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Characterization and CFD-DEM modelling of a prismatic spouted bed

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A B S T R A C T
In this study a prismatic spouted bed was characterized experimentally and modelled by means of 3D CFD-DEM simulations. The main focus was on the investigation of the influence of the gas flow rate on the bed dynamics and spouting stability. Pressure drop time series obtained at different gas velocities were used for the identification of flow regimes by means of the frequency domain and of chaotic properties such as the correlation dimension and Kolmogorov entropy. The gas and particle dynamics were investigated through simulations of different operational regimes: the spouting onset, as well as stable and unstable regimes. A 3-D bed behaviour, typical for slot-rectangular beds, was found. A good agreement between simulations and experiments in the particle flow patterns, bed expansion and dynamics of characteristic gas pressure fluctuations was achieved. The particle dynamics as a function of the gas velocity was investigated for the entire bed. For one of the stable regimes, the bed regions showing different particle dynamics (spout, fountain and annulus) were characterized in detail. A regime map showing the stable operational window in dependence on an inlet-to-bed size ratio and gas velocity is also provided.

1. Introduction

A spouted bed is a very effective and widely used gas–solid or liquid–solid contactor. In this investigation a prismatic spouted bed apparatus described in our previous work [1] was investigated experimentally and modelled by using a Discrete Element Model (DEM) coupled with Computational Fluid Dynamics (CFD). The investigated apparatus can be affiliated with the family of slot-rectangular spouted beds, which are the subject of considerable academic and industrial research with respect to overcoming the scale-up problem of conventional axisymmetric reactors [2]. Conventional axisymmetric spouted beds can be distinguished according to conical–cylindrical and entirely conical beds. For a conical apparatus the static bed heights within the cone section are used. Analogously, we term this slot-rectangular configuration as a prismatic spouted bed, since the used height of the static beds is usually lower than the height of the prismatic regions. A specific feature of the apparatus is the flexible gas inlet, which is implemented as two horizontal slits and the gas is deflected in the vertical direction by a central profile (Fig. 1a). The gas inlet area can be adjusted by rotation of the gas throttle shafts, which changes the height of the slits. This allows for some flexibility in finding of the appropriate inlet size for optimum spouting conditions for different bed materials and bed masses. Furthermore clogging of the inlet by particles and a creation of dead zones can often be eliminated without interrupting the process. Moreover, the apparatus can be comfortably filled with the bed material keeping the slits closed. The apparatus is operated by underpressure, i.e. the gas is sucked through the bed. This concept was adopted by industry and applied as laboratory and large scale plants for spray granulation, particle agglomeration, coating, encapsulation and drying (ProCell spouted bed technology, [3]). In practice a scale-up of the system is usually realized by extending the depth of the bed β (y-direction in Fig. 1), which can optionally be combined with partitioning of the apparatus along the depth.

As pointed out by Mathur and Epstein [4] for conventional axisymmetric spouted beds the occurrence of the spouting regime and the spouting stability depend on: (i) the particle bed height, (ii) solid properties, such as the particle size, size distribution and the interparticle friction, (iii) geometrical parameters, such as the inlet size, the column diameter and the cone angle, and (iv) the gas velocity. For a given apparatus geometry and particle properties the stable spouting region (if one exists) is limited on the one hand by the particle inventory (so-called minimum and maximum spoutable bed heights) and on the other hand the spouting appears only in a limited range of the gas velocity (minimum and maximum spouting velocities). In the previous experimental investigations, it was found that to achieve stable spouting conditions in this apparatus the static bed height should not exceed the height of the prismatic region [1]. The range of the ratio between the gas inflow area and apparatus cross-section at the static bed height, where the initiation of stable spouting in this apparatus is possible, was identified and correlated with the Archimedes number of particles. For lower or higher inlet-to-bed size ratios the unstable fluidization regimes were found and the stable spouting did not appear at all. A map describing this transition was provided, from which the gas velocity...
necessary for the onset of stable spouting (expressed as particle Reynolds number at the gas inlets) can be obtained depending on the inlet-to-bed size ratio and Archimedes number.

The gas flow rate has a pronounced influence on the spouting stability. For a given apparatus geometry and solid inventory, a range exists where spouting is initiated and remains more or less stable. If the gas velocity is further increased, spouting disappears, being replaced by a less stable regime. Depending on the particle properties and the static bed height this regime can be incoherent spouting, bubbling or slugging [4]. Thus the area of spouting is closed also from the gas velocity side and a domain of the stable dense spouting is formed. For the apparatus modelled in this work, Gryczka et al. [1] obtained quickly a growing process instability by increasing the gas flow rate. Thus this apparatus deserves a further optimization regarding the flow stability, to enlarge the stable spouting domain to higher gas velocities.

1.1. Pressure drop fluctuations

Besides visual observations the pressure drop fluctuations can be used for an identification of the existing flow regime in a spouted bed. Freitas et al. [5], Liu et al. [6], Chen [7], Piskova and Mörl [8] and others used a Fast Fourier Transform (FFT) of the pressure drop signal for the analysis of the flow regimes in rectangular spouted beds. Freitas et al. [5] report a well-defined dominant frequency between 5 and 7.5 Hz as a characteristic attribute for the dense spouting regime in a slot-rectangular bed with one vertical gas inlet. In the previous study on this apparatus geometry by Gryczka et al. [1], the stable dense spouting was also correlated with a narrow peak in the frequency domain with a characteristic frequency of about 6 Hz. The occurrence of further pronounced peaks at different frequencies was attributed to instabilities. Leu and Pan [9] used the amplitude of the pressure drop fluctuations...
to identify the initiation of dilute spouting in a conical spouted bed. Besides statistical methods, several approaches based on the deterministic chaos theory were developed and applied for fluidized and spouted beds to extract the information about the bed behaviour hidden in the pressure fluctuations. Van der Bleek and Schouten proposed to use the deterministic chaos theory for the design and operation of fluidized beds [10]. The correlation dimension and Kolmogorov entropy of a strange attractor reconstructed from the pressure time series were used to identify the flow regimes. It was shown that the information about the evolution of these properties with increasing of the gas velocity is applicable for the identification of points of the minimum fluidization and the onset of bubbling. It was also found that after the fluidization onset (sudden increase in the chaos order) some flow reorganisation (a disorder decrease) takes place. For the bubbling regime a pronouncedly chaotic behaviour was characteristic. Schouten et al. [11] developed a method to treat strange attractors obtained from time series corrupted by a noise. Likewise for spouted beds, the reconstructed attractors, mutual information, Lyapunov exponent and Hurst’s rescaled range analysis were used to identify the flow regimes [5,8,12].

1.2. Numerical investigations on spouted beds

Several research groups modelled different spouted bed configurations by using coupled CFD-DEM simulations, often termed as Discrete Particle Method (DPM) or Euler–Lagrange Method, e.g. [13–17]. The important advantage of DPM, where the movement and interactions of each individual particle are calculated, is that the bed dynamics can be analysed on the scale of the whole bed, in different regions of the apparatus and on the level of the individual particles. Furthermore, the values, such as the particle rotation, interparticle collision velocities and forces can be analysed, which are hardly accessible for measurements with non-intrusive techniques. Takeuchi et al. [14] pointed out the extreme difficulty in establishing stable spouting by using DPM, regardless of adjustments of particle diameter, gas velocity, and inlet-to-bed size ratio. The basic principles of DPM were described in detail and reviewed by Deen et al. [18]. An overview on numerical investigations on spouted beds can be found in [19]. For the investigated apparatus configuration, Gryczka et al. [20] and Jacob [21] reported 2D-CFD studies by using an Euler–Euler approach. The simulations were compared with experiments by means of the bed expansion and particle flow patterns, particle velocities obtained by the Particle Image Velocimetry (PIV), and the pressure drop signal. The continuum approach showed a high sensitivity to the used drag model. Very different bed expansions, flow structures, and pressure drop behaviour were simulated. However, no model was able to predict simultaneously the bed expansion, flow patterns and the pressure drop behaviour. Regarding all three criteria in combination, a reasonable resemblance was achieved by the oldest of the used drag correlations; however the bed expansion and velocities of particles in comparison with the PIV results were underpredicted. A 3D-CFD investigation (Euler–Euler-approach) was done by Gryczka et al. [22] to study the influence of the apparatus depth on the prevailing gas–solid hydrodynamics. An apparatus with the same plane geometry as investigated experimentally [1] and modelled in 2D [20,21], and a high extension in the depth direction was simulated. The simulations showed only minor differences in the flow structure, particle velocities and pressure drop behaviour along the apparatus depth.

The aim of this work was to investigate the hydrodynamics of this apparatus by variation of the gas inlet velocity in more detail with the main focus on the identification of the apparatus-specific mechanisms which terminate spouting. In the numerical part, the bed behaviour was characterized for a fixed particle bed mass and inlet size and the gas flow rate was varied beginning from the spouting initiation point towards the fully unstable flow regime at high gas velocities. The particle dynamics was resolved by the Discrete Particle Model to gain a deeper insight in the spouting event. The simulations were performed for the prototype apparatus geometry, described in [1]. For the comparison with experiment the apparatus was rebuilt. The particle dynamics, the frequency domain of the pressure fluctuations and the changes in chaotic properties occurring with increasing gas flow rate were studied. In the experimental investigations both the inlet-to-bed size ratio and the gas flow rate were varied.

2. Material and methods

A transparent spouted bed was installed (wall material Europlex® SDX, Evonik, Germany) to visually observe the particle motion. The particle flow patterns were recorded by means of a high-speed video camera (MotionPro Y4, Imaging Solutions, Germany). A flow chart of the experimental setup is shown in Fig. 1b. Air was sucked through the apparatus by an exhaust fan (SKG 420-2V, Elmo Ritschle, Germany). The air throughput was regulated by a frequency converter. The gas flow rate was calculated from the air velocity in the connecting pipe between the apparatus and the fan, measured by using an anemometer (E665, E + E Elektronik, Austria). The pressure drop was measured in the freeboard above the particle bed (Pos. 1 in Fig. 1a) by means of a high-speed differential pressure detector (PD-23/8666.1, Keller, Germany). The sensor was connected to a signal convertor and a data acquisition system, and the measured pressure drop fluctuations were analysed by using the Fast Fourier Transform (FFT) algorithm in Matlab. Nearly monosized spherical γ-Al₂O₃ particles with a mean diameter of 1.8 mm (Sasol, Germany, Fig. 1c) were used in experiment and ideally monosized particles were assumed in the simulations. A pressure sampling frequency of 1 kHz was used both in the experiments and in the simulations. The number of sample points used to obtain the frequency spectrum was determined by the FFT algorithm, which needs 2ⁿ data points (4,096 s corresponds to 2¹² sampling points). The experimental pressure signal was less smooth in comparison to simulations, due to the gas fluctuations produced by the sensor noise and by the fan. Therefore the signal length for the FFT was extended to 2¹³, which corresponds to a measurement period of 8.192 s. Since the FFT power is a quadratic function of the number of data points in the input, the spectrum was normalized by dividing it by the square of the signal length, as proposed by Link et al. [23]. For calculation of the correlation dimension and Kolmogorov entropy the method proposed in [10] was applied (KRCHAOS). In this method, the embedding time window is set equal to the average cycle time, and the time delay to 1/ IRC. This approach uses the so-called maximum likelihood estimation for the calculation of the correlation dimension and Kolmogorov entropy. A detailed description of the method can be found in [10,11,24]. In case of time series, corrupted by a noise, an alternative routine using a rescaled correlation integral can be applied. It was used for the noisy experimental data. The requirement that the number of sampling points per cycle time is in the range 50–200 was always fulfilled, both for the time series obtained in experiments and simulations. In most cases, this parameter was in the range between 120 and 170. For the analysis of the experimental time series, a signal length of 10,000 points was used. The time series were pre-cleaned by a low-pass filtering. The frequencies exceeding 100 Hz were removed. This is the value still exceeding the 10-fold of the dominant frequencies of the time series, obtained from frequency domain of the unfiltered data (Figs. 3–5), as suggested in [10].

3. Numerical model and simulation conditions

Fig. 1d shows the dimensions of the geometry used in the simulations. The commercial codes ANSYS Fluent 12.0.16 and EDEM 2.3.1 were used in conjunction to solve the fluid and the particle dynamics, respectively. The gas inlet areas were set as two velocity inlets and the outlet area on the apparatus top was defined as a pressure outlet with a gauge pressure of zero. Thus the model represents rather an apparatus
operated with compressed gas, than one operated by underpressure.
Under these boundary conditions, the simulated pressure drop fluctuations above the particle bed have the smallest amplitudes. The maximum overpressure is located in the slits (Pos. 2 in Fig. 1a), where this was recorded during the simulations. The pressure drops over the entire particle bed were obtained in this way both in the experiments and in the simulations. Each time, the simulations started from a fixed bed state with a bed mass of 0.75 kg. All particles were randomly generated in a domain in the bottom part of the apparatus, settled under the influence of the gravity on a fictitious plate placed above the gas inlets until the particle velocities were close to zero. Subsequently, the particles were completely decelerated, the plate was removed, and the gas was introduced into the bed. The gas flow rate was increased in discrete steps with increments of 0.004 m³/s and time intervals of 0.01 s, respectively. For each gas flow rate a period of 7.096 s was simulated. However, to exclude start-up effects the bed dynamics were analysed only after 3 s.

A detailed introduction of the DPM can be found in [18]. Here, a short introduction is given and deviations from above reference are described in more detail. The geometry was meshed by means of the software GAMBIT 2.3.16. The RNG-κ-ε-model (RNG: Renormalization Group) proposed by Yakhot and Orszag [25] was used for the turbulence modelling because of a high gas streamline curvature in the apparatus inlet channels. The Semi-Implicit Method for Pressure-Linked Equations (SIMPLE) algorithm was applied to solve the volume-averaged Navier–Stokes equations (Eqs. (1), (2)).

\[
\frac{\partial}{\partial t} (\varepsilon g \rho g) + \nabla \cdot (\varepsilon g \rho g \mathbf{u}_g) = 0, \tag{1}
\]

\[
\frac{\partial}{\partial t} (\varepsilon g \rho g \mathbf{u}_g) + \nabla \cdot (\varepsilon g \rho g \mathbf{u}_g \mathbf{u}_g) = -\varepsilon g \nabla p_g - \nabla \cdot (\varepsilon g \mathbf{u}_g) - \mathbf{u}_g \cdot \nabla \varepsilon g + \varepsilon g \rho g \mathbf{g}. \tag{2}
\]

where \(\varepsilon g, \rho g, \mathbf{u}_g\) and \(\mathbf{u}_g\) are the volume fraction, density, pressure and velocity of the gas phase, respectively. \(\mathbf{g}\) denotes the gas phase stress tensor and \(\mathbf{g}\) the gravity. The reaction forces resulting from the drag forces \(F_d\) on particles affect the gas phase. The momentum sink term \(S_p\) in Eq. (2) considers this influence:

\[
\mathbf{S}_p = \frac{1}{V_{cell}} \sum_i \mathbf{R}_{di} = \frac{1}{V_{cell}} \sum_i \frac{V_i}{V_{cell}} \mathbf{R}_{di}, \tag{3}
\]

with \(\mathbf{R}_{di} = \mathbf{u}_i - \mathbf{v}_i\).

\(V_{cell}\) is the volume of the corresponding CFD cell. \(V_i\) and \(\mathbf{v}_i\) are the particle volume and velocity. The inter-phase momentum transfer coefficient \(\beta\) is calculated by means of the widely used combined Ergun and Wen & Yu drag correlations [26,27], as proposed by Gidaspow [28]. The gas volume fraction \(\varepsilon g\) in CFD cells was calculated as [29]:

\[
\varepsilon_{g, cell} = 1 - \frac{1}{V_{cell}} \sum_i x_i \mathbf{V}_i, \tag{4}
\]

where \(x_i\) is the volumetric fraction of the particle \(i\) in the corresponding cell.

This method is well applicable when the cell volume is larger than the particle volume, but causes numerical instabilities in CFD solver, if a particle approaches the cell volume [23]. However, to approximate the complex geometry of the apparatus bottom and to resolve the gas dynamics in this area with high gas velocity gradients, a fine computational mesh is advantageous. Since usually no particles reside in the inlets’ area, a gradually increasing mesh size was used, starting from fine cells in the inlet area and larger ones in the freeboard and the outlet regions. An unstructured mesh was used because of the complex geometry of the bottom part. The minimum and maximum size of the cells and the used CFD time steps are given in Table 1. Nevertheless, several times the solution diverged, due to an unfavourable configuration in the particle positions. The problem could be solved by rewinding the simulation to the previous saving step, increasing the resolution of the particle contours and setting the CFD time step temporarily to a smaller value of \(10^{-5}\) s.

The particle dynamics are calculated by Newton’s and Euler’s equations (Eqs. (5), (6)). Forces due to the pressure gradient, drag, gravity, shear lift, particle–particle and particle–wall collisions are included, respectively:

\[
m_i \frac{d\mathbf{v}_i}{dt} = -\nabla \mathbf{p}_g + \frac{V_i}{1 - \varepsilon_g} \mathbf{v}_rel + m_i \mathbf{g} + \mathbf{T}_d + \mathbf{f}_c, \tag{5}
\]

where \(m_i\) is the mass of the particle \(i\).

\[
I_i \frac{d\omega_i}{dt} = \mathbf{T}_i, \tag{6}
\]

where \(I_i\) is the momentum of inertia, \(\omega_i\) the angular velocity of particle \(i\) and \(\mathbf{T}_i\) the torque. The shear lift force \(F_{sl}\) is calculated as:

\[
\mathbf{T}_d = 1.61 C_d \frac{1}{2} \rho \mathbf{u}_g^2 \left( \frac{\mathbf{V}_i}{|\mathbf{v}_rel|} \right)^{0.5} \mathbf{v}_rel \times \mathbf{u}_i, \quad \text{for} \quad 0.005 \leq \beta_L \leq 0.4 \tag{7}
\]

where

\[
\beta_L = 0.5 \frac{Re_s}{Re_p}, \quad \text{with} \quad Re_s = \frac{|d\mathbf{u}_g/dy| |d^2\mathbf{v}_i}{\mathbf{g}}, \quad Re_p = \frac{|\mathbf{v}_rel|}{\mathbf{g}}, \quad \mathbf{v}_rel = \nabla \times \mathbf{u}_i,
\]

\[
C_d = \begin{cases} 
1 - 0.3314 \beta_L^{0.5} \exp \left( - \frac{Re_p}{10} \right) + 0.3314 \beta_L^{0.5}, & \text{for} \quad Re_p \leq 40 \\
0.0524 \left( \beta_L Re_p \right)^{0.5}, & \text{for} \quad Re_p > 40
\end{cases}
\]
A soft sphere contact model [32] based on correlations of Hertz [33], Mindlin [34], and Tsuji [35] was applied. The forces acting on the contact partners \( i \) and \( j \) (Eqs. (9) and (10)) consist of the elastic and inelastic (damping) components and the tangential force is limited by static friction (Eq. (11)).

\[
\begin{align*}
F_{c,n} &= -k_n \delta_{n,ij} - \eta_n \dot{\delta}_{n,ij} - n_{d,n} \ddot{\delta}_{n,ij} \\
F_{c,t} &= -k_t \delta_{t,ij} - \eta_t \dot{\delta}_{t,ij} - n_{d,t} \ddot{\delta}_{t,ij} \\
F_{c} &= -\mu_i |F_{c,n}| \dot{\delta}_{ij}, \quad \text{for} \quad |F_{c,t}| \leq |\mu_i| F_{c,n},
\end{align*}
\]

where \( \mu_i \) is the coefficient of the static friction. The stiffnesses \( k_n \) and \( k_t \) are functions of the elastic and shear moduli \( E_n, E_t \) and \( G_n, G_t \) as well as the radii \( R_n, R_t \) of contact partners:

\[
\begin{align*}
k_n &= \frac{4}{3} E_n \sqrt{R_n} \\
k_t &= 8 G_t \sqrt{R_t} \delta_{n,ij}
\end{align*}
\]

The contact force is the sum of the normal and tangential components:

\[
F_c = F_{c,n} + F_{c,t}.
\]

There is little information about the composition and properties of the layer material; therefore the wall properties as well as frictional properties were estimated. An overview of the used parameters and settings is given in Table 1.

4. Results and discussion

4.1. Dense flow regimes

In a dense stable regime spouted beds show a structured particle flow with three distinct regions: (i) the dilute spout, where particles move upwards, (ii) the fountain region, where the change of particle flow direction occurs, and (iii) the dense annulus, where particles flow downwards under the influence of the gravity (Fig. 1a). Furthermore, depending on the amount of particles in the apparatus and the superficial gas velocity, the dense and the dilute stable spouting regimes can be distinguished [38]. For the simulated operational conditions the investigated spouted bed behaves as a dense system. In this case the gas flow is highly influenced by the particles and pronounced fluctuations in the particle and gas dynamics can be observed (Figs. 3–5, 9b, 10 and 12). Following flow regimes were observed beginning from the fixed bed state:

(a) **Fixed bed and internal cavity:** The bed remains completely static up to a gas flow rate of about 0.007 \( \text{m}^3/\text{s} \). The pressure drop signal and the FFT power plot shown in Fig. 2 correspond to a gas flow rate of 0.006 \( \text{m}^3/\text{s} \). The measured fluctuations have no regularity and very small amplitudes, which results in a value of the FFT power smaller than 4 Pa\(^2\). This power level is within the level of the sensor noise. At gas flow rates higher than 0.007 \( \text{m}^3/\text{s} \), a small cavity with an internal circulation of a small number of particles is forming above the gas inlet. The cavity formation does not influence the pressure drop behaviour significantly.

(b) **Irregular bubbling:** At a gas flow of about 0.009 \( \text{m}^3/\text{s} \), the cavity forms the first bubble, which is able to ascend through the particle bed. With further increasing of the gas flow rate no qualitative changes in the bed dynamics can be observed: bubbles of different sizes pass through the bed at different time intervals, which results in an irregular pressure drop behaviour (different amplitudes of fluctuations occurring at different time intervals). In Fig. 3 the typical pressure drop behaviour and the corresponding FFT power plots for this gas flow rate interval are shown. The non-regularities in the pressure drop fluctuations also become noticeable in a broad distribution of the FFT power spectrum. With increasing gas flow rate the regularity of the pressure signal grows and the power functions become narrower. Fig. 6 shows the evolution of the chaotic properties as function of the gas flow rate. The correlation dimension provides for some evidence about the complexity of a dynamic system and the Kolmogorov entropy describes the predictability of the system behaviour with time. For a completely ordered system the Kolmogorov entropy is equal to zero and for a completely stochastic system it goes to infinity. Values between both extrema characterize a deterministic chaos. An introduction in the deterministic chaos theory and its application for fluidized bed design and operation can be found in [10]. High values of the correlation dimension and the Kolmogorov entropy in this range of the gas flow rate indicate very chaotic bed behaviour. However with increasing gas flow rate, the system behaviour becomes less chaotic, which results in a strong decrease in the correlation dimension and Kolmogorov entropy (Fig. 6). The estimated values of the correlation dimension for the area of irregular bubbling are in the range of 3–5 (slightly higher than the values of 3–4 reported in [10,11] for fluidized beds). The main fluctuations’ frequency within this interval is 3–4 Hz.
Dense spouting: At gas flow rates exceeding 0.015 m$^3$/s a spouting is established. The photographs taken of this operational point, the corresponding pressure drop signal and the FFT power plots are presented in Fig. 4. The gas fluctuations show nearly the same amplitudes and frequencies, which results in single narrow peaks in the FFT power plots. The gas flow rate, at which the regular periodical pressure drop signal first time occurs, corresponds according to Gryczka et al. [1] to the point of the initiation of the stable spouting. This is some kind of the minimum spouting velocity determined in a procedure based on the behaviour of the pressure drop fluctuations under conditions of the increasing gas velocity. The system becomes significantly less chaotic than in the previous regime. When the gas flow rate is further increased, the pressure fluctuations remain regular for a while. In the spouting area the Kolmogorov entropy and the correlation dimension have the smallest values (Fig. 6); the state is quite ordered and (at least to some extent) predictable. The spouting is not completely steady-state because of the bed fluctuations, but similar flow patterns are reproduced with time. However, at a certain point, slight alternating spout oscillation to the left and to the right from the central axis arises, which grows in intensity with the gas flow rate, as also reported by Gryczka et al. in [1]. This can be recognized visually (Fig. 4), for example for a gas flow rate of 0.023 m$^3$/s, which is close to the upper limit of this regime (a point between this air flow rate and 0.026 m$^3$/s, the first pressure drop shown in Fig. 5). The increase in the correlation dimension and Kolmogorov entropy with increasing of the gas flow rate shows an increase in the system complexity and growing disorder in the bed behaviour (Fig. 6). The main frequency of the pressure fluctuations in this interval is about 6 Hz.

Instable region: In this regime, the abovementioned spout oscillations reach a high intensity. The particle flow is less structured and shows random events such as spontaneous changes in the expansion of the particle bed, as can be seen in Fig. 5. Due to the spout deflection, a large amount of the bed material can be accumulated from time to time on one side of the apparatus and the main gas flow passes through the apparatus on the opposite side. In Fig. 5 the corresponding pressure drop behaviour and FFT power plots are also shown. The instabilities can be recognized in the pressure drop signal by irregular fluctuations with different amplitudes and frequencies, which become apparent in additional random peaks of a smaller magnitude in the FFT power spectrum. The main frequency is about 7 Hz. The flow structure of a spouted bed with regular circulating patterns is terminated. Higher values of the correlation dimension and Kolmogorov entropy in this region show a disorder increase (high flow complexity and a loss in the system predictability). However, these values continue to grow only in the first part of this region and show a tendency to decrease at the highest of used gas flow rates (Fig. 6). This indicates the onset of a second reorganisation of the system, which will later result in the second stable regime of a spouted bed (dilute spouting), occurring at high air flow rates. More information about the dilute stable regime can be found in Section 4.3 (Regime map).

As one can see in Figs. 2–5 by comparison of the FFT power plots, the transformations between regimes proceed quite continuously. The domain of stable dense spouting can be characterized as the area with a strongly reduced order of the deterministic chaos (Fig. 6).
4.2. DPM simulations

The simulations were performed for gas flow rates corresponding to:

• Case 1, the minimum spouting velocity (0.015 m$^3$/s),
• Case 2, a gas velocity close to the upper limit of the dense spouting range (0.023 m$^3$/s), a regime with a vigorous but yet quite stable spouting, as a preferable regime for practical applications such as coating,
• Case 3, the instable regime (0.032 m$^3$/s).

4.2.1. Particle flow patterns

Figs. 4 and 5 show the instantaneous particle flow patterns, captured from the experiments and the corresponding simulations with time.

Fig. 4. Pressure drop and bed behaviour for the dense spouting regime at different gas flow rates: Left: pressure time series and FFT power plots; Right: snapshots obtained from experiments and simulations in time interval of 0.1 s. The colour bars represent the vertical particle velocity.
intervals of 0.1 s. The bed fluctuates in accordance with the pressure drop. The simulation results for Cases 1 and 2 are in very good agreement with the experimental results. For Case 3 the bed expansion is highly irregular and therefore difficult to compare. It seems to be slightly under predicted by the simulation in the average. The increase of the alternating spout oscillation with the gas flow rate is well predicted by the model. The irregular bed expansion and heavy spout deflections in the instable regime (Fig. 5) are also in a good agreement.

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**Fig. 5.** Pressure drop and bed behaviour in the instable region at different gas flow rates: The snapshots were obtained from the experiment and the simulation in the time interval of 0.1 s. The colour bars represent the vertical particle velocity.

**Fig. 6.** Correlation dimension and Kolmogorov entropy as function of the gas flow rate. Crosses indicate the simulated Cases 1, 2 and 3 (from left to right).
4.2.2. Gas dynamics

The simulations were performed with four-way coupling, which includes the reaction forces of the particles on the gas phase. This allows for an analysis of the gas dynamics in the spouted bed. Figs. 4 and 5 show also the evolutions of the gas pressure drop plotted versus simulation time for three simulated gas flow rates, in comparison with the corresponding experiments.

Case 1, minimum spouting velocity (0.015 m³/s). After the start-up time, regular pressure fluctuations were obtained in the simulation (Fig. 4, Case 1), just as in the corresponding experiment. The pressure fluctuations result in a clean sharp peak in the FFT power spectrum. The obtained frequency of the fluctuations is slightly higher compared to the experiment.

Case 2, the upper range of the stable spouting domain. The simulated fluctuations produce a clean sharp peak in the FFT plot. The frequency of the pressure fluctuations is in a good agreement with the experiment (Fig. 4, Case 2).

Case 3, instable regime. Fig. 5, Case 3 shows the pressure drop time series from the simulation of the gas flow rate of 0.032 m³/s. The simulated pressure fluctuations are as highly irregular as in the corresponding experiment shown in the same figure. This results in the appearance of additional random peaks in the FFT power plot.

In general, the simulated pressure drop behaviour and the main frequencies of the pressure fluctuations are in accordance with the experiments. The predicted magnitude of the pressure fluctuations is slightly higher in the simulations than in the experiments. Although the pressure drop over the entire bed was analysed both in the experiment and in the simulation (as described in the chapter “Material and methods”), the fluctuations were measured at different locations, which may cause this deviation. A comparison of the values of the correlation dimension and Kolmogorov entropy can be seen in Fig. 6. A growth in the value of the Kolmogorov entropy indicates a loss in the predictability and an increase in system disorder with the air flow rate, as in the corresponding experiments. The correlation dimensions show a good agreement for Cases 1 and 2, but indicates that the simulated instable regime at 0.032 m³/s (Case 3) possesses a more complex flow behaviour than in the experiment.

4.2.3. Particle dynamics

In this section, the particle dynamics will be described on the entire bed scale (the influence of the apparatus depth and of the gas flow rate on the particle dynamics and flow stability), as well as locally for three distinct regions of the spouted bed (spout, fountain and annulus) that essentially differ in the particle flow.

4.2.3.1. Influence of the apparatus depth. In this study true three-dimensional behaviour could be proven also for this configuration of a slot-rectangular apparatus. In the industrial practice with this apparatus configuration, a process is designed empirically by performing experiments on small lab scale beds. Initially, process feasibility and parameter studies are done by using apparatuses with small depths (usually $\beta = 200$ mm) followed by a small number of experiments on large scale plants with the same apparatus width $\alpha$ and an increased depth (width to depth ratios $\alpha/\beta \leq 0.25$) for finding the best process parameters. The prototype investigated by Gryczka et al. experimentally and by means of Euler–Euler model [1,20], has a depth of 100 mm ($\alpha/\beta = 2.5$). In [20], a 2D behaviour of the particle bed was assumed and particle velocities measured by means of Particle Image Velocimetry (PIV) were applied for the comparisons with a 2D model. However, this apparatus has a depth that is larger than usual for pseudo-2D beds [e.g. 15,17,23,29]. In this 3D-DPM investigation the bed dynamics in the third dimension could be analysed as well. Due to the fluctuating bed behaviour, the time averaged particle data are used. Fig. 7a shows the bed expansion (vertical position of particles) and the corresponding particle velocities are plotted in Fig. 7b. Both of them were time-averaged within slices of 5 mm thickness along the depth direction. At the lowest of the applied gas flow rates, both the bed height and the particle velocities are higher in the vicinity of the front wall. With increasing gas flow rate, the bed expansion is higher in the vicinity of both vertical walls forming a “valley” in the apparatus middle. A very similar behaviour was found experimentally by Freitas et al. [39] for slot-rectangular spouted beds with one vertical gas inlet and an apparatus depth $\beta$ in the range of $29–100$ mm ($\alpha/\beta$ varied in the range of 1.5...5). They termed this as multiple spouting (MS). Chen [7] investigated experimentally several configurations of slot-rectangular spouted beds and also sketched this effect qualitatively. The height of both fountains can be different, which was also observed in experiments. This is also in accordance with

![Fig. 7. Behaviour of the particle bed in the direction of the apparatus depth. (a) Bed expansion (time-averaged vertical positions of particles), (b) time-averaged particle velocities. The error bars are standard deviations.](image-url)
the experimental results by Freitas et al. [39] and Chen [7] for slot-rectangular beds. A probable explanation for this phenomenon is that the gas forms spouting channels in the particle bed, which are quite stable due to the influence of interparticle friction in the peripheral dense annulus area. These can have different cross-sections, due to the initial random packing structure of the fixed bed. The effect is smaller at the highest of the investigated gas flow rates (Fig. 7), because the entire bed structure is more aerated by gas. Thus, the discrepancy between 2D simulations and PIV measurements reported in [20] (under-predicted bed expansion and particle velocities) can be probably explained with the help of a 3D simulation, since the bed expansion and the particle velocities are higher in the vicinity of the vertical walls than in the centre of the apparatus, which does not appear in a 2D model. However, another 3D CFD study [22] carried out on this apparatus to investigate the influence of the third dimension, by means of a model with a significantly higher depth of 400 mm ($\alpha/\beta = 0.625$), showed only minor variations in the bed height, particle velocities and pressure behaviour along the depth direction. Therefore it was assumed, that the influence of the depth dimension on the flow structure is quite low and that the particle dynamics in this apparatus can be assumed to be independent on the depth [22,40]. However, this DPM study shows that this is not always the case and a low distance between vertical walls can cause three-dimensional behaviour (at least in dense regimes). In summary, this has the following consequences:

(i) The apparatus cannot be simulated with a 2D method,
(ii) PIV is not sufficient for a complete characterization, since only the information about the bed behaviour in areas next to the vertical walls is provided,
(iii) The depth of the model used in this study ($\beta/d_p < 55.6$) is probably too small to be sufficient to predict the bed behaviour in industrial scale plants, up-scaled by a simple extension of this dimension. In investigation of Freitas et al. [39] the bed depth was varied in the range 29–100 mm. They found that 3D behaviour was accompanied by a change in the minimum spouting velocity with the apparatus depth. The minimum spouting velocity was found to grow if the vertical walls become closer to each other (and vice versa). There is no reason to assume that the apparatus depth used in this study (100 mm) is sufficient and the trend of a decreasing in the minimum spouting velocity with the bed depth will not continue for a while.

The influence of the vertical walls on the particle dynamics is high in apparatuses of a small depth and it does not consist of only the effect of (at least in dense regimes). In summary, this has following consequences: the wall. Therefore it was assumed, that the in

\[ \frac{\text{particle trajectories in the spout region follow the gas flow. Some dependence of the gas flow profile on the distance between walls exists already in the fixed bed state. The presence of the walls locally influences the bed packing structure. Schwartz and Smith investigated the gas flow through a fixed particle packing in a pipe [41]. The reduced gas velocity above the central area of the bed and a velocity maximum at the distance of about one particle diameter from the wall were found, with a difference up to 100%. The flow channels at a wall are larger simply from geometrical considerations and thus the near-wall area offers a lower resistance for the gas flow than the central region. The location of the velocity maximum was found to be virtually independent on the bed diameter (about one particle diameter from the wall). The effect decreases for larger bed diameters. It was proven that a larger pipe diameter (the distance between “walls”) results in a more uniform distribution of the gas velocity. For ratios of the pipe to the particle diameters more than 30, the deviation from a uniform flow profile was less than 20%. This gas flow profile through the fixed bed may explain the initiation of the observed 3D bed behaviour by an increasing

Fig. 8. Time-averaged distribution of the particles in the spout region in the direction of the apparatus depth.

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(iv) The shear lift. The shear lift may also have an effect on the establishing of a gap with the reduced particle concentration in the wall vicinity. Due to the gas velocity gradient at the wall surface, also a particle moving parallel to the wall will be pushed away. However the shear lift did not cause this 3D behaviour and was not a dominant effect. After the “main” simulation of Case 2, the calculation was continued for 2 additional seconds without using this model part (Eq. (7)). After this simulation period, the 3D behaviour did not disappear nor markedly reduced.

The upward motion of a small number of particles being in a long term contact with vertical walls takes place by rolling and sliding, and therefore the vertical velocity of these particles is lower due to a deceleration by the particle-wall friction. This is probably the reason for some particle accumulation and a slight anew increase in particle concentration directly at the walls (Fig. 8).

4.2.3.2. Influence of the gas flow rate. In this sub-section, the influence of the gas flow rate on the particle dynamics and flow stability will be described.

4.2.3.2.1. Particle dynamics. Fig. 9a shows the evolution of translational and angular particle velocities, time-averaged over the entire particle bed and plotted against the applied gas flow rates. The simulation showed that both the particle velocities and the rotation in apparatus increase slightly non-linearly with the gas flow rate and can be fitted with a quadratic or logarithmic function (see the inserted quadratic fits). The quite detailed and thus computationally expensive model used in this work predicts average particle rotation in range of 30–90 rad/s. In terms of the kinetic energy, the contribution of the particle rotation is rather low (the percentage in the total kinetic energy is 3.6% for 0.015 m³/s, 1.2% for 0.023 m³/s, and 1% for 0.032 m³/s). Recently, Pepiot and Desjardins [43] and Jajcevic et al. [44] neglected the particle rotation in DPM to simulate fluidized and spout-fluidized beds with a large particle number and nevertheless found a good agreement with experiment. This seems to be a plausible simplification. However, sometimes the information about the tangential contact forces and the particle rotation is of importance for understanding of a process and can assist for an advanced apparatus designing. For instance in case of a coating process, a high particle rotation in the spray zone of the apparatus contributes to an enhanced distribution and spreading of the liquid on the particle surface and thus to a more homogeneous coatings. The tangential force contributes to the breakage of agglomerates.

4.2.3.2.2. Flow stability. In general, the representation of the particle velocity as the mean and standard deviation over the entire particle bed is quite crude, particularly in case of a spouted bed. Due to the slow downwards motion of high number of particles (annulus area) and high upwards velocity in the lower loaded spout the particle velocity shows a non-symmetrical density distribution. Under steady-state spouting conditions, the shape and the location of this distribution should be nearly constant with time and can be well fitted by a skewed probability density function (pdf), e.g. the Gumbel function used in [40]. Chen [7] considered a steady-state, symmetrical spouting with minimal fluctuations as an ideal (most stable) case for slot-rectangular spouted beds. In case of very strong spout pulsations the spouting is often termed as incoherent [42]. Under dense spouting conditions simulated in this work the location and the shape of (still skewed) pdf-curves are progressively not constant with time due to the growing amplitude of the fluctuations with gas flow rate. Therefore in the next sub-section the particle dynamics was characterized more locally for one of the simulated cases. Fig. 9b shows the evolution of the bed expansion with increasing gas flow rate. This increase is accompanied by a growth in the amplitude of the bed fluctuations. With increasing of the gas flow rate, the spouting stability is affected not only by the alternating spout deflection but also by a decrease in the flow coherence.

4.2.3.3. Local particle dynamics (Case 2). This case can be distinguished by a satisfactorily structured vigorous spouting, whereas Case 1 shows a structured particle flow, but a very slow particle motion and therefore it is less interesting for a practical application. The particle flow patterns at the high gas flow rate in Case 3 are highly unstructured and the three spouted bed regions (annulus, fountain and spout) can hardly be distinguished for a separate analysis.

In Case 2, as mentioned above, the deviations from the ideally steady-state spouting are the pronounced fluctuations of both spouts (cluster-wise particle transport) and the alternating deflections from the vertical axis, as can be seen by means of simulation snapshots in Fig. 4. The spouts fluctuate periodically not only in the vertical, but also in the lateral direction from fully developed state to a shape

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Fig. 9. Overall trends. (a) Average particle velocity and angular velocity magnitudes in dependence on the gas flow rate, (b) bed expansion (average vertical position of particles in bed) in dependence on the gas flow rate. The error bars are standard deviations.
constricted above the central profile. Fig. 10 shows the event of a single spout pulsation by means of simulation snapshots and the corresponding evolution of the slit pressure. In the middle snapshot the spout is partially choked; the sudden change in the cross-section is the origin of a fluctuation in the gas velocity and pressure. Gryczka et al. [1] interpreted the regular pressure fluctuations as an effect of “bubbles” of nearly equal size ascending through the particle bed and bursting on the bed surface in regular time intervals, and Freitas et al. [39] for a slot-rectangular bed with one vertical gas inlet as oscillations in the spout diameter. The latter can be confirmed. Actually, a spouting state presupposes the existence of a more or less continuous spout. Bubbles can be observed in the area of irregular bubbling, prior to the dense spouting (Section 4.1), because the gas velocity is not sufficient to form spouts. Other cases, where this behaviour can be observed, are when a spouted bed is “overloaded” by particles, or it is used in dense regime with too fine ones. In these cases the spout is completely disrupted (chocked) by particles and the gas passes through the particle bed as well-formed bubbles.

Fig. 11a shows the average absolute and relative particle velocities for different spouted bed regions, separately. The relative (collision) velocity is about an order of magnitude smaller than the absolute velocity. The annulus is only slightly expanded (mean porosity of 43.3 ± 1.2%), compared to the porosity of 41.8% in the fixed bed state. The particles move as a bulk and are rather in long time contact than in a colliding state. Therefore the particle translational and angular velocities as well as the contact forces have a minimum in this bed zone: the averaged particle relative velocity is about 0.02 m/s, and the mean contact force of about 1 mN. At these intense operating conditions the fountain region plays an important role. The average amount of the particles permanently residing in both fountains is quite high (27% of all particles in the apparatus). The particle translational and angular velocities, as well as the contact forces achieve their maxima in this region (Fig. 11).

### 4.3. Regime map

The first reports about rectangular spouted beds with a tangential gas supply through a slit can be found in [45]. In our configuration, the gas is also introduced tangentially and the height of both slits can be varied by rotation of flatten cylinders (inclination towards the apparatus inner) in the range of 0–3.5 mm; this is virtually a variation from thin to very thin slits. The gas flow channels narrow along the gas flow direction and wider again. For a simplification the heights of both slots was summed to an actual inlet width. For the construction of a regime map this inlet width, the bed mass, and the gas velocities were varied. With increasing in the static bed height the instability due to the growing alternating spout deflections is only slightly reduced. However, simultaneously the incoherence level grows. The spout becomes more pulsating. This influence can be seen in Fig. 12 in the increasing of the amplitude of the pressure fluctuations, expressed as the standard deviation of the pressure time series. However, one can also extract from the shown diagrams, that the increase in incoherence with the bed height can be suppressed to some extent by the reduction of the inlet size. Thus, higher static beds can be spouted in a smoother manner. However, a higher pressure drop due to the apparatus geometry has to be accounted for. Fig. 13, right shows the regime map for the investigated particles, inlet heights $h$ in the range of 1–3.5 mm and the static bed heights, which do not exceed the prismatic apparatus part. As ordinate the particle Reynolds number in slits $Re_{p,in}$ (Eq. (16)) and as
The abscissa the ratio between the inlet width $2h$ and the static bed height $H_{st}$ (Eq. (17)) were used.

$$Re_{p,in} = \frac{v_{g,in} d_p}{\nu}$$  \hspace{1cm} (16)

$$H = \frac{2h}{H_{st}}.$$  \hspace{1cm} (17)

Note, the used two-dimensional inlet-to-bed size ratio has no connection to the apparatus depth and the illustrated map is valid only for the investigated apparatus depth of 100 mm. As mentioned above, some shift of the transition lines between regimes with an increasing of the apparatus depth cannot be excluded. Therefore, for a more general description, additional dimensionless groups considering this influence are necessary and for the graphical representation a 3D map seems to be reasonable, where the changes in dependence on the used apparatus depth can be traced.

The main goal of this diagram is to show the location of the stable operating window. As described in the numerical part, the stable dense regime is the spouting of MS-type, described previously by Freitas et al. [39] for slot-rectangular beds with one vertical gas inlet. The particle Reynolds number is nearly inversely proportional to the used inlet-to-bed size ratio for the initiation of the dense spouting ($Re_{p,in} \approx H^{-0.987}$, the line AB in Fig. 13). It is remarkable, that this dependence is comparable to the prevalent conditions in axisymmetric spouted beds, whereas the entirely conical beds should be referred,
because the static bed height $H_s$ in both configurations is always located within the prismatic/cone sections. An overview of the dimensionless equations describing the spouting initiation in different conical beds can be found in [46]. It can be seen from equations using the static bed height in the inlet-to-bed size ratio, that the initiation of the dense spouting occurs at $Re_{in} = (D / H_s)^{-1.25... - 0.82} (D$ is the inlet diameter). All states within the operational window of the dense spouting feature quite regular periodical pressure drop behaviour, but differ slightly in the level of incoherence, in dependence on the inlet-to-bed size ratio and the gas velocity. For the investigated range of the static bed height the spout deflection seems to have the dominating effect on the spout termination, particularly at low and intermediate static bed heights. The boundary between the irregular bubbling regime and the instable region for shallow beds is difficult to recognize both by the visual observations and the pressure drop behaviour, it is shown as a dashed line. In principle, it should be possible to suppress both instability sources, the oscillations in the spout diameter and alternating spout deflections, by an introduction of appropriately designed and positioned draft plates. Furthermore, the 3D behaviour should be influenced by introduction of additional vertical walls. On this way, the spout region is surrounded by vertical wall from all sides.

At high gas velocities the second stable flow regime, which was not reported by Gryczka et al. [1], the dilute or jet spouting was ascertained. The regime can also be identified by means of the pressure drop signal. This flow type can be characterized as a uniform and continuous entrainment of particles coming down in a very thin (but at this prismatic angle still present) annulus. Although, the particles are highly dispersed in the apparatus, the spout (from visual observations it seems to be a single jet) can be clearly distinguished (Fig. 13, left). No oscillations or deflections of the jet can be observed. The achieving of this spouting state can be recognized in the frequency domain by the absence of other peaks than measured in the apparatus in the corresponding interval of the air flow rates. Fig. 13, left shows the FFT power spectrum measured in the area of dilute spouting (0.040 m$^3$/s). Contrary to the pressure signal measured in the foregoing instable region (0.032 m$^3$/s), the pressure drop in this regime shows no fluctuations, which can be distinguished from the noise measured in the apparatus without any particles. This regime can be used for low to intermediate bed masses in large apparatuses, because of the increased risk of the solid elutriation. The dilute spouting also provides for a possibility for a stable spouting of very fine particles. Recently, we report the using of this regime in an apparatus with a prismatic process chamber and a very large freeboard for a granulation of µm-sized pre-structured and entirely ceramic particles with the aim of a synthesis of novel composite materials [47,48].

5. Conclusions and outlook

In this work, the gas–solid hydrodynamics of a prismatic spouted bed with two horizontal gas inlets was systematically investigated in experiments and by means of coupled CFD-DEM simulations. Initially the bed behaviour for the modelled particle type, bed mass and range of the gas flow rate was characterized experimentally by means of high speed recordings and the FFT of the measured pressure drop signals. Different dense operational regimes (the fixed bed and internal cavity, irregular bubbling, dense spouting and the instable region) could be identified. The hydrodynamic regimes differ also significantly in the chaotic properties. For the domain of the dense spouting a decrease in the system disorder was found to be characteristic, whereas bed behaviour at the lower and higher gas velocities was very chaotic. Simulations were performed at the gas flow rate corresponding to the onset of spouting (minimum spouting velocity), as well as the flow rates corresponding to the upper end of the spouting domain and to the instable region. The simulations satisfactorily predict the particle flow patterns, the expansion of the particle bed and characteristic pressure drop fluctuations of all studied regimes in the spouted bed. Single sharp peaks in the FFT power plots, characteristic to the dense spouting, were obtained, with a good agreement in the frequency of the pressure fluctuations. The irregular pressure behaviour resulting in many additional peaks in FFT plots were also predicted accurately by the DPM model. The comparison of chaotic properties showed a good agreement with experiments for the area of the dense spouting and a higher complexity of the simulated instable regime. The evolution of the particle dynamics with increasing gas flow rate was investigated at the entire bed level. A three-dimensional behaviour of the particle bed in apparatus was found for all three simulated cases. The average bed height and the particle velocities are increased in the vicinity of the vertical walls, which is a typical behaviour reported in literature for slot-rectangular beds on the basis of experiments. One of the simulated regimes was also characterized regarding the particle micromechanics in apparatus regions with different particle dynamics, such as the annulus, fountain and spout. The mechanisms governing the spouting termination are the growing spout instability by an alternating deflection and the incoherence. The influence of the inlet-to-bed size ratio was investigated experimentally. A regime map was constructed, where the location of the domain of the dense spouting and the transition lines between other regimes can be obtained.

This work covers the first part of our investigations regarding the influence of the gas velocity on the behaviour of a prismatic spouted bed. The next part will contain the investigation on the contribution of the particle properties and of the prismatic angle. Furthermore, an optimization study, performed with the aim to enlarge the stable dense operational window to higher gas flow rates will be reported [45].

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References
