Graphical abstract:

Demonstration of simultaneous high-G-intensified gas-solids contact, gas-solids separation and segregation in a bi-disperse rotating fluidized bed in a vortex chamber by means of coupled discrete particle method – computational fluid dynamics simulations. Left: Gas entering through the tangential gas inlets slots and strong vortex in the near-chimney region; Right: Dense and uniform rotating fluidized bed of large/heavy particles against the cylindrical wall and somewhat less dense and faster rotating fluidized bed of small/light particles radially more inward. Black tracer to visualize the flow path of gas injected via one of the slots.

Qualitative Numerical Study of Simultaneous High-G-Intensified Gas-Solids Contact, Separation and Segregation in a Bi-Disperse Rotating Fluidized Bed in a Vortex Chamber

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Abstract:

Coupled discrete particle method – computational fluid dynamics simulations are carried out to demonstrate the potential of combined high-G-intensified gas-solids contact, gas-solids separation and segregation in a rotating fluidized bed in a static vortex chamber. A case study with two distinct types of particles is focused on. When feeding solids using a standard solids inlet design, a dense and uniform rotating fluidized bed is formed, guaranteeing intense gas-solids contact. The presence of both types of particles near the chimney region reduces, however, the strength of the central vortex and is detrimental for separation and segregation. Optimization of the solids inlet design is required, as illustrated by stopping the solids feeding. High-G separation and segregation of the batch of particles is demonstrated, as the strength of the central vortex is restored. The flexibility with respect to the gas flow rate of the bed density and uniformity and of the gas-solids separation and segregation is demonstrated, a unique feature of vortex chamber generated rotating fluidized beds. With the particles considered in this case study, turbulent dispersion by large eddies in the gas phase is shown to have only a minor impact on the height of the inner bed of small/light particles.

Keywords: Fluidization, Process Intensification, Segregation, High-G, Vortex chamber.

1. Introduction

Vortex chambers have recently re-gained attention as efficient gas-solid contactors or reactors. In a vortex chamber, gas is injected tangentially via multiple slots and evacuated via a centrally positioned chimney. This leads to the formation of a free vortex in the chamber¹ and the chimney is sometimes referred to as vortex finder. When suspended in the rotational gas flow, particles cannot follow the gas due to their inertia and form a dense rotating fluidized bed against the outer cylindrical wall of the chamber. The particles experience two counteracting forces in the radial direction, the drag force by the gas flowing to the chimney and the (apparent) centrifugal force due to inertia. In certain cases the centrifugal force is dominant and the bed is radially nearly packed. Even then, it remains in a fluidized state. This was demonstrated by step response experiments with colored particles, showing efficient mixing, also radial, with a bed of mono-disperse particles.² In rotating fluidized beds in vortex chambers, in contrast with cyclones, the process gas is, while driving the particle bed rotational motion, continuously flowing through the bed at high velocity, resulting in efficient gas-solids contact, as explained in more detail hereafter. Characteristic for rotating fluidized beds in vortex chambers is also the flexibility with respect to the gas flow rate, the latter affecting the radial drag force and centrifugal force in similar ways.³

The centrifugal acceleration can be much stronger than earth gravity, operation referred to as high-G. The latter allows high gas-solid slip velocities and intensifying interfacial transfer of mass, momentum and energy through increased values of the coefficients of gas-solid mass (k_G), momentum (β) and heat (h_f) transfer, on a per m^2 interface basis. The intensification of interfacial momentum transfer and the flexibility with respect to the gas flow rate allow generating dense and more uniform fluidized beds at high slip velocities and fluidizing particles that cannot be easily fluidized in conventional fluidized beds, such as small/light cohesive Geldart C-type particles and large/heavy Geldart D-type particles. Dense and more uniform fluidized beds with reduced or no bubble formation are crucial for efficient gas-solids contact by increasing the specific interfacial surface area, a_v (m^2 interface per m^3 reactor), further intensifying interfacial transfers on a per m^3 reactor basis, as well as reactions. So taking as an example interfacial mass transfer with the amount of species A transferred between gas and particles per m^3 reactor and per second written as $k_G \cdot a_v \cdot (C_A - C_A^{s,s})$, where k_G is the coefficient of mass transfer in m^3 fluid per m^2 interface per second, high-G operation allows increasing both k_G and a_v . Application to drying of

granular materials, including biomass, was studied by Kochetov et al.,⁴ Volchkov et al.^{5,6} and Eliaers and De Wilde.⁷ Eliaers et al.⁸ numerically studied optimization of the vortex chamber dryer design to improve the product quality/uniformity and the air usage efficiency. Other applications of gas-solid rotating fluidized beds in vortex chambers studied include colloid core nuclear rockets,⁹ gas phase polymerization,¹⁰ fluid catalytic cracking (FCC),¹¹ biomass pyrolysis and gasification,¹² combustion processes,¹³ SO₂/NO_x adsorption from flue gas¹⁴ and low-temperature wet coating of cohesive particles.¹⁵ Use of vortex chambers with a liquid has also been considered.¹⁶

High-G operation in rotating fluidized beds in vortex chambers not only allows intensifying gas-solids contact, but also gas-solids separation and segregation. The latter and the combination of these features has not received much attention so far, but is of importance for specific potential applications, such as chemical looping combustion (CLC) of coal. In CLC, a typically metallic oxygen carrier is transported between an air reactor where the oxidation of the carrier takes place and a fuel reactor in which combustion of a hydrocarbon proceeds with the oxygen provided through the oxidized carrier.¹⁷ Different reactor technologies have been proposed and demonstrated, fluidized bed fuel reactor based¹⁸ and countercurrent moving bed fuel reactor based.¹⁹ Most of the research in the field of CLC focuses on the development of efficient and reliable oxygen carriers,²⁰ reaction kinetics²¹ and reactor and process design.^{19,22} Aspects that remain critical when converting coal are carrier-coal and carrier-ash separation. At the high temperatures encountered, magnetic separation is excluded. For the ash separation, ex-situ separation by elutriation is typically proposed, either from the reduction²³ or oxidation²⁴ zone. Little information is available on the separation efficiency and operational issues. Furthermore, conventional elutriation methods require a subsequent separation of the entrained particles from the conveying gas stream. In contrast, efficient segregation in a high-G rotating fluidized bed, with drains from distinct regions, could provide in-situ solids separation in one unit operation. No studies of segregation in rotating fluidized beds in vortex chambers have been reported so far. With mono-disperse particles, intense particle bed mixing in the radial and axial directions was observed.² In an experimental study of low-temperature wet coating of cohesive particles with limited agglomeration, however, no losses of coated particles were reported, whereas losses of (lighter) uncoated particles through the chimney were observed,¹⁵ giving a clear indication segregation takes place.

In the present paper, the possibility of using a rotating fluidized bed in a vortex chamber as a combined efficient gas-solids contactor, gas-solids separator and solids segregator is qualitatively studied by

means of discrete particle method – computational fluid dynamics (DPM-CFD) simulations. A case study with two distinct types of particles is focused on and operation with continuous solids feeding and with a batch of particles fed to the vortex chamber is considered to evaluate the influence of solids feeding using the standard solids inlet design on the particle bed density and uniformity and on the gas-solids separation and segregation. The flexibility with respect to the gas flow rate is addressed next, as well as a possible effect of large eddies on the particle trajectories. The simulation model and code are discussed next. Some preliminary design considerations and the simulation geometry and conditions are described thereafter.

2. Simulation model

A limited number of mono-disperse simulations of vortex chamber generated rotating fluidized beds have been reported. Comparing a conventional fluidized bed with a rotating fluidized bed in a vortex chamber, De Wilde and de Broqueville³ conducted a two-fluid model (TFM) study on the potential intensification of interfacial heat transfer. The very different range of operating conditions that could be used with the two technologies was stressed. Dutta et al.²⁵ used TFM-based CFD simulations to derive some guidelines for design and optimizing the operating conditions. Trujillo and De Wilde¹¹ carried out coupled reaction-flow simulations to evaluate the use of vortex chamber reactor technology for fluid catalytic cracking (FCC). A similar approach was taken by Ashcraft et al.¹⁴ for a process for simultaneous adsorption of SO₂ and NO_x (SNAP). TFM-type CFD models are, however, not sufficiently accurate to describe the crucial interfacial transfer of momentum taking place, in particular for cases where the size of the gas inlet slots is of the same order of magnitude as the size of particles. This may be necessary in order to generate a sufficiently strong centrifugal force, as described above, and is the case in the simulations presented. The discrete particle model (DPM) described hereafter, allows tracking the motion of each individual particle, including its own rotational motion, and collisions with other particles and walls. DPM simulations are computationally more expensive than TFM simulations, but efficient parallel computing algorithms and the availability of a supercomputer at NETL²⁶ today allows application to some practical cases as in this case study. The basic model equations are presented in Appendix I.

In this DPM approach, a constant time step is used to update the particle velocities through a first order integration scheme for Newton's law. The particle position is then updated based on its velocity. Fluid-coupled simulations essentially proceed in two parts. First, the continuum fluid equations, Eqs. (1) and

(2), are solved for a fluid time step, wherein the particles are at given positions with given velocities. The discrete particle simulation then follows, wherein the particles are advanced in time using Eqs. (5)–(7) until the time elapsed equals the fluid time step to calculate the corresponding particle positions and velocities. At this point, the fluid and particles are advanced to the same time and the process is repeated. The gas phase and particle velocities affect one another through the distribution of the gas phase pressure gradient over the phases and interphase momentum exchange, as shown in Appendix I. The continuum fluid equations are solved on a fixed (Eulerian) grid using a first order time integration scheme and both the first order upwind (FOU) and the second order superbee numerical schemes for the convective terms (see for example Syamlal and Benyahia²⁷). Using a second-order scheme leads to excessive calculation times, the fluid time step required for convergence being at least two orders of magnitude smaller than with a first-order scheme.

No turbulence models were included in this study. Turbulence in the gas phase was observed to have a relatively small effect on the behavior of heavily loaded gas-solids systems.²⁸ In such systems, the solids flow pattern, such as clusters and streamers, dictates the behavior of the gas and not vice-versa. The operating conditions shown in Table 1 are discussed later, but with the expected velocities, the particle Reynolds number, $Re_p = d_p \cdot u_{slip} \cdot \rho_g / \mu_g$, is around 180 for the large/heavy particles and 140 for the small/light particles, values typical for the beginning of the transition region between laminar and fully turbulent flow. For the large particles, the Stokes number based on the gas-solid contact time, that is, the gas phase residence time in a bed of thickness t_b , $St = \tau_p(\text{response}) \cdot u_{slip} / t_b$ with $\tau_p(\text{response}) = \rho_p \cdot d_p^2 / (18\mu_g)$, is larger than 10^3 . For the small particles, it is still somewhat larger than 10. Hence, the gas phase turbulence is expected to have a negligible effect on the motion of the large particles and only a limited effect on that of the small/light particles. Gas phase turbulence modulation by particles (Elgobashi³⁰) is neglected in this study. Only in a dilute particle bed or particle bed freeboard region, the presence of particles is expected to increase turbulence. The presented simulations apply refined spatial and temporal domain discretization that potentially allow resolving the most energetic large eddies in the gas flow and their effect on particle dispersion. Simulations were carried out using the NETL-developed MFI-X-DPM code (mfix.netl.doe.gov) and NETL's High Performance Computer (HPCEE).²⁶ Running on 256 cores, a simulation takes about one week when using a first-order upwind scheme for the gas phase convective terms. The DPM-CFD model and MFI-X-DPM code were previously described and validated – see Garg et al.³¹ and Benyahia and Galvin²⁹ and references therein.

3. Simulation geometry and operating conditions

Table 1 summarizes the vortex chamber dimensions, the operating conditions and the physical and numerical parameters used in the simulations. Figure 1 shows the computer-aided design (CAD) of the static geometry of the vortex chamber as well as the generated computational mesh. The system geometry described in Table 1 is that of a simple block in which the actual geometry used in the simulations (Figure 1) is created by intersection with an STL file containing the information on the position of the walls that can be generated with any CAD software. This so-called Cartesian cut-cell method has been described by Dietiker et al.³² A 24 cm-diameter (D_{vc}), 5 cm-long (L_{vc}) vortex chamber with 8 gas inlet slots (n), 4 mm wide each (s), and with an 8 cm-diameter chimney (D_c) was simulated – dimensions close to those typically used in experimental and pilot scale studies.^{4,7,15} The gas is injected nearly tangentially. The chimney-to-vortex chamber diameter ratio is 0.33, the vortex chamber length-to-diameter ratio 0.21. This is within the optimal ranges $0.3 < D_c/D_{vc} < 0.5$ and $L_{vc}/D_{vc} < 0.5$ reported by Kochetov et al.⁴ The fraction of the chamber circumference taken by the gas inlet slots, λ , is 0.042, about the upper limit reported by Kochetov et al.⁴ This λ is an important design parameter as it allows adjusting the gas inlet velocity/particle bed rotation speed for a given gas flow rate and as such the ratio centrifugal force-to-radial gas-solid drag force and the resulting bed density and uniformity. Trujillo and De Wilde³³ and De Wilde et al.¹⁵ showed that with fine particles λ must be sufficiently small, see also De Wilde.² For optimal bed uniformity, a high number of gas inlet slots is preferred and so the slot size is decreased if λ is to be reduced, see e.g. Eliaers et al.¹⁵ Slot sizes smaller than the particle diameter are excluded as this leads to inefficient gas-solid momentum transfer in the vicinity of the gas inlet slots. If reducing the slot size is not possible, decreasing the number of slots to reduce λ can be considered, see e.g. Anderson et al.⁹ Simulations were carried out feeding air and a mixture of two distinct types of particles. As a case study, large/heavy 1 mm particles with a density of $2700 \text{ kg}_p/\text{m}^3_p$ and small/light 0.4 mm particles with a density of $200 \text{ kg}_p/\text{m}^3_p$ were used, referred to as large and small in what follows. The mass ratio of the large and small particles is as such 210, about the ratio for oxygen carrier and ash in CLC. For visualization purposes and throughout this study, the large and small particles are colored blue and red, respectively. The slot size was then chosen 4 times the diameter of the large particles. To guarantee a sufficiently low λ , the number of slots was reduced to 8, a minimum to achieve uniform operation. The restitution coefficient, e , the friction coefficient, μ , and the spring constant, k , were assumed to be respectively 0.9, 0.1 and 100 kg/s^2 . Similar values have been used in previous studies.²⁹ Their influence on the particle trajectories was beyond the scope of this case study. The particles and a

small amount of gas are fed through a perforation in one of the end walls of the vortex chamber, the most widely used solids inlet design.^{2,15,34-36} The particles are fed under an angle to pre-accelerate them in the tangential direction. For given chamber design and gas flow rate, this allows operation at higher solids feeding rates, as only a small fraction of the tangential momentum supplied with the gas has to be used for the acceleration of freshly entering particles. Atmospheric pressure is imposed at the outlet/chimney.

A minimum gas flow rate requirement follows from the required tangential momentum supply to compensate for shear with the wall and keep the particle bed of given mass rotating. An estimate can be made based on the time the bed keeps rotating when abruptly stopping the gas supply. As an example, consider a 2 cm thick bed (t_b) with a solids volume fraction ($\epsilon_{s,b}$) of $0.5 \text{ m}^3_s/\text{m}^3_r$ of the heavy particles in the vortex chamber as described above, containing about 1 kg of particles, that rotates at $V_{s,t} = 3 \text{ m}_r/\text{s}$ – a typical value found in the literature² – and keeps rotating for 1 s when the gas flow is stopped, based on experimental observations. Thus, the gas must supply tangential momentum at a rate of minimum $3 \text{ kg}\cdot\text{m}_r/\text{s}^2$ to keep the bed rotating at the given speed. The minimum required gas flow rate, $F_{g,\min}$, then follows from $\rho_g \cdot F_{g,\min} \cdot V_{g,\text{in}} = 3 \text{ kg}\cdot\text{m}_r/\text{s}^2$. With the gas inlet velocity, $V_{g,\text{in}}$, given by $V_{g,\text{in}} = F_{g,\min}/(n \cdot s \cdot L_{vc})$, a value of $F_{g,\min} \approx 200 \text{ m}^3_g/\text{h}$ is found, value initially imposed in the simulations. The corresponding $V_{g,\text{in}}$ is 35 m/s, value imposed in the base simulations (Table 1). In this case, a lower gas flow rate could not keep rotating the given bed at $3 \text{ m}_r/\text{s}$. In practice, an equilibrium is found between the gas flow rate, the solids loading and the bed rotation speed, particles being lost through the chimney when the bed rotation speed becomes too low. In the example considered, no solids losses through the chimney are expected as the centrifugal force density $f_{\text{centr}} = \epsilon_s \cdot \rho_s \cdot (V_{s,t})^2/R_{vc} \approx 1 \cdot 10^5 \text{ N}/\text{m}^3_r$, whereas the radial gas-solid drag force density is $f_{\text{drag},r} = \beta \cdot V_{g,r} \approx 3 \cdot 10^4 \text{ N}/\text{m}^3_r$, with the interstitial radial gas velocity $V_{g,r} = F_g/(\pi \cdot D_{vc} \cdot L_{vc} \cdot \epsilon_g) \approx 3 \text{ m}_r/\text{s}$ and the gas-solid momentum transfer coefficient β calculated by the Ergun equation.³⁷ Note that the gas phase residence time in the bed is $\tau_{\text{res},g,b} = t_b/V_{g,r} \approx 6 \cdot 10^{-3} \text{ s}$. With an equally dense bed of light particles rotating at the same speed, radially inward motion of the particles is expected as $f_{\text{centr}} \approx 8 \cdot 10^3$ and $f_{\text{drag},r} \approx 1 \cdot 10^5 \text{ N}/\text{m}^3_r$. Of course, it remains to be seen at what speed the particles will actually rotate. With a mixture of heavy and light particles, segregation should take place and could be intensified by high-G operation. The light particles can then either be entrained into the chimney, as was experimentally observed by Eliaers et al.,¹⁵ or form a faster rotating particle bed radially inward from the rotating bed of heavy particles, allowing to avoid entrainment of light particles by the gas into the chimney and to combine in-situ solid-solid and gas-solid separation. The simulations

presented in this work will allow gaining insight in the complex fluid dynamics and optimizing the concept, in particular the design of the solids inlet and eventual solids outlet(s), closed in the present case study.

The simulations follow a procedure similar to the one used experimentally^{7,15} and start feeding gas only. After the vortex flow develops, a mixture of heavy and light particles is fed at respectively 4.864 and 0.032 kg_p/s and the formation of the rotating fluidized bed and eventual segregation studied. After a stable flow pattern develops, the solids feeding is stopped to study the solids retention in the vortex chamber, the flow pattern and eventual effects of solids feeding on the flow, and more particular on the bed stability, density and uniformity, on the gas-solids separation and on segregation. Simulations were run for about 1 second, which is sufficiently long to reach a statistically steady state. Next, the influence of the gas flow rate and an eventual influence of large eddies on the particle trajectories are studied.

4. Results and discussion

Establishing a single-phase free vortex

Before feeding solids, it is of interest to verify if a free vortex forms in the vortex chamber of given design with the gas entering tangentially through the eight 4-mm slots. Figure 2 shows the formation of a free vortex with the gas velocity increasing as expected when going radially inwards from the cylindrical wall towards the chimney, similar to a tornado observed in nature. The free vortex is observed to form rapidly, in about 0.1 sec. Grid independency of the simulation results was verified and a fine computation grid was used with a total of 2.6 million cells. The radial profiles of the tangential and radial gas velocity are shown in Figure 3a. After an initial decrease in the immediate vicinity of the gas inlet slots, both the tangential and radial gas velocity increase when going radially inwards as a result of the reducing volume and surface area for flow in the cylindrical geometry. In the chimney region itself, the free vortex is destroyed by the outflow of gas, as experimentally observed by Volchkov et al.⁵ At the center of the chimney region, the flow field is relatively calm as in the eye of a cyclone and some backflow of gas from the outlet towards the chamber is seen. The decrease of the tangential and radial velocity in the immediate vicinity of the gas inlet slots is the result of the difficulty for the injected gas to penetrate the vortex and the not completely tangential injection of the gas in the chamber. Figure 3b shows the radial profile of the gauge pressure in the chamber, scaled with the kinetic energy supplied through the 8 gas inlets. The total pressure drop over the vortex chamber is seen to equal the latter. It is

noticeable that a major contribution to the pressure drop comes from the penetration of the injected gas into the vortex and from the acceleration of the flow when approaching the chimney. Inside the chimney region, the gauge pressure becomes slightly negative, causing the observed reversed gas flow (backflow) from the outlet into the chamber. Different systems have been developed to eliminate such backflow, see De Wilde.²

Behavior when feeding a bi-disperse particle mixture into the vortex chamber

After establishing a free vortex, a bi-disperse particle mixture is introduced in the chamber via the solids inlet. Figure 4 shows instantaneous plots of the bi-disperse particle positions 0.025 sec and 0.85 sec after starting the solids injection. Initially the solids inlet performs as designed; i.e. particles are tangentially pre-accelerated and directed toward the cylindrical wall of the vortex chamber, away from the chimney, also as a result of the strong centrifugal force still reigning in the vortex chamber. It is clear that the smaller and lighter particles (red) are accelerated faster than the larger and heavier ones (blue). Some of the smaller/lighter particles have almost completed a first revolution after only 0.025 sec (Figure 4a). As the solids feeding proceeds (Figure 4b), particles accumulate near the cylindrical wall and a rotating fluidized bed is formed. The particles are axially uniformly distributed in the chamber and no significant bubbling is observed. Segregation is taking place, with the larger/heavier particles concentrating against the cylindrical wall and the smaller/lighter particles moving radially more inwards in the chamber. As the rotating fluidized bed is formed, the rotational speed drastically decreases, in agreement with experimental observations showing a loss of the free vortex behavior in the dense particle bed region.^{5,9,35,38} This results in a decrease of the pressure drop over the chamber. The pressure drop from the weight of the bed in the high-G field remains also relatively small because of the limited bed height. The jet of particles coming from the solids inlet is less pronounced and particles are dispersed radially inwards, on the one hand because of the reduced centrifugal force, on the other hand due to collisions of incoming particles with particles already rotating in the bed. The presence of particles in the freeboard and chimney regions causes solids losses via the chimney and a loss of free vortex behavior in these regions as well. Figure 5 shows an instantaneous plot of the gas velocity 0.85 sec after starting the solids feeding. Comparison with Figure 2 clearly shows that the vortex is significantly weakened in the entire chamber by the presence of the particles. The loss of solids via the chimney is to a certain extent self-sustaining as it leads to reduction of the strength of the vortex and of the related centrifugal force, which is believed to be one of the factors at the origin of solids losses via the chimney. As the bed rotational speed increases with decreasing solids loading, a design- and particle

type-dependent equilibrium is found in which a given solids loading can be built up in the vortex chamber for given gas and solids feeding rates. In their study of continuous biomass drying in a vortex chamber using a similar solids inlet design, Eliaers and De Wilde⁷ noticed a certain degree of bypassing, a fraction of the particles going nearly directly from the solids inlet into the chimney. The DPM simulations confirm this phenomenon, but show that this could also be the result of collisions of the incoming particles with the particles in the rotating bed. This also explains that both losses of the large and small particles via the chimney are observed soon after starting the solids feeding, detrimental for segregation of these particles in the vortex chamber. The rotating chimney, proposed to eliminate solids losses via the chimney³⁸⁻⁴⁰ does not resolve the problem of the presence of particles in the freeboard region. The action of the rotating chimney replaces, however, to a certain extent that of the strong central vortex that is generated in the absence of particles in the freeboard and chimney regions.

Behavior after stopping solids feeding to the vortex chamber

The influence of solids feeding on the bed stability, solids losses via the chimney and segregation was verified by continuing the simulation after stopping the solids feeding. A statistically steady state is quickly reached, after which fluctuations in the particles flow field were found to be minor, confirming experimental observations.^{7,15,34-36} Snapshots of the particle profiles are as such representative for the time-averaged behavior. The effect of fluctuations in the gas flow field is discussed in a separate section. Figure 6b shows that already 0.17 sec after stopping the solids feeding solids losses via the chimney have stopped. The standard solids inlet design is seen to have a negative effect on solids losses via the chimney and dispersing particles in the entire vortex chamber. With the particles evacuated from the freeboard and chimney regions, a strong vortex is seen to re-appear around the chimney region (Figure 6a) which strengthens and stabilizes the rotational motion in the entire vortex chamber. Furthermore, segregation of the large and small particles improves drastically. The losses of small particles via the chimney are also eliminated and the formation of two distinct rotating fluidized beds is seen, a dense and uniform rotating fluidized bed concentrated in large particles against the cylindrical wall of the vortex chamber and a somewhat less dense but uniform rotating fluidized bed of mainly small particles more radially inwards in the vortex chamber.

The intensification of segregation by high-G operation should be noticed, the total bed height being only 2 to 3 cm. It is remarkable, as with a mono-disperse rotating fluidized bed in a vortex chamber, efficient particle mixing in all directions was observed in experiments with colored particles.² Looking at the

particle velocities (not shown) in the segregated bed shows that the large particles rotate at about 3 m/s (corresponding to about 4 revolutions per second), whereas the small particles rotate at twice that speed. The latter is due to the dilute nature of the inner bed of small particles, allowing a free vortex type behavior, lost in the dense outer bed of large particles, to redevelop, as will be illustrated later. The large and small particles are as such subject to a centrifugal acceleration of respectively about 8G and 32G, in the range of typically experimentally observed values.² Due to their significantly higher mass (mass ratio of 210), however, the large particles are subject to a larger centrifugal force, explaining their concentration against the cylindrical wall of the chamber.

Figure 6c shows the tangentially averaged radial profiles of the volume fraction of large and small particles in the vortex chamber. Whereas the outer bed of large particles is dense, the inner bed of small particles is dilute, despite the relatively high number density. This dilute nature of the inner bed allows the vortex to regain strength, explaining the higher particle bed rotation speed. Efficient gas-solids separation is confirmed. The somewhat lower bed density in the immediate vicinity of the wall seen in Figure 6c is the result of the tangential averaging of non-uniformities in the void fraction following the interaction with the different gas inlet slots. Although segregation is seen to be pronounced, accounting for the couple of cm bed height, some contamination of the outer bed of large particles by small particles which are captured between the large particles seems unavoidable. Contamination of the inner bed of small particles by large particles is, however, minor and a quite sharp interface in the heavy particle volume fraction profile is observed. The contamination of the inner bed seen in the tangentially averaged profiles in Figure 6c is the result of a local phenomenon. As seen from Figure 6b, contact of the particle bed with a perforation in one of the end walls foreseen as solids outlet (at the left end of the particle bed) disturbs the particle bed and leads to radial mixing of large and small particles. The large particles are, however, quickly evacuated from the inner bed and returning to the periphery. Optimization of the solids outlet design is required, e.g. making use of a disc behind which solids outlets can be located. Finally, the particle position profiles in Figures 6b and 6c show that, when aiming at operation with continuous solids feeding and removal, separate evacuation of large and small particles via two distinct solids outlets in one of the end walls of the vortex chamber is possible, one against the cylindrical wall of the vortex chamber, the second close to the freeboard region. This is important as evacuating the small particles via the chimney is excluded in view of the reduced vortex strength in the presence of particles in the freeboard and chimney regions. Operation with continuous solids feeding

will, however, require the development of a solids inlet design preventing a significant presence of particles in the freeboard and chimney regions during solids feeding.

Figures 3 and 7 allow quantitatively comparing the impact of the presence of the particle bed (after stopping the solids feeding) on the (a) radial and tangential gas velocity and on the (b) pressure drop over the vortex chamber. The radial gas velocity profile is not much affected in the major part of the vortex chamber as it is determined by the gas flow rate, the circumference at given radial position and the length of the vortex chamber. Only in the dense particle bed region, an increase of the radial gas velocity is logically observed. The tangential gas velocity, on the other hand, is significantly reduced by the presence of the particle bed and this also in the particle bed freeboard region. A free vortex type behavior is, however, restored in this region. In the dense particle bed region, the tangential gas velocity decreases to about 10% of the gas injection velocity and the free vortex type behavior is lost. The velocity profiles and the way they are affected by the presence of a particle bed are in line with those experimentally measured, e.g. by Volchkov et al.⁵ Figures 3b and 7b clearly illustrate the significant, more than 40%, decrease of the pressure drop over the chamber as a result of the reduced vortex strength in the presence of the particle bed. Such a strong decrease of the pressure drop was experimentally observed by different groups.²

Flexibility with respect to the gas flow rate

The gas flow rate affects both the radial gas-solid drag force and the centrifugal force on the particles. The resulting flexibility of rotating fluidized beds in vortex chambers with respect to the gas flow rate is an important feature of the technology. In experiments with mono-disperse particles, the flow regime or fluidized bed state was unchanged in a wide gas flow rate range.^{2,35} In this numerical study, the impact of the gas flow rate on the fluidization characteristics of a bi-disperse bed was studied by doubling the gas flow rate starting from the flow field obtained after stopping the solids feeding, discussed in the previous section. Figure 8a shows that the abrupt change in the gas flow rate, i.e. increasing the inlet gas velocity from 35 to 70 m/s, leads to the formation of waves and mixing of large and small particles. After about 0.1 sec, however, (Figure 8b) the waves have dampened, a stable and uniform bed of comparable density is again formed, and segregation of the large and small particles is nearly completely restored. No losses of any particles are observed in this time. As seen from the tangentially averaged radial profiles of the volume fraction large and small particles in the vortex chamber shown in Figure 6c, doubling the gas flow rate improves slightly the gas-solid separation and segregation. In particular the

inner rotating fluidized bed of small particles is somewhat better confined. The minor influence of the gas flow rate on the flow regime and the quality of segregation is a unique advantage of vortex chamber technology and opens perspectives for applications requiring high gas throughputs. This flexibility with respect to the gas flow rate combined with the possibility to evacuate gas and two distinct types of particles separately from the vortex chamber is important as it allows independently controlling the gas and particle residence times, important for specific reactor applications of the technology, e.g. chemical looping combustion.

Effect of large eddies on the particle trajectories

Because of the relatively high gas velocity in the vortex chamber and the bi-disperse and segregated nature of the bed with an inner dilute rotating fluidized bed of small particles with a Stokes number of somewhat larger than 10 (gas phase residence time based), eventual influence of large-scale most energetic turbulent structures or eddies in the gas phase on the trajectories of the particles, neglected so far, was studied. Calculations using a second-order (superbee) scheme for the gas phase convective terms and a fine spatial and temporal discretization steps were carried out to simulate large eddy formation. No sub-grid-scale model was applied, which can be considered as coarse direct numerical simulations (DNS).^{41,42} The fluid time step had to be reduced by at least two orders of magnitude with respect to the one used in the simulations with the FOU scheme. Figure 9 shows the effect of large eddies on the bi-disperse particles flow pattern and the segregation in the vortex chamber. As well instantaneous (Figures 9a and 9b) as time-averaged (Figures 9c and 9d) profiles are shown and the gas phase flow pattern is illustrated by showing the motion of an inert black tracer injected through one of the gas inlet slots. The gas injected via a given gas inlet slot is seen to be deflected radially inwards and out of the dense particle bed region when reaching the next gas inlet slot (in the flow rotational direction). This confirms experimental observations using smoke.² Once reaching the inner dilute rotating fluidized bed of small particles and the particle-lean freeboard region, the gas is seen to be tangentially re-accelerated by the strong vortex in this region, leading to an S-shaped profile in the gas phase flow path. The time-averaged profiles (Figures 9c and 9d) clearly show that gas dispersion increases with the use of higher order discretization scheme (superbee), even though this scheme is less diffusive than the FOU scheme. This can only be due to large turbulent eddies that are better resolved by improved spatial/temporal numerical resolution. The large eddies that ultimately lead to increased dispersion in the time-averaged plot are clearly seen in the instantaneous plot (Figure 9b), in particular in the inner dilute bed of small particles and the freeboard region where the gas is re-accelerated. Figure

9 shows that the effect of large eddies on the trajectories of the large particles is negligible, as expected from the Stokes number of more than 10^3 (gas phase residence time based). The possible effect of large eddies on the small particles is confirmed, but the effect is limited. The inner bed height increases somewhat by turbulent dispersion, in particular in the top and down-flowing part of the bed (at the right in Figures 9b&d).

5. Conclusions

The possibility of intensifying simultaneously gas-solids contact, gas-solids separation and segregation by high-G operation in a rotating fluidized bed in a static vortex chamber was qualitatively studied by means of coupled discrete particle model – computational fluid dynamics simulations and focusing on the case of a bi-disperse particle bed. Using the standard solids inlet design with the solids fed via a tube in one of the end walls of the chamber, solids feeding is seen to result in a significant presence of particles in the particle bed freeboard and chimney regions. This strongly reduces the strength of the vortex in these regions and the related centrifugal force on the particles and is detrimental for particle losses via the chimney and for segregation. Dispersion of particles entering the vortex chamber after collision with particles in the rotating fluidized bed explains the high concentration of particles in the freeboard and chimney regions during solids feeding. Nevertheless, the formation of a dense and uniform rotating fluidized bed with a certain degree of segregation is observed. When stopping the solids feeding, particles are immediately evacuated from the freeboard and chimney regions. This eliminates particle losses via the chimney and allows the vortex in these regions to regain strength. The latter has a positive effect on the particle bed rotation speed and on segregation. With a total bed height of less than 5 cm, efficient segregation is demonstrated. A dense and uniform rotating fluidized bed of large particles is formed against the cylindrical wall of the vortex chamber and a somewhat less dense and faster rotating fluidized bed of small particles more radially inward. With a batch of particles fed to the vortex chamber, the flexibility of the gas-solids separation and the segregation with respect to the gas flow rate was also demonstrated – a unique characteristic of vortex chamber generated rotating fluidized beds impossible to achieve in conventional fluidized beds operating under constant earth gravity. Doubling the gas flow rate initially formed waves that are quickly dampened and the dense and uniform bed and segregation can be maintained without significant solids losses via the chimney. Large eddies in the gas phase are seen to have a negligible impact on the motion of the large particles and on segregation. The height of the bed of small particles slightly increases by turbulent dispersion. The

simulations open perspectives for the development of a vortex chamber type rotating fluidized bed reactor that combines in-situ and efficient separation of different types of particles, efficient gas-solids separation and efficient gas-solids contact by the generation of a dense and uniform rotating fluidized bed at high gas-solid slip velocities. This could, for example, facilitate ash separation in chemical looping combustion of coal. Future research will focus on operation with continuous solids feeding and removal with two well-positioned solids outlets and a novel solids inlet design that could prevent significant dispersion of particles in the freeboard and chimney regions during solids feeding.

Appendix I

In the DPM model, the fluid flow is described as a continuum by the single-phase Navier-Stokes equations modified to include the fluid volume fraction as well as the fluid-particle interaction due to the drag force. The fluid continuity equations for mass and momentum can then be written as

$$\frac{\partial(\rho_g \varepsilon_g)}{\partial t} + \nabla \cdot (\rho_g \varepsilon_g \vec{V}_g) = 0 \quad (1)$$

$$\left[\frac{\partial(\rho_g \varepsilon_g \vec{V}_g)}{\partial t} + \nabla \cdot (\rho_g \varepsilon_g \vec{V}_g \vec{V}_g) \right] = -\varepsilon_g \nabla P_g + \nabla \cdot \vec{\tau} - \sum_{p=1}^{N_T} \beta_p \frac{\phi_p}{\phi_c} (\vec{V}_g(\vec{x}_p) - \vec{V}_p) + \varepsilon_g \rho_g \vec{g}, \quad (2)$$

where ε_g is the fluid volume fraction, ρ_g is the fluid-phase density, P_g is the fluid phase pressure, $\vec{\tau}$ is the fluid viscous stress tensor, $\vec{g}$ is the specific gravity force, $\vec{V}_g$ is the local average velocity of the fluid phase, $\vec{V}_g(\vec{x}_p)$ is the fluid velocity at the particle location, $\vec{V}_p$ is the velocity of the p^{th} particle, and β_p is the interphase momentum exchange coefficient. N_T represents the total number of particles in the system, and ϕ_p and ϕ_c are the volume of the p^{th} particle and the fluid cell, respectively. The fluid is assumed to be Newtonian and the standard Wen-Yu⁴³ model for the interphase momentum exchange coefficient for the p^{th} particle in a fluid cell is used to calculate the drag force.

$$\beta_p = \frac{3}{4} C_D \frac{\rho_g \varepsilon_g |\vec{V}_g(\vec{x}_p) - \vec{V}_p|}{d_p} \varepsilon_g^{-2.65} \quad (3)$$

where d_p is the particle diameter and C_D is the drag coefficient expressed as

$$C_D = \begin{cases} 24 / \text{Re} (1 + 0.15 \text{Re}^{0.687}) & \text{Re} < 1000 \\ 0.44 & \text{Re} \geq 1000 \end{cases} \text{ and } \text{Re} = \frac{\rho_g \epsilon_g |\vec{V}_g(\vec{x}_p) - \vec{V}_p| d_p}{\mu_g} \quad (4)$$

The position, linear velocity, and angular velocity of each individual particle are calculated using Newton's laws of motion

$$\frac{d\vec{x}_p}{dt} = \vec{V}_p \quad (5)$$

$$\frac{d\vec{V}_p}{dt} = \vec{g} - \frac{\nabla P_g}{\rho_p} + \frac{\beta_p}{\rho_p} (\vec{V}_g(\vec{x}_p) - \vec{V}_p) + \vec{F}_{c,p} / m_p \quad (6)$$

$$I_p \frac{d\vec{\omega}_p}{dt} = \vec{T}_p \quad (7)$$

where $\vec{x}_p$ is the position of the p^{th} particle, ρ_p is the density of the particle, and m_p its mass, $\vec{F}_{c,p}$ is the net contact force due to collisions of particle p with other particles and walls, $\vec{\omega}_p$ is the angular velocity of the particle, $\vec{T}_p$ is the sum of all torques acting on the particle, and the other terms are as defined earlier. The forces acting on a particle, on the right-hand-side of Eq. (6), are the gravitational force, a generalized buoyancy force, the drag force, and the collisional forces. The traditional soft-sphere approach is used to model collisions. The approach is described in detail by Garg et al.³¹ as well as by Benyahia and Galvin.²⁹

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Tables & Figures:

Geometry	Symbol	Unit	Value
Vortex chamber diameter	D_{vc}	m_r	0.24
Vortex chamber length	L_{vc}	m_r	0.05
Chimney diameter	D_c	m_r	0.08
Number of gas inlet slots	n	-	8
Gas slot width (individual)	s	m_r	4×10^{-3}
System geometry	$L_x \times L_y \times L_z$	$m \times m \times m$	$0.26 \times 0.102 \times 0.26$
Eulerian grid	$i \times j \times k$	-	$178 \times 81 \times 178$
Eulerian & DPM time steps	dt & dt_p	s	1.0×10^{-5} & 1.0×10^{-7} (base case)
Operating conditions / Properties	Symbol	Unit	Value
Gas density	ρ_g	kg_g/m^3_g	Uses ideal gas law (~ 1.2)
Gas phase viscosity	μ_g	$Pa \times s$	1.8×10^{-5}
Particle density	ρ_p	kg_p/m^3_p	2700 (large/heavy) and 200 (small/light)
Particle diameter	d_p	mm	1 (large/heavy) and 0.4 (small/light)
Total number of particles	n_t	-	$> 210,000$
Restitution coefficient	e	-	0.9
Friction coefficient	μ	-	0.1
Spring constant	k	kg/s^2	100
Inlet gas velocity	$V_{g,in}$	m_r/s	35 (base case) and 70
Superficial gas velocity	$V_{g,sf}$	$m^3_g/m^2_r/s$	1.49 (base case) and 2.98
Particle feed rate (during solids injection)	$\dot{m}_p$	kg_p/s	4.864 (large/heavy) and 0.032 (small/light)

Table 1. CFD-DPM geometry specifications, simulation conditions and properties assumed in the presented case study.

Figure 1. Geometry and mesh of the static vortex chamber. Specifications: see Table 1.

Figure 2. Gas velocity vectors in the vortex chamber prior to solids feeding at $t = 0.2$ sec showing two views of the formation of a free vortex. Red velocity vectors indicate a gas velocity of 35 m/s or higher. For clarity, only 10k velocity vectors are plotted. Geometry specifications and operating conditions: see Table 1.

(a)

(b)

Figure 3. Radial profile of the (a) tangential and radial gas velocity scaled with the gas inlet velocity and (b) pressure scaled with the kinetic energy of all 8 gas inlets ($V_{g,in} = 35$ m/s) in the absence of particles at $t = 0.2$ sec (see Figure 2). Geometry specifications and operating conditions: see Table 1.

Figure 4. Instantaneous plots of the bi-disperse particle positions (a) 0.025 sec and (b) 0.85 sec after the start of solids injection. Blue large/heavy and red small/light particles. Geometry specifications and operating conditions: see Table 1.

Figure 5. Instantaneous plot of the gas velocity vectors 0.85 sec after the start of solids injection (gas velocity coloring scheme as in Figure 2). Geometry specifications and operating conditions: see Table 1.

Figure 6. Instantaneous side-by-side plots of (a) the gas velocity vectors and (b) the bi-disperse particle positions 0.17 sec after stopping the solids injection (gas velocity coloring scheme as in Figure 2). Blue

large/heavy and red small/light particles. (c) Tangentially averaged radial profiles of the volume fraction large/heavy and small/light particles with $V_{g,in} = 35$ and 70 m/s. Geometry specifications and operating conditions: see Table 1.

Figure 7. Radial profile of the (a) tangential and radial gas velocity scaled with the gas inlet velocity and (b) pressure scaled with the kinetic energy of all 8 gas inlets ($V_{g,in} = 35$ m/s) 0.17 sec after stopping the solids injection (see Figure 6). Geometry specifications and operating conditions: see Table 1. Scales as in Figure 3.

Figure 8. Instantaneous plots of the bi-disperse particle positions after solids injection and (a) 0.01 sec and (b) 0.095 sec after doubling the gas flow rate by increasing the inlet gas velocity from 35 to 70 m/s. Blue large/heavy and red small/light particles. Geometry specifications and operating conditions: see Table 1.

Figure 9. Evaluation of the influence of large eddies on the particle trajectories. Bi-disperse particle positions after stopping the solids injection with (a)&(b) instantaneous ($t = 1.2$ sec) and (c)&(d) time-averaged plots of an inert black tracer (e.g. smoke) flowing with the gas injected at only one of the gas inlet slots (bottom-right in the figure). (a)&(c) First order upwind discretization scheme and (b)&(d) second order superbee and highly improved spatial/temporal resolution. Blue large/heavy and red small/light particles. Geometry specifications and operating conditions: see Table 1 (base case).