JOURNAL OF COMPUTATIONAL PHYSICS **135,** 1–7 (1997)
ARTICLE NO. CP975719

Simulation of Fluidized Beds with Lattice Gas Cellular Automata

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Received September 5, 1996; revised April 14, 1997

This paper introduces an approach for the simulation of the hydrodynamic behaviour of gas–solid fluidized beds via the use of lattice gas cellular automata. This approach is based on a two-speed model, developed by U. Frisch, B. Hasslacher, and Y. Pomeau. Simulation runs for different configurations of the automaton produce results that can be compared to actual data. The simulations show when and how bubbling will occur. Values for the bubble diameters as a function of bed height, as well as bed porosities in two horizontal planes have been obtained from the simulations. From these results correlation diagrams and the Kolmogorov entropy are calculated. Generally, the results of the simulations are qualitatively in good agreement with experimental observations, showing that this new approach could provide a useful tool in predicting the fluid dynamic behaviour of fluidized beds. © 1997 Academic Press

1. INTRODUCTION

A lot of research has been done to predict the behaviour of fluidized beds. Unfortunately there is still much confusion and contradiction in the reported literature. The reports often produce recommended correlations, but little in the way of unifying theory [12]. In this research a physical model is developed and implemented into a cellular automaton. This approach can be used to predict some of the aspects of the physical behaviour of the fluidized bed. This model, however, cannot yet be compared to all quantitative measurements, and therefore more research will be needed on this field.

Cellular automata (CA) were first introduced by von Neumann [24], describing idealized selfreproducing systems. Hereafter the CA models have been used for numerous applications, from the evolution of spiral galaxies [8] to phase transitions [14].

The usage of cellular automata became popular for simulating fluids, when a new family of cellular automata were developed: the lattice gas cellular automata (LGCA) [6]. This type of cellular automata is mainly used for the simulation of fluids, i.e., the Navier–Stokes equation. Rothman [17] has used this method to look at multiphase flow, a similar subject of this paper.

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An ever newer development in the CA is the lattice Boltmann (LB) technique [13]. The standard LB technique only describes averaged behaviour, whereas in fluidized beds fluctuations are important. For this reason the more classical LGCA technique is used. Nowadays also fluctuating LB techniques are used, but this has not been researched in this work.

The simulation of fluidized beds differs from the simulation of the Navier–Stokes equation as for the latter there is a well-developed differential equation. No real unifying and exact differential equations, describing the complete behaviour of fluidized beds, exist. Anderson and Jackson [1] and Pritchett *et al.* [16] were one of the first to develop the two-fluid model, describing both the gas and solid phase as continuous and fully interpenetrating. Later many others [4, 15] reformulated so-called granular kinetic theory into the solid stresses and viscosity to resemble the solid flow behaviour. The description of the solid phase by a continuous phase, however, will only be valid under certain assumptions. Another drawback of these models, is the large computational cost.

Another approach to simulate fluidized beds is the approach from molecular dynamics. Particles are described as ideal round spheres, as described by Hoomans *et al.* [10], and Seibert and Burns [21]. These models have very high computational costs and can only be used for small systems and a short period of time.

The behaviour of a fluidized bed is similar to fluid behaviour. The two fluid model uses this property of the fluidized bed to simulate its behaviour. The LGCA model presents macroscopic fluid behaviour and could also be suitable for the simulation of fluidized beds. This is researched in this paper.

To simulate fluidized beds with a LGCA model, the microscopic behaviour of the fluidized bed is implemented into the LGCA. Therefore the standard LGCA is modified to include gravity and gasflow. The results of the simulations will hopefully represent the macroscopic behaviour of a fluidized bed. The result is a computationally very inexpensive model.

0021-9991/97 $25.00

The presented topics in this paper are:

1. LGCA,
2. fluidized beds,
3. modification of the LGCA to incorporate superficial gas flow and gravity,
4. results.

2. LGCA

The simulation model is an automaton that can be defined as a D-dimensional Bravais lattice with fixed points, called nodes. Every node has a state, which is determined by the previous state of that node and the states of its neighbors. The nodes are connected via links, which cannot be occupied by more than one particle. Particles travel along the links and collide at each node. Usually all particles have the same speed and the same mass. The state of one node is then defined as

$$n(\mathbf{r}) = \{n_i(\mathbf{r});\ i = 1, ..., b\}, \tag{1}$$

where $\mathbf{r}$ is the position vector of the node, n_i is the state of link i, and b is the number of links, which is the same as the number of neighbours.

At every time step the automaton is updated in two steps: (a) the collision step, and (b) the propagation step. The collision step is defined as

$$s' = \mathscr{C} \cdot s, \tag{2}$$

where $\mathscr{C}$ is the collision operator, s' is the output state, and s is the input state. Each transition is assigned a probability: $A(s \to s') \geq 0$. The probability only depends on s and s' and does not depend on the position of the node. The collision step only redistributes the particles at a node. The particles are only given a new direction and are not moved. A collision operator must conserve certain physical quantities, like mass and momentum. The collision operator must also agree with the exclusion principle, stating that every link can only be occupied by one particle at the most, and the Stueckelberg condition, leading to a reversible solution. It is important, however, not to conserve too many quantities, so-called spurious conserved quantities. For this a stochastic behaviour of the model is important.

Moving the particles is done by the propagation step. The propagation step is defined as

$$n_i(\mathbf{r}_*) \to n_i(\mathbf{r}_* - \mathbf{c}_i \cdot \Delta t), \tag{3}$$

where Δt is the amount of time for one time step, and $\mathbf{c}_i$ is defined as the velocity of the particles in direction i. One time step consists of a collision step and a propagation step.

Three LGCA models are: (a) the Hardy, Pomeau, and Pazzis (HPP) model [11], (b) the Frisch, Hasslacher, and Pomeau (FHP) model [6], and (c) the face-centered hyper cubic (FCHC) model [3]. The HPP model is not suitable for realistic simulations. The FHP model is used for two-dimensional simulations. It is built up from a two-dimensional triangular lattice, where each node has six nearest neighbours and one rest particle. A two-speed model was also used in this research. Then each node has 12 neighbours which particles can reach in one time step. The FCHC model is a pseudo four-dimensional model which is used for three-dimensional simulations. It has 24 nearest neighbours.

It can be easily seen that the two-speed FHP model has the same isotropic characteristics as the classic FHP model. The proof that this model is isotropic is given by Frisch *et al.* [6].

Strictly speaking LCGA models lack Galilei invariance. There is no Galilei transformation that maps an allowed microstate of the LGCA onto another one. However, within the fluidized bed we consider flow velocities much less than the particle velocity, so that nonGalilean invariance is not a serious difficulty.

The collision operator is a square matrix, when a lookup algorithm is used during simulation. For the two-speed FHP model, the collision operator thus is a $2^{13} \times 2^{13}$ matrix. This size still fits well into computer memory. The FCHC model, however, requires a $2^{24} \times 2^{24}$ matrix. It is generally not possible to fit matrices of this size into hard- or software.

3. GAS–SOLID FLUIDIZED BEDS

To implement gas–solid fluidized beds into cellular automata, the microscopic influences are approximated. The main forces on a single particle in a gas–solid fluidized bed, are the drag force from the upward flow and the gravity force. These forces are defined as

$$F_g = \frac{\pi}{6}(\rho_p - \rho_g)\, g d_p^3 \tag{4}$$

$$F_d = \left(\frac{200(1-\varepsilon)}{\mathrm{Re}\,\varepsilon^3} + \frac{2.33}{\varepsilon^3}\right)\frac{\pi}{4} d_p^2 \frac{\rho_g u^2}{2}, \tag{5}$$

where F_g is the gravity force, F_d is the drag force, ρ_p is the density of the particles, d_p is the average particle diameter, ε is the local porosity, ρ_g is the density of the flow, Re is the Reynolds number, and u is the velocity of the flow. Equation (4) is the buoyancy force and Eq. (5) is an empirical equation for the drag force on a particle, based on the correlation by Ergun [5] for the frictional pressure drop through a bed of particles.

The fluidization condition where the drag force equals the gravity force, is called *minimum fluidization.* From Eq. (5) one can see that at high local porosity the drag force is relatively low. This means that areas with high local density will go up, and areas with high local porosity will go down.

In Eq. (5), the basic assumption is made that the pressure from the flow is the same at every point in the bed. When voids, called bubbles, occur in the bed, however, the gas tends to flow into the bottom part of the bubbles. This leads to extra drag on the top of a bubble, increasing the bubble growth.

The hydrodynamic behaviour of bubbling gas–solid fluidized beds can be described as chaotic [22, 23, 20]. Chaotic systems are governed by nonlinear interactions between the system variables. Due to this nonlinearity, these deterministic systems are sensitive to small changes in initial conditions and are, therefore, characterized by a limited predictability. In other words, information about the initial state of the system is lost when it evolves in time. The chaotic dynamics of a system are fully represented by its attractor in the phase space, which describes the time evolution of the system and which can be quantified by characteristic invariants.

The low-dimensional chaotic behavior of fluidized beds is due to the behaviour of the rising and interacting bubbles which is a phenomenon that takes place at relatively large scale. This particular behaviour with a small number of dynamic modes is actually a result of the high-dimensional behaviour of the particles due to the interaction with the flowing gas and to particle collisions and friction. These gas–solid and solid–solid interactions that are represented by a large number of dynamic modes at small scale thus finally lead to low-dimensional chaotic behaviour at larger scale. A similar phenomenon may be present in the model in this paper, where very high dimensional (stochastic) behaviour of simulated particles at the small scale finally lead to large scale chaotic structures (i.e., bubbles).

These chaos characteristics of dynamical systems can be estimated from time series of only one of the system's characteristic variables, such as pressure fluctuations in bubbling gas–solid fluidized beds, via a technique called (attractor) reconstruction [22].

One of the most important chaos characteristics is the Kolmogorov entropy [9], which measures the rate of loss of information (expressed in bits of information per unit of time), and which quantifies the limited predictability of chaotic systems. In general, the Kolmogorov entropy is large for very irregular dynamic behaviour (like pressure fluctuations in turbulent gas flow), while it is small in case of more regular, periodic-like, lower dimensional behaviour (like in slugging beds). The limiting values for Kolmogorov entropy are infinity for complete random sets, and zero for completely periodic systems. A practical maximum likelihood method to estimate Kolmogorov entropy from (measured) time series has been reported by [18].

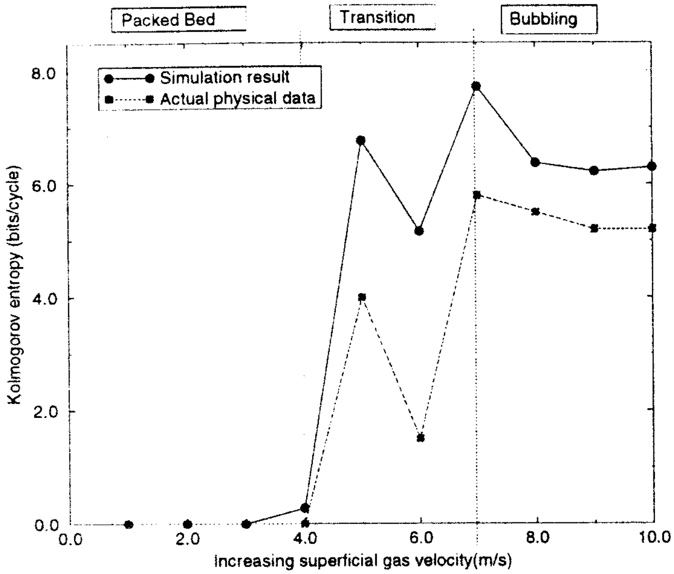

FIG. 1. The Kolmogorov entropy as a function of configurations in increasing superficial gas velocity (actual data are taken from [22]). The lines are drawn to guide the eyes.

Schouten *et al.* [20] have derived an empirical relationship between the Kolmogorov entropy and characteristic fluidized bed properties, such as the superficial gas velocity U_0, the minimum fluidization velocity U_{mf}, the bed diameter d_{t}, and the settled bed height H_s, according to

$$K(\text{bits/s}) = 10.7 \left(\frac{U_0 - U_{\mathrm{mf}}}{U_{\mathrm{mf}}} \right)^{0.4} \frac{d_{\mathrm{t}}^{1.2}}{H_{\mathrm{s}}^{1.6}}. \tag{6}$$

The Kolmogorov entropy was estimated from time series of pressure fluctuations that were measured in the center of a bed of fluidized Geldart B particles [7], at the position of the settled bed height.

Vander Stappen *et al.* [23] have also performed experiments in which they measured the Kolmogorov entropy as a function of the superficial gas velocity in the vicinity of minimum fluidization to investigate the onset of chaos in gas-solid fluidized beds. It was found that between minimum fluidization and the freely bubbling state, an intermediate regime exists, where the Kolmogorov entropy first increases and then decreases but always is lower than in the fully developed regime. This is illustrated in Fig. 1.

Numerous empirical relations have been determined for bubbles in gas–solid fluidized beds. These equations are widely accepted in present fluidized bed sciences and form a good basis to check the results of a fluidized bed model. A correlation between the bubble rise velocity and the bubble diameter is [2]

$$u_{br} = 0.711\sqrt{gd_b}, \quad \frac{d_b}{d_t} < 0.125. \tag{7}$$

The bubble diameter versus the bubble height fits the equation [12]

$$d_b = A_0 + A_1 \cdot h_b^{A_2}, \tag{8}$$

where the literature value of A_2 is between 0.75 and 1.0.

4. SIMULATING FLUIDIZED BEDS WITH LGCA

When simulating fluidized beds with LGCA, the microscopic behaviour is estimated and implemented into the cellular automaton. This is done for the three influences discussed in the last section:

1. Gravity force. The gravity force is equal for all particles because it is not a function of the porosity.

2. Drag force. The drag force is a function of the porosity, and thus, it is a function of the number of particles at a node. At high local porosity, the drag force will be small per particle. If, however, the local porosity is low, the drag force will be larger per particle. The drag force is only accounted for in the z direction. This assumption can be made if most gas travels straight upward to the top of the bed, only moving in one direction. Around solid concentration gradients, like bubbles, this is not completely true.

3. Pressure gradients near bubbles. The top of a bubble is detected in the system, if all links going up are occupied by particles travelling upwards and all links going down are unoccupied. If the top of a bubble is detected, momentum is added, because such places attract gas also from the sides [12]. This is to correct the error in the assumption made under point 2 above for bubbles.

The total momentum change only affects the z direction.

When constructing the collision operator, all possible input states are taken into account and linked to an appropriate output state. During the simulation, an output state for the input state is looked up in the collision table. Sometimes one input state can lead to multiple output states. To ensure the stochastic behaviour of the system, a condition for the simulations with LGCA, a random choice of the possible output states is made.

During the simulation various quantities are measured: (a) the porosities of two horizontal planes in the system, and (b) the size and location of certain bubbles. The computed porosities in two planes can be correlated. The correlation between these two planes gives insight into the velocity and the uniformity of the velocity of the particles in the bed. Time series of the calculated porosity in a plane can be used for the estimation of the Kolmogorov entropy [18, 19]. The bubble quantities are used to verify bubble correlations which were discussed in the previous section.

5. SIMULATION RESULTS AND DISCUSSION

The two-speed FHP model was introduced to improve the simulation results of the one-speed model. The number of possible velocity gradients in the one-speed model proved to be too small. The results of the two-speed model predict the actual behaviour much better than the standard FHP model. The visual representation resembles photographs of fluidized beds very well.

To simulate the fluidized bed system, first, a momentum is defined for all directions, upward links having a positive momentum and downward links a negative one. The rest particle has zero momentum. A rest particle is included to increase the number of possibilities of momentum and velocities at a node. Hereafter the momentum change is calculated for every possible particle distribution. This is done by adding the momentum change according to the three effects described in the previous section. For instance, for every particle at a node one unit of momentum is subtracted for gravity.

Then the collision operator is constructed. This is a large matrix, linking all input momentum possibilities to a calculated output possibility, regarding required conservations (mass) and the required momentum change. If more than one output possibility exists, this is stored in a separate matrix. When such a condition is needed, one is randomly picked from the possibilities. This is to ensure the needed stochastic character of the system.

Ten different systems with different configurations were simulated, visually compared, and the porosities calculated in the two horizontal planes were correlated. This was done to give insight into the consequence of different configurations and to determine if different regimes could be simulated. Figure 2 shows a correlation diagram of a system. Figure 4 shows the visual representation of the system; 50 bubbles were measured in each system, and the averaged results are shown in Table I and in Figs. 5 and 6.

The 10 systems are different regarding momentum definition on the links between the nodes and the influence of the drag force and the bubble pressure gradient correction.

The ratios of the bubble diameter versus the height of the bed correspond to literature values, up to 80% of the bed height. The curves representing bubble velocity versus the bed height, however, do not correspond with data from the literature. The bubble velocity is almost constant and the same in all simulated configurations. This can be seen from the bubble velocity and from the correlation diagrams. LGCA do not allow large velocity gradients, because the momentum at a node is limited to certain values. If the required momentum becomes greater than that certain value, the model does not allow this increase.

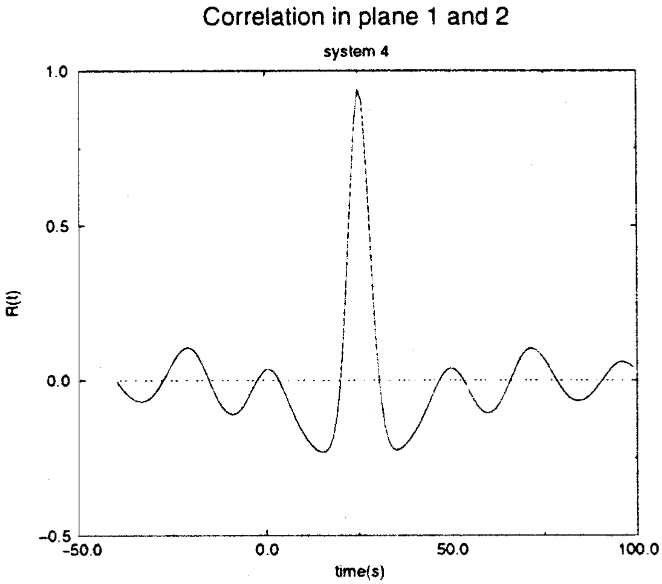

FIG. 2. The correlation of the porosities measured in two horizontal planes.

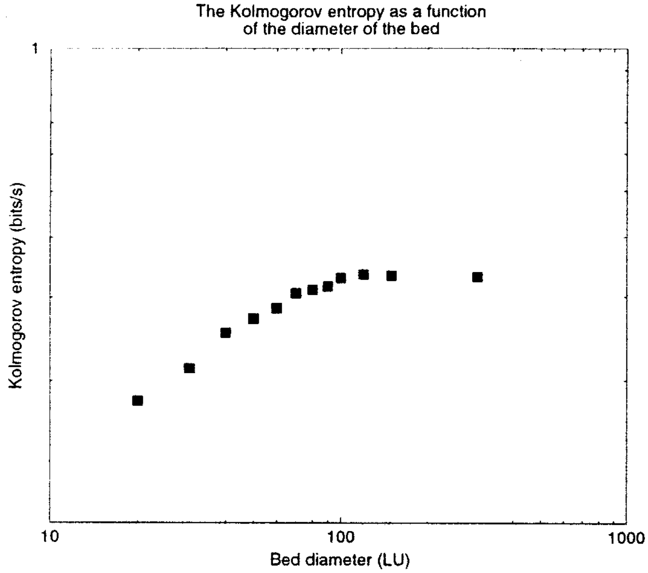

FIG. 3. The Kolmogorov entropy as a function of the bed diameter.

Ten systems in increasing superficial gas velocity were simulated. The superficial gas velocity is increased, by increasing the drag force on the particles. The exact superficial gas velocity, however, cannot be extracted from this increase, and thus, the superficial gas velocity is not linear with the system number. The Kolmogorov entropy was determined for all 10 systems. The result is shown in Fig. 1. The calculated Kolmogorov entropy from the simulations behaves in the same way as the Kolmogorov entropy that was estimated from pressure fluctuations in a real fluidized bed of 10 cm ID [23]. This means that the two-speed FHP model is able to reproduce actual trends in the chaotic dynamics of gas–solid fluidized beds.

The Kolmogorov entropy was determined for 12 simulated systems in increasing bed diameter. The result is shown in Fig. 3, which clearly shows an increase of the Kolmogorov entropy with the bed diameter up to 100 LU, where LU stands for lattice unit. Beyond 100 LU saturation takes place. This saturation is not visible in Eq. (6), but maybe this is due to the fact that this equation has been obtained from measuring in-bed diameters only up to 40 cm ID.

Storing the whole FCHC collision table in memory is not possible. The implementation of the FCHC model thus requires the computation of all possible collisions of particles in each node at every time step. This is done in the

TABLE I

The Fit Parameters of Bubble Diameter vs Bed Height for Systems 1 through 9

Fit-parameter	*System number*								
	1	2	3	4	5	6	7	8	9
A_2	0.82	0.86	0.84	0.81	0.76	0.82	1.0	1.0	0.81

FIG. 4. Visual representation of simulated fluidized bed.

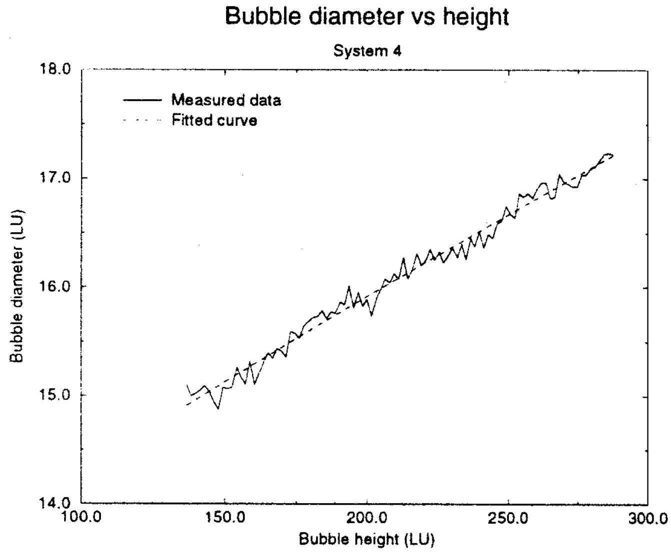

FIG. 5. The bubble diameter versus the bubble height.

same way the collision operator is constructed: a possible output state is computed, taking into account the input state and the required momentum change. Mass is conserved. This is a very time-consuming way of simulation, so only a few results were obtained for this model.

Only two types of particle behaviour could be simulated. If bubbles form in the bed, the bubbles continue to grow, without reaching a maximum size. This resembles the behaviour of Geldart B particles [7]. Configurations where the bed fluidized without bubbles were also found. This resembles some of the behaviour of Geldart A particles.

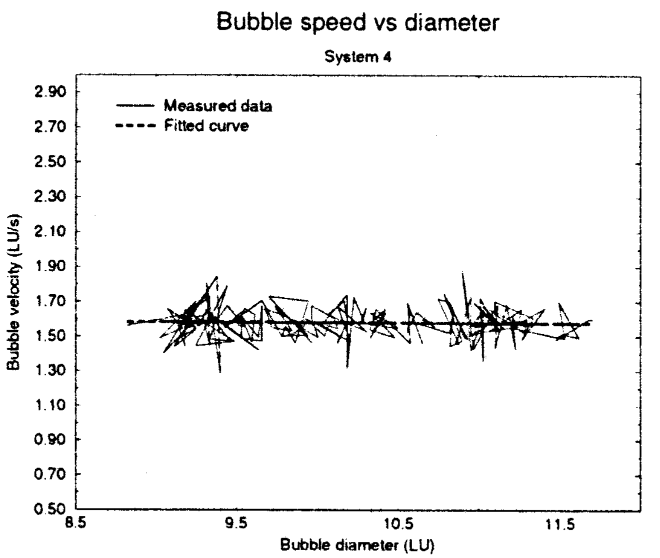

FIG. 6. The bubble velocity versus the bubble diameter.

The main and surprising result of the simulation runs, is that bubbles form in the fluidized bed, even though this macroscopic phenomenon was not implemented beforehand. Also the chaotic properties and some bubble correlations of the calculated system resemble actual parameters.

A problem of LGCA models is that they do not allow large velocity gradients. This results in a constant bubble velocity in all the simulated systems. This can be seen in the fact that Fig. 6 does not correspond with Eq. (7). Another drawback is that all the configurations behave alike. The bulk of the fluidized bed has the same velocity in all simulated configurations. This is because the freedom of the particles is limited.

The simulation of fluidized beds, however, can give insight into and predict some important features of real fluidized bed reactors. After more research into the influence of the configuration and into the behaviour of the chaotic properties of the simulated fluidized bed, using this method could provide a useful additional tool to predict the behaviour of gas–solid fluidized beds.

ACKNOWLEDGMENTS

B. G. M. van Wachem gratefully acknowledges the assistance of C. M. van den Bleek and M. L. M. vander Stappen at the department of Chemical Process Technology, Faculty of Chemical Technology and Materials Science, Delft University of Technology giving more insight into the models of fluidized beds and discussing the obtained results.

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