Boltzmann Method, induces considerable parasite current despite the absence of any external force. Gunsing [27] suggested another method to calculate the surface tension force, which is linked to the VOF method, where the parasite current was successfully reduced.

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The wetting of fluid interfaces on a solid surface can be modelled easily within the framework of the CSF model. In order to consider the dynamic contact angle, Fukai et al. [4] suggested selectively using advancing and receding contact angles in their Marker Particle simulation. Yabe et al. [25] also suggested an alternative approach to consider the wetting and dynamic contact angle.

In this paper, liquid–gas two-phase flow is solved by the CIP method and the interaction between fluid phases and solid phase is calculated by the body force IB method since these methods are very accurate and the implementation is relatively easy compared to the other methods. The surface tension and wetting is taken into account by the CSF model linked with the Fukai's approach for the dynamic contact angle. The effect of the numerical cell size has been intensively investigated to find the criteria to obtain a reasonable flow field and interaction force. It is stressed here that, although only static particle cases are presented in this paper, the model can be easily extended to a dynamic case by incorporating it with the discrete particle model [28]. The outline of the paper is as follows. The fundamental idea of the CIP method is explained and compared with conventional schemes in Section 2. Then the numerical solution method is explained in Section 3. Several simulation results are shown to examine the accuracy of the present model in Section 4, followed by the conclusions in Section 5.

## 2. Numerical solution of an advection equation and the CIP method

### 2.1. Advection equation

An advection equation is used to describe transportation of arbitrary quantities or waves. It is, in the general form, written as

$$\frac{\partial f}{\partial t} + (u \cdot \nabla) f = H \tag{1}$$

where $f$ is the function to be transported, $u$ the transportation velocity, and $H$ any other term on the right-hand side. To make the explanation easier, only the 1-dimensional case is discussed here. However, the discussion below can be easily extended to the 2- or 3-dimensional cases. The 1-dimensional advection equation is written as

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} = H \tag{2}$$

If $f$ has a sudden change in value at any point, it is generally difficult to solve Eq. (2) accurately by conventional numerical schemes. Fig. 1 (a) shows a square wave propagation after 200 seconds computed by the up-wind [29] and Lax–Wendroff schemes [30] with $u=1$ and $H=0$. It can be seen that the result of the upwind scheme suffers from serious numerical diffusion and the profile becomes lower and broader compared to the exact solution, whereas the result of the Lax–Wendroff scheme suffers from overshooting. The results of other conventional schemes are discussed by Takewaki et al. [31].

### 2.2. CIP method

In order to overcome the problem above, Yabe et al. [21] proposed the constrained interpolation profile (CIP) method and the concept of "multi-moment". In the CIP method, the profile between the neighbouring cells is interpolated by a high-order polynomial function, and the coefficients of the interpolation function are determined by employing different kinds of quantities such as data values, space derivatives, and cell-integrated values. These quantities are collectively called *moments*.

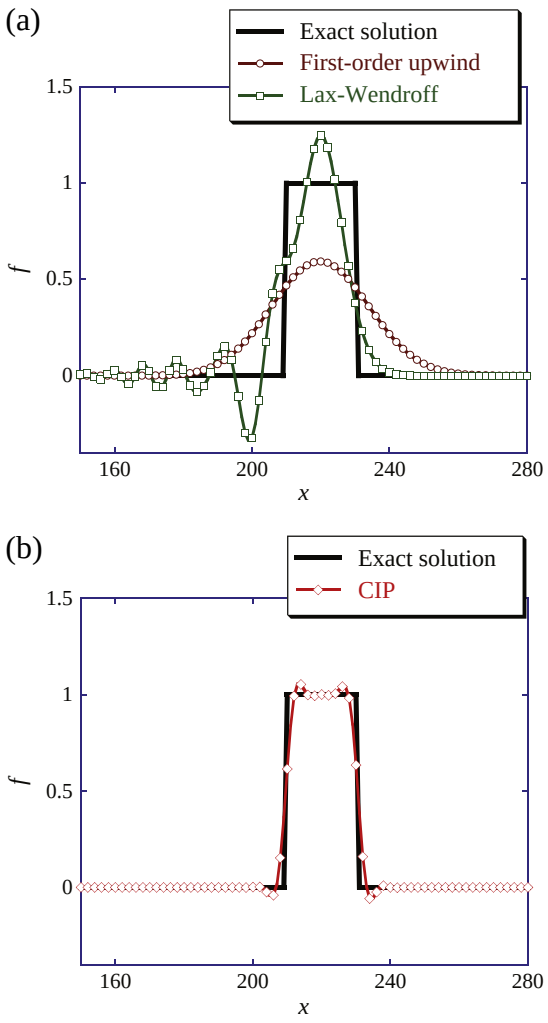


**Fig. 1.** Square wave propagation solved (a) by the first-order upwind and Lax–Wendroff schemes and (b) by the CIP method.

In the original CIP method, the space derivatives are used as the moment. When Eq. (2) is differentiated with respect to $x$, it gives

$$\frac{\partial f_x}{\partial t} + u\frac{\partial f_x}{\partial x} = \frac{\partial H}{\partial x} - f_x\frac{\partial u}{\partial x} \tag{3}$$

where $f_x = \partial f/\partial x$. Eqs. (2) and (3) are solved by use of the fractional step method: the equations are split into the advection and non-advection phases and each of the phases is solved in turn.

- Advection phase

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} = 0 \tag{4}$$

$$\frac{\partial f_x}{\partial t} + u\frac{\partial f_x}{\partial x} = 0 \tag{5}$$

- Non-advection phase

$$\frac{\partial f}{\partial t} = H \tag{6}$$

$$\frac{\partial f_x}{\partial t} = \frac{\partial H}{\partial x} - f_x\frac{\partial u}{\partial x} \tag{7}$$