Available online at www.sciencedirect.com
SCIENCE DIRECT®
ELSEVIER
Computers and Chemical Engineering 27 (2003) 681–687
Computers & Chemical Engineering
www.elsevier.com/locate/compchemeng

Particle packing constraints in fluid–particle system simulation

Z. Chen [a], L.G. Gibilaro [b,*], N. Jand [b]

[a] Reaction Engineering International, 77 W. 200 E., Suite 210, Salt Lake City, UT 84101, USA
[b] Department of Chemical Engineering, University of L'Aquila, Monteluco di Roio, 67040 L'Aquila, Italy

Received 24 April 2002; received in revised form 9 October 2002; accepted 11 November 2002

Abstract

A procedure is described for limiting the void fraction in fluid particle systems, computed by means of numerical multiphase flow simulation codes, to values which do not fall below those realisable in practice. It is based on a computation of the particle–particle contact forces which come into play only when computed void fractions fall to values below those corresponding to random packing of the particles. The general method is illustrated with reference to the process of sedimentation using a specific fluid-dynamic formulation of the equations of change for fluidization. Without the particle contact force algorithm, the particles compact to the physically meaningless void-fraction of 0.17; with the algorithm the random packing value of 0.4 is achieved.

Keywords: Multiphase flow; Fluidization; Fluid–particle systems; Simulation

1. Introduction

A serious problem that arises in the application of numerical multiphase-flow codes to the two- and three-dimensional simulation of fluid–particle interaction systems concerns the lower void fraction limit. This corresponds to the situation of the particles coming into contact with one another, giving rise to contact forces which return the void fraction to the value corresponding to that in a randomly packed bed (typically, 0.4 for spherical particles of a uniform size). Formulations in terms of a continuum description of the particle phase pay no heed to this phenomenon unless possessed of a specific mechanism which comes into play as this limit is approached. Without such a term, void fractions may fall unrealistically, resulting in physically meaningless solutions. The problem becomes particularly acute for the simulation of gas-fluidized beds of moderately sized particles (above about 100 μm in diameter), which tend to give rise to almost completely void gas bubbles rising through a particle phase which remains at a void fraction very close to the packing limit.

The resolution of this problem is by no means straightforward. Shih, Gidaspow and Wasan (1987) and Gidaspow, Shih, Bouillard and Wasan (1989) have confronted it by including a term for solids stress in the particle momentum equations expressed in the form:

$$\frac{d\tau}{dx} = \frac{d\tau}{d\varepsilon}\frac{d\varepsilon}{dx}, \tag{1}$$

where $d\tau/d\varepsilon$ is specified as a function of void fraction $G(\varepsilon)$ which grows sharply as the packing limit is approached and remains negligibly small elsewhere:

$$\frac{d\tau}{d\varepsilon} = G(\varepsilon) \tag{2}$$

$G(\varepsilon)$ is typically assumed to be a power or exponential function of void fraction. Many forms for $G(\varepsilon)$, representing orders of magnitude differences, have been proposed in the literature (Massoudi, Rajagopal, Ekmann & Mathur, 1992). The problem with this approach is that, to be effective, $G(\varepsilon)$ must increase enormously over a narrow range of void fraction at the approach to the packing condition. In contrast to the notion of such a term being necessary for system stability (Gidaspow, 1986), its inclusion in the equations may well lead to numerical instability. A close reading of reported applications (see for example Gidaspow, 1994), supports these misgivings.

* Corresponding author.

0098-1354/02/$ - see front matter
PII: S0098-1354(02)00258-2

Nomenclature

C_{d0}	unhindered particle drag coefficient
D_p	residual of the particle continuity equation (kg/m^3)
d_p	particle diameter (m)
F	net force on a phase (N/m^3)
G	modulus of particle elasticity (Pa)
g	gravitational field strength (N/kg)
i	computing cell index in x-direction
j	computing cell index in z-direction
K	fluid–particle friction coefficient (kg/(m^3 s))
p	fluid pressure (Pa)
p_s	particle pressure (Pa)
t	time (s)
u	lateral velocity (m/s)
u_{mf}	minimum fluidization velocity (m/s)
v	axial velocity (m/s)
x	lateral distance (m)
z	axial distance (m)
Δt	time step (s)
Δx	computing cell size in x-direction (m)
Δz	computing cell size in z-direction (m)
ε	void fraction
ρ	density (kg/m^3)
τ	solids stress (Pa)
Superscript	
n	index for time step
Subscripts	
f	fluid
p	particle
x	lateral direction
z	axial direction
Bold type	vector quantities

2. Computation of particle–particle contact forces

The proposed method is conceptually very straightforward. No additional terms enter into the basic system equations until required. The simulation is allowed to proceed normally, values of the variables (fluid and particle velocities, fluid pressure and void fraction) being computed at the spatial grid points for successive time increments. If at a certain time increment the void fraction at one or more of the grid points is found to have fallen below the packing limit, say 0.4, the computation is halted, the off range void fractions are set to 0.4, and an iterative procedure is used to determine the contact force at each affected grid point necessary to sustain this condition and also satisfy particle continuity. This procedure effectively mimics the physical reality of contact forces coming into play only when particle concentration attempts to exceed that for random packing.

The particle contact forces are referred to in terms of 'particle pressures' p_s, by analogy with fluid pressure which enters into the momentum equations in a similar manner. They are set everywhere to zero and held at zero under normal conditions. The derivatives of p_s ($\partial p_s/\partial x$, $\partial p_s/\partial z$) are included in the particle momentum equations but only assume non zero values where the corresponding p_s values contain a non zero value. As the magnitude of the additional force is just sufficient to maintain the void fraction at 0.4, the procedure avoids the problems of numerical instability referred to above.

'Particle pressure' measurements have been reported in the literature in recent years (see for example Zenit, Hunt & Brennen, 1997). These however concern particle bombardment, usually on the wall of a fluidized bed, and therefore represent a very different phenomenon to that of the effectively static contact forces considered in this paper.

2.1. Determination of particle pressures p_s

The particle pressure p_s at each grid point at which the void fraction has been changed from an off range value to 0.4 is chosen to satisfy particle phase continuity. This