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EMMS-based modeling of gas–solid generalized fluidization: Towards a unified phase diagram

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ABSTRACT

Hydrodynamic features of gas–solid generalized fluidization can be well expressed in the form of phase diagrams, which are important for engineering design. Mesoscale structure presents almost universally in generalized fluidization and should be considered in such phase diagrams. However, current phase diagrams were mainly proposed for cocurrent upward flow according to experimental data or empirical correlations with homogeneous assumption. The energy-minimization multiscale (EMMS) model has shown the capability of capturing mesoscale structure in generalized fluidization, so EMMS-based phase diagrams of generalized fluidization were proposed in this article, which describe more reasonable global hydrodynamics over all regimes including the important engineering phenomena of choking and flooding. These characteristics were also found in discrete particle simulation under various conditions. For wider range of application, the typical hydrodynamic parameters of the phase diagrams were correlated to non-dimensional numbers reflecting the effects of material properties and operation conditions. This study thus shows a possible route to develop a unified phase diagram in the future.

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1. Introduction

Gas–solid fluidization systems are widely found in industrial processes. Classical fluidization refers to the particle–fluid systems in which the fluid flows upwards and suspends the particles with negligible entrainment. Kwauk [1] extended the classical concept of fluidization to generalized fluidization which operates in three modes identified by the moving directions of the gas and the solids: cocurrent upward, cocurrent downward and counter-current downward flows.

No matter in which mode, both axial and radial heterogeneities are always displayed [2–4]. In the cocurrent upward flow, there are typical regime transitions such as bubbling, turbulent and fast fluidization corresponding to different gas velocities [5,6]. At a particular gas velocity, a bottom dense region coexists with a top dilute region and a transition zone in between, which is called choking [6,7]. While in the counter-current downward flow, flooding is observed when the downward particle movement is prevented by the upward gas flow to form a dense suspension [1,8–10]. The hydrodynamic features are dependent on operating conditions as well as gas and particle properties, which can be characterized by the phase diagrams of fluidization. For instance, the variation of voidage (ε) or pressure drop gradient (d_p/d_z) with

superficial gas velocity (U_g) or slip velocity (U_s) for specific particle properties in gas–solid risers was plotted by many researchers [11–14]. Grace [5] introduced non-dimensional numbers to consider the effects of gas and particle properties in the phase diagram of cocurrent upward flow. Bi *et al.* [15] further incorporated pneumatic transport regime in the phase diagram of classical fluidization. Sun *et al.* [16] reclassified fast fluidization as high- and low-density circulating fluidization regimes and consolidated the phase diagram for cocurrent upward flow. According to experimental data, Rabinovich *et al.* [17] proposed a phase diagram with modified Archimedes and Reynolds numbers. Based on the Richardson–Zaki correlation, Kwauk [1] proposed a generalized fluidization phase diagram and defined the flooding gas velocity in the counter-current downward flow. However, these phase diagrams are mainly based on empirical correlations or experimental data and few of them can predict choking as the homogeneity of the flow is assumed.

Taking into account the particle clustering phenomenon in gas–solid flow, the energy-minimization multiscale (EMMS) model was established to predict the axial and radial heterogeneous distributions as well as regime transitions in the cocurrent upward gas–solid flow [6,7]. This global EMMS model was further improved by introducing particle acceleration and avoiding the limit of empirical correlation of cluster diameter [18,19], and then extended to predict global hydrodynamics in bubbling fluidization [20] and downer fluidization systems [9,21]. In this work, therefore, a phase diagram of similar to Kwauk's

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chart [1] was redrawn by using the EMMS model and its extensions. As a result, both choking and flooding are located in the phase diagram.

To validate this phase diagram, an EMMS-based coarse-grain discrete particle method (EMMS-DPM) [22,23] was employed to simulate typical flow regimes in the phase diagram. The DPM can facilitate following the trajectory of each particle, but the particles should be coarse-grained to acquire well balance between calculation accuracy and efficiency in the simulation of industrial-scale reactors [22]. In this study, the particles were coarse-grained by using the EMMS model. Recognizing the significant effect of mesoscale structure on gas–solid interaction in the EMMS-DPM, the structure-dependent drag coefficient was calculated with the method proposed by Hu *et al.* [19,24].

To generalize the application of the phase diagrams, the main hydrodynamic parameters in the phase diagram were correlated to both the operating parameters and material properties in the form of non-dimensional numbers. These non-dimensional correlations were validated by the experimental and simulation results in a wide range of material properties and operating conditions.

2. EMMS-based Modeling Method of Generalized Fluidization

For cocurrent-up gas–solid flow with different fluidization regimes such as bubbling, turbulent and fast fluidization, the original EMMS model [6] based on particle clusters and the EMMS bubbling model [20] based on gas bubbles are regime-specific. Two critical velocities (e.g., terminal velocity U_t and choking velocity U_{tr}) can demarcate the above-mentioned three flow regimes successively. With increasing superficial gas velocity (U_g) from minimum fluidization velocity (U_{mf}) gradually, the EMMS bubbling model (Table A1) is applicable for bubbling fluidization at $U_g \leq U_t$, whereas the original EMMS model (Table A2) can be applied to fast fluidization at $U_g \geq U_{tr}$. When U_g varies from U_t to U_{tr} , the gas–solid flow experiences the transition from bubbling to turbulent fluidization, which can be further defined as another transition velocity U_c for Geldart A particles, corresponding to the intersection point of the two curves of voidage vs. gas velocity calculated by the original EMMS and EMMS bubbling models respectively. However, as shown in Table 1, increasing particle sizes (e.g., for Geldart A/B particles), the EMMS bubbling model can be used at $U_t \leq U_g \leq U_{tr}$, as gas bubbles form readily in these two flow regimes. For Geldart B particles, the simulation results of the both models tend to be consistent with each other at $U_t \leq U_g \leq U_{tr}$, so either of them can be used approximately in the two flow regimes. [20,25].

Table 1
Modeling of cocurrent-up flow regimes for different particle types

Particle type	$U_{mf} \leq U_g \leq U_t$	$U_t \leq U_g \leq U_c$	$U_c \leq U_g \leq U_{tr}$	$U_g \geq U_{tr}$
Geldart A	EMMS bubbling	EMMS bubbling	original EMMS	original EMMS
Geldart A/B	EMMS bubbling	EMMS bubbling		original EMMS
Geldart B	EMMS bubbling	EMMS bubbling or original EMMS		original EMMS

To simulate the axial flow structure in the cocurrent and counter-current downward gas–solid flow, the EMMS model, as summarized in Tables A3 and A4 in Appendix A, was further extended to downward fluidization systems by improving stability condition and cluster description [9,21]. The hydrodynamic parameters in the fully developed section of downer reactor, which are dominated by operating parameters such as superficial gas and solids velocities (U_g and U_p), can be predicted well by the extension models, but the axial distribution in the entrance region can only be determined at the specified entrance voidage in the downer reactor.

However, neither of the two extension models works at $U_g = 0$ since the total energy consumption in this case is zero. Therefore, as indicated in Fig. 1, the hydrodynamic parameters (e.g., voidage ε_{full}) in the fully

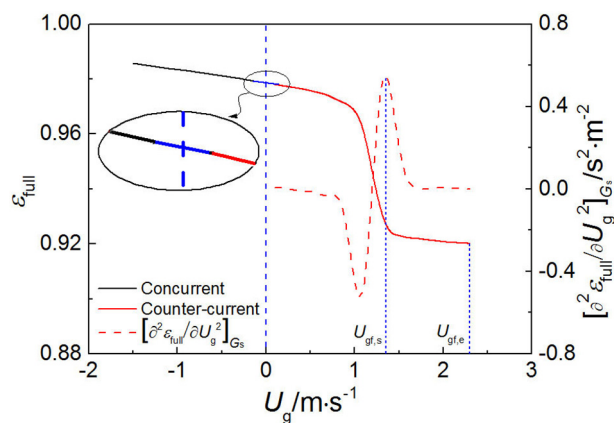


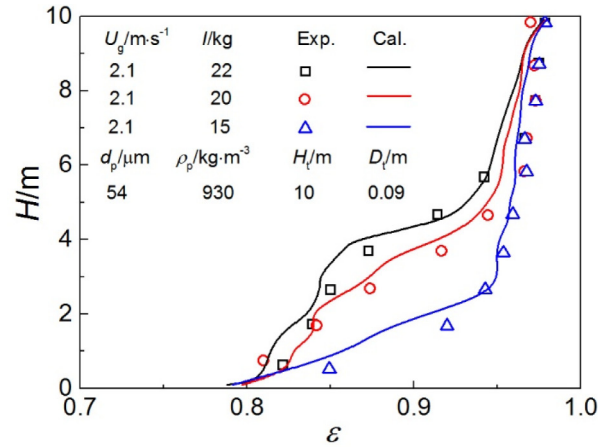
Fig. 1. Variation of ε_{full} with U_g in gas–solid downer systems.

developed sections of cocurrent and counter-current downers were calculated by the EMMS extension models for cocurrent and counter-current downward flow, respectively. When U_g approaches zero from either a positive or negative direction, the variation of ε_{full} with gas velocity can be determined by smoothly connecting the two ε_{full} vs. U_g curves obtained from the two extension models respectively.

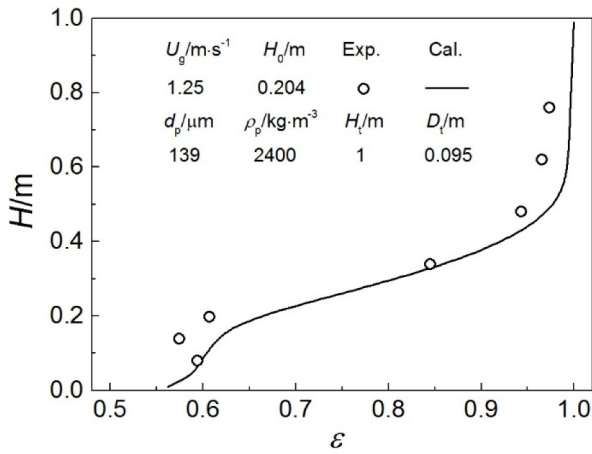
An important but unsolved engineering problem about the counter-current downward gas–solid flow is the accurate prediction of flooding. Liu *et al.* [9] investigated the variation of ε_{full} with U_g and found its general tendency. As illustrated in Fig. 1, with the increase of U_g , the decreasing of ε_{full} is not noticeable initially but then becomes significant because flooding may happen. Finally, ε_{full} remains nearly invariable until the particles begin to be carried out of the downer bed. That is, flooding is not an abrupt, but a gradual process. Therefore, increasing U_g from zero, the gas velocity corresponding to the point at which ε_{full} remains nearly constant beyond the inflection point of the ε_{full} vs. U_g curve was defined as the start of flooding ($U_{gf,s}$), while the point at which the particle entrainment occurs was taken as the end of flooding ($U_{gf,e}$) [9]. In order to determine $U_{gf,s}$ accurately in practical operation, as indicated by the dashed line in Fig. 1, the second-derivative curve of the ε_{full} vs. U_g curve is plotted, and the gas velocity corresponding to the maximum derivative value can thus be defined as $U_{gf,s}$.

In order to verify and display the typical gas–solid flow structures described by the phase diagram, the EMMS-DPM simulations were firstly compared with experimental data to test its applicability for generalized fluidization. In the EMMS-DPM, the coarse-graining ratio (k) and internal voidage (ε_{CGP}) of the coarse-graining particles (CGP) are two basic parameters. According to Lu *et al.* [22], for fast fluidization k should be large enough to reduce computational cost but less than minimum cluster diameter to describe mesoscale structure, which was determined by taking into account the calculation accuracy and efficiency in this study. The parameter ε_{CGP} was set as minimum fluidization voidage (e.g., = 0.5 in this study). It is to specify gas velocity (U_g) and solids inventory (I) to predict solids flux (G_s) or axial voidage profile for cocurrent upward flow. To maintain I invariable, the particles blown out of the reactor top were recirculated to the bottom with the same particle number in the cocurrent upward flow. While specifying U_g and G_s to predict axial voidage profiles in the cocurrent and counter-current downward flow, a certain number of particles equivalent to G_s were fed from the reactor top entrance and allowed to leave freely from reactor bottom in the downer reactor simulations. The statistical results were conducted for 10 s physical time.

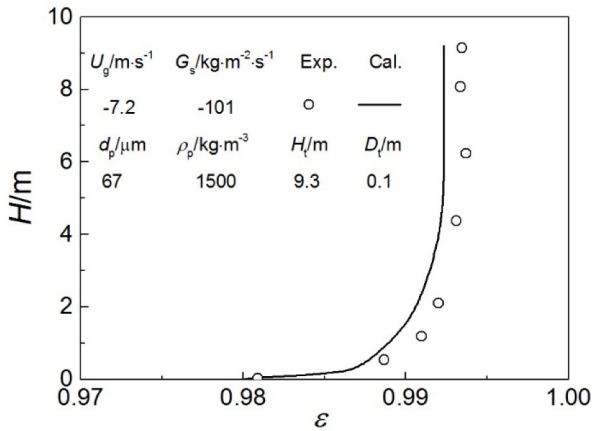
Fig. 2 indicates the comparison between the EMMS-DPM simulations and the experimental results of choking [6], turbulent fluidization [26] and cocurrent downward flow [27]. The value of k in the above three cases is respectively 30, 8 and 20 in the simulations. It can be seen from Fig. 2(a) that a bottom dense region coexists with a top dilute region, and the axial voidage displays an S-shaped profile in choking.



(a) Choking



(b) Turbulent fluidization



(c) Cocurrent downward flow

Fig. 2. Comparison between calculated and experimental axial voidage profiles in (a) choking, (b) turbulent fluidization and (c) cocurrent downward flow.

With the increase of I , the inflection point of axial voidage profile is gradually moving upward. For turbulent fluidization and cocurrent downward flow, as shown in Fig. 2(b) and (c), the axial voidage profiles calculated by the EMMS-DPM are generally in accordance with the experimental results.

To support the calculation results of the global EMMS models, the EMMS-DPM simulations were further performed for Geldart B ($d_p = 300 \mu\text{m}$, $\rho_p = 2500 \text{ kg} \cdot \text{m}^{-3}$) and Geldart A particles ($d_p = 100 \mu\text{m}$, $\rho_p = 1500 \text{ kg} \cdot \text{m}^{-3}$) in a fluidized bed of $H_t = 5 \text{ m}$ and $D_t = 0.1 \text{ m}$. Tables 2 and 3 indicate the operating conditions and the calculation results for generalized fluidization. The value of k for choking, pneumatic transport, cocurrent and counter-current downward flow is respectively 5, 3, 3 and 4 for Geldart B particles, while the value for Geldart A particles is 12, 8, 8 and 10 respectively. It is to compare G_s for cocurrent upward flow and $\varepsilon_{\text{full}}$ for cocurrent and counter-current downward flow. As shown in Tables 2 and 3, both G_s and $\varepsilon_{\text{full}}$ calculated by utilizing the two methods are consistent under the various operating conditions, since mesoscale interaction is taken into account in the both methods.

Table 2

Simulation results for cocurrent upward flow

Particle type	Case	$U_g/\text{m} \cdot \text{s}^{-1}$	I/kg	G_s (EMMS)/ $\text{kg} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$	G_s (DPM)/ $\text{kg} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$
Geldart B	Choking	2.8	7.7	5.6	5.9
	Transport	6.3	0.14	16.8	13.7
Geldart A	Choking	1.2	4.6	2.7	2.4
	Transport	2.0	0.12	5.4	3.5

Table 3

Simulation results for cocurrent and counter-current downward flow

Particle type	Case	$U_g/\text{m} \cdot \text{s}^{-1}$	$G_s/\text{kg} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$	$\varepsilon_{\text{full}}$ (EMMS)	$\varepsilon_{\text{full}}$ (DPM)
Geldart B	Cocurrent	-3.4	-56	0.9955	0.9962
	Counter-current	0.5	-56	0.9854	0.9898
Geldart A	Cocurrent	-1.1	-10.8	0.9945	0.9949
	Counter-current	0.1	-5.4	0.9846	0.9873

3. EMMS-based Phase Diagram of Generalized Fluidization

As discussed above, for generalized fluidization, the cocurrent upward flow was simulated by incorporating the original EMMS model and the EMMS bubbling model, while the cocurrent and counter-current downward flow were modeled by using the EMMS extension models for cocurrent and counter-current downward flow, respectively. Integrating the simulation results under various operating conditions, a so-called EMMS-based phase diagram is thereby possible to be proposed for generalized fluidization.

The phase diagram of fluidization can be drawn in various styles for different flow regimes and purposes. In this article, the style of Kwauk [1] was still used to redraw the phase diagram of generalized fluidization according to the calculated results of the EMMS model and its extensions. In the EMMS-based phase diagram, the system voidage was plotted as the function of normalized superficial gas velocity ($U_g^* = U_g/U_t$) at various normalized superficial solids velocity ($U_d = U_p/U_t$). It should be noted that the voidage in the fully developed section instead of the average voidage in the whole system was used in the cocurrent and counter-current downward flow in order to exclude the effect of entrance condition.

As a reference, Kwauk's phase diagram [1] was also plotted in this article. Based on the Richardson-Zaki correlation for homogeneous particulate fluidization, Kwauk [1] proposed

$$\varepsilon^n = \frac{U_g}{U_t} - \frac{U_p}{U_t} \frac{\varepsilon}{1-\varepsilon} \quad (1)$$

for generalized fluidization, where n is a function of the terminal Reynolds number [1]. That is, if only U_g and G_s are given at the specific fluidization system, the system voidage can be calculated by Eq. (1) in the

overall fluidization regime under all operation modes. Based on this generalized empirical correlation, the flooding gas velocity was further defined as

$$[\partial U_g / \partial \varepsilon]_{G_s} = 0 \quad (2)$$

implying that the superficial gas velocity reaches its maximum at a given solids circulation rate in a free fluidized system.

Figs. 3 and 4 (a) show the Kwauk's and EMMS-based phase diagrams of generalized fluidization for Geldart B particles ($d_p = 300 \mu\text{m}$, $\rho_p = 2500 \text{ kg} \cdot \text{m}^{-3}$) in a fluidized bed of $H_t = 5 \text{ m}$ and $D_t = 0.1 \text{ m}$. It can be seen that the voidage in the EMMS-based phase diagram is always lower than that in the Kwauk's phase diagram under the same operating conditions, especially in the cocurrent upward flow. This is because the formation of particle clusters in the cocurrent upward flow leads to the reduction of the interphase drag between the gas and solids phases [19]. However, although the clustering phenomenon still exists in the cocurrent and counter-current downward flow, its influence on the interphase drag becomes less important than that in the cocurrent upward flow due to the unstable and loose structures of particle clusters [28,29].

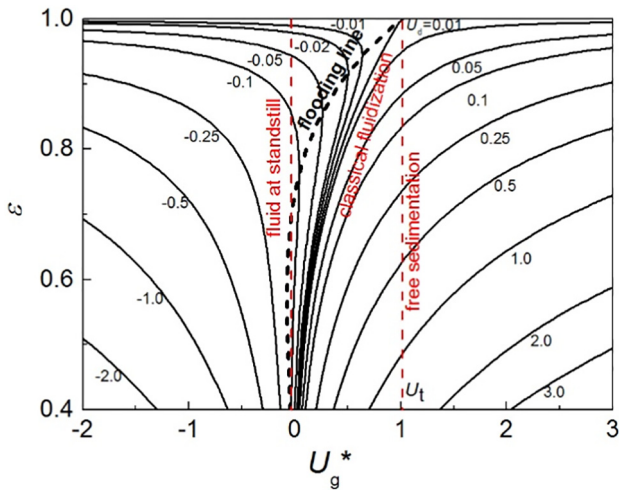
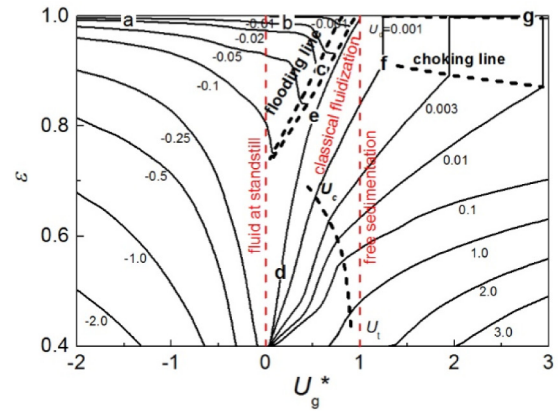


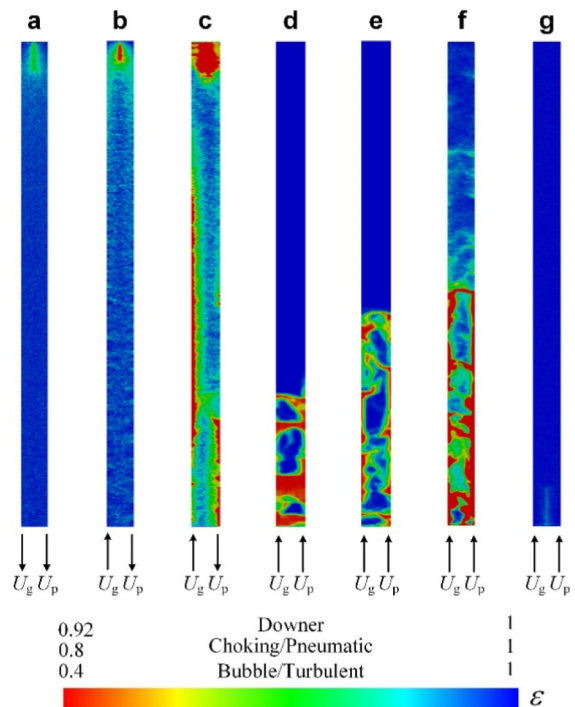
Fig. 3. Kwauk's phase diagram for Geldart B particles.

In Kwauk's phase diagram (Fig. 3), the bold dotted line marked as the flooding line was obtained by connecting all points defined by Eq. (2) under the simulated operating conditions. It is clear that at the flooding point the voidage shows an abrupt decrease with increasing U_g , indicating that the downer reactor is instantaneously blown out. Corresponding to the flooding line in Kwauk's phase diagram, a flooding zone formed in the EMMS-based phase diagram (Fig. 4(a)), where the top and bottom boundary lines represent the onset and end gas velocities of flooding respectively. That is, the downward movement of particles was prevented partly at the flooding onset velocity, while prevented completely and even blown out of the reactor at the flooding end velocity [9].

Different from the Kwauk's phase diagram, the bubbling/turbulent transition line and the choking zone were also plotted in the EMMS-based phase diagram (Fig. 4(a)). It can be found that the transition velocity U_c increases with the increase of U_d , but is always less than U_t for Geldart B particles, which is consistent with the experimental results [30]. The top and bottom choking lines represent the top dilute phase voidage and the bottom dense phase voidage at the choking state respectively. It is clear that the EMMS-based phase diagram characterizes well the detailed hydrodynamics of gas–solid generalized fluidization, thus providing a reference for engineering design and scale-up.



(a) EMMS-based phase diagram for Geldart B particles

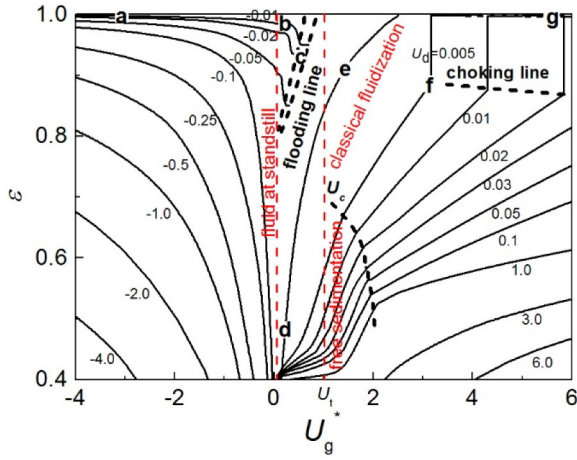


(b) Typical flow structures for Geldart B particles

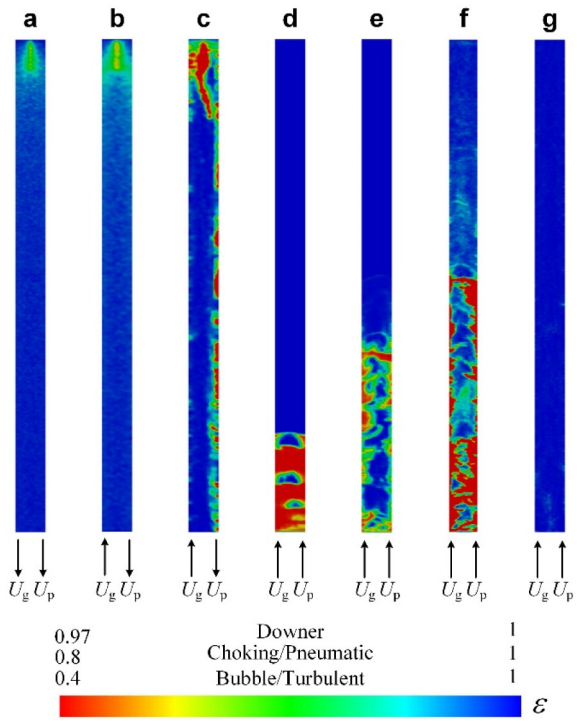
Fig. 4. (a) EMMS-based phase diagram and (b) typical flow structures for Geldart B particles.

Fig. 5(a) illustrates an EMMS-based phase diagram of generalized fluidization for Geldart A particles ($d_p = 100 \mu\text{m}$, $\rho_p = 1500 \text{ kg} \cdot \text{m}^{-3}$) in a fluidized bed of $H_t = 5 \text{ m}$ and $D_t = 0.1 \text{ m}$. Compared with the EMMS-based phase diagram for Geldart B particles, U_c becomes higher than U_t , and even the U_c line completely moves to the cocurrent upward regime with a narrow range of gas velocity [30,31]. Correspondingly, the flooding zone also becomes narrow for Geldart A particles, implying the difficulty involved in the operation of counter-current downer of Geldart A particles.

To display the gas–solid flow structure of phase diagram, utilizing the EMMS-DPM we simulated several typical operation regimes and some classic engineering phenomena. For Geldart B and A particles, the simulated voidage contour graphs corresponding to different operating conditions denoted as a, b, c, d, e, f, g in Figs. 4(a) and 5(a) were



(a) EMMS-based phase diagram for Geldart A particles



(b) Typical flow structures for Geldart A particles

Fig. 5. (a) EMMS-based phase diagram and (b) typical flow structures for Geldart A particles.

shown in Figs. 4(b) and 5(b), respectively. It can be seen that the voidage firstly increases along the axial direction and then almost maintains invariable in the fully developed region of cocurrent and counter-current flow. With the increase of U_g or G_s , the homogeneous gas-solid flow structure is destroyed and the flooding phenomenon appears in the counter-current downward flow. The particles move to the peripheral location and accumulate at the reactor top. With increasing gas velocity in the cocurrent upward flow, discrete gas bubbles are surrounded by continuous dense phase in bubbling fluidization, followed by a phase inversion beyond which discrete particle clusters are suspended by continuous dilute phase in turbulent fluidization. It is indicated that the top dilute phase region coexists with the bottom dense phase region at choking, while particle clusters disappear and

the gas-solid flow is nearly uniform in pneumatic transport. These qualitative phenomena for Geldart A and B particles are all consistent with published data [4,6,8,9], indicating the reasonability of the global EMMS models and the EMMS-DPM as well as the EMMS-based phase diagram.

4. EMMS-based Non-dimensional Correlations

The new phase diagrams summarize well the hydrodynamic characteristics of gas-solid generalized fluidization, but only incorporate the influences of operating conditions. In order to take into account the effects of material properties further, some typical hydrodynamic parameters were correlated in the form of non-dimensional numbers according to the EMMS-based simulation results. These parameters include choking gas velocity (U_{gc}), flooding onset velocity ($U_{gf,s}$), flooding end velocity ($U_{gf,e}$), choking bottom voidage (ε_b), choking top voidage (ε_t), voidage in the fully developed cocurrent downward flow ($\varepsilon_{full-co}$), and voidage in the fully developed counter-current downward flow ($\varepsilon_{full-ct}$).

Taking length, mass and time as independent physical dimensions, as listed in Table 4, four dimensionless quantities such as U_{pg} , ρ_{pf} , Re_p and Ar can be obtained in gas-solid fluidization systems according to the dimensional analysis method. It is clear that U_{pg} and ρ_{pf} represent operating conditions and material properties respectively, while Re_p and Ar are essentially Reynolds and Archimedes numbers, respectively. Therefore, as shown in Table 5, those critical variables were firstly calculated in the wide ranges of operating conditions and material properties by using the original EMMS model and/or its extensions, and further correlated to the preceding dimensionless numbers. The regression correlations were evaluated by the statistical parameter of fit goodness (R^2).

Table 4

Expressions and physical meanings of dimensionless quantities

Dimensionless number	Mathematical expression	Physical meaning
U_{pg}	$\frac{G_s}{U_g \rho_p} = \frac{U_p}{U_g}$	Ratio of solids to gas velocity
ρ_{pf}	$\frac{\rho_p}{\rho_g}$	Ratio of particle to fluid density
Re_p	$\frac{G_s d_p}{\mu_g} = \frac{\rho_p d_p U_p}{\mu_g}$	Reynolds number
Ar	$\frac{d_p^3 \rho_g (\rho_p - \rho_g) g}{\mu_g^2}$	Archimedes number

Table 5

Dimensionless correlations of typical hydrodynamic variables

Dimensionless correlations	R^2	Variable range
$U_{gc} = 11.1166 \frac{G_s}{\rho_p} (\rho_{pf})^{0.5513} (Re_p)^{-0.5143} (Ar)^{0.3418}$	0.999	$U_{gc} (0.1, 10) \text{ m} \cdot \text{s}^{-1}$
$\varepsilon_b = 0.7325 (\rho_{pf})^{0.0091} (Re_p)^{0.0175} (Ar)^{0.0137}$	0.956	$G_s \varepsilon (10, 400)$
$\varepsilon_t = 0.9845 (\rho_{pf})^{0.0051} (Re_p)^{-0.0084} (Ar)^{0.0033}$	0.930	$\text{kg} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$
$\varepsilon_{full-co} = 0.9256 (U_{pg})^{-0.0136} (\rho_{pf})^{0.0008} (Re_p)^{-0.0002} (Ar)^{0.0002}$	0.974	$d_p \varepsilon (50, 300) \mu\text{m}$
$\varepsilon_{full-ct} = 0.8428 (U_{pg})^{0.0014} (\rho_{pf})^{0.0293} (Re_p)^{-0.0257} (Ar)^{0.0141}$	0.963	$\rho_p \varepsilon (500, 3500) \text{ kg} \cdot \text{m}^{-3}$
$U_{gf,s} = 0.2389 \frac{G_s}{\rho_p} (\rho_{pf})^{1.0457} (Re_p)^{-1.0576} (Ar)^{0.6278}$	0.971	$\mu \varepsilon (0.1, 10) \text{ kg} \cdot \text{m}^{-3}$
$U_{gf,e} = 0.3047 \frac{G_s}{\rho_p} (\rho_{pf})^{1.0445} (Re_p)^{-1.0488} (Ar)^{0.6192}$	0.955	$\mu \varepsilon (1, 5) \times 10^{-5} \text{ kg} \cdot \text{m}^{-1} \cdot \text{s}^{-1}$
		$G_s \varepsilon (10, 500)$
		$\text{kg} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$
		$d_p \varepsilon (100, 2000) \mu\text{m}$

As shown in Fig. 6(a), the prediction of choking gas velocity in this article is in good agreement with the experiments as well as the calculation of Bi & Fan [32], while the other two correlations show discrepancies from the experimental data. Fig. 6(b) indicates that the top and bottom voidage of choking predicted by this article and the

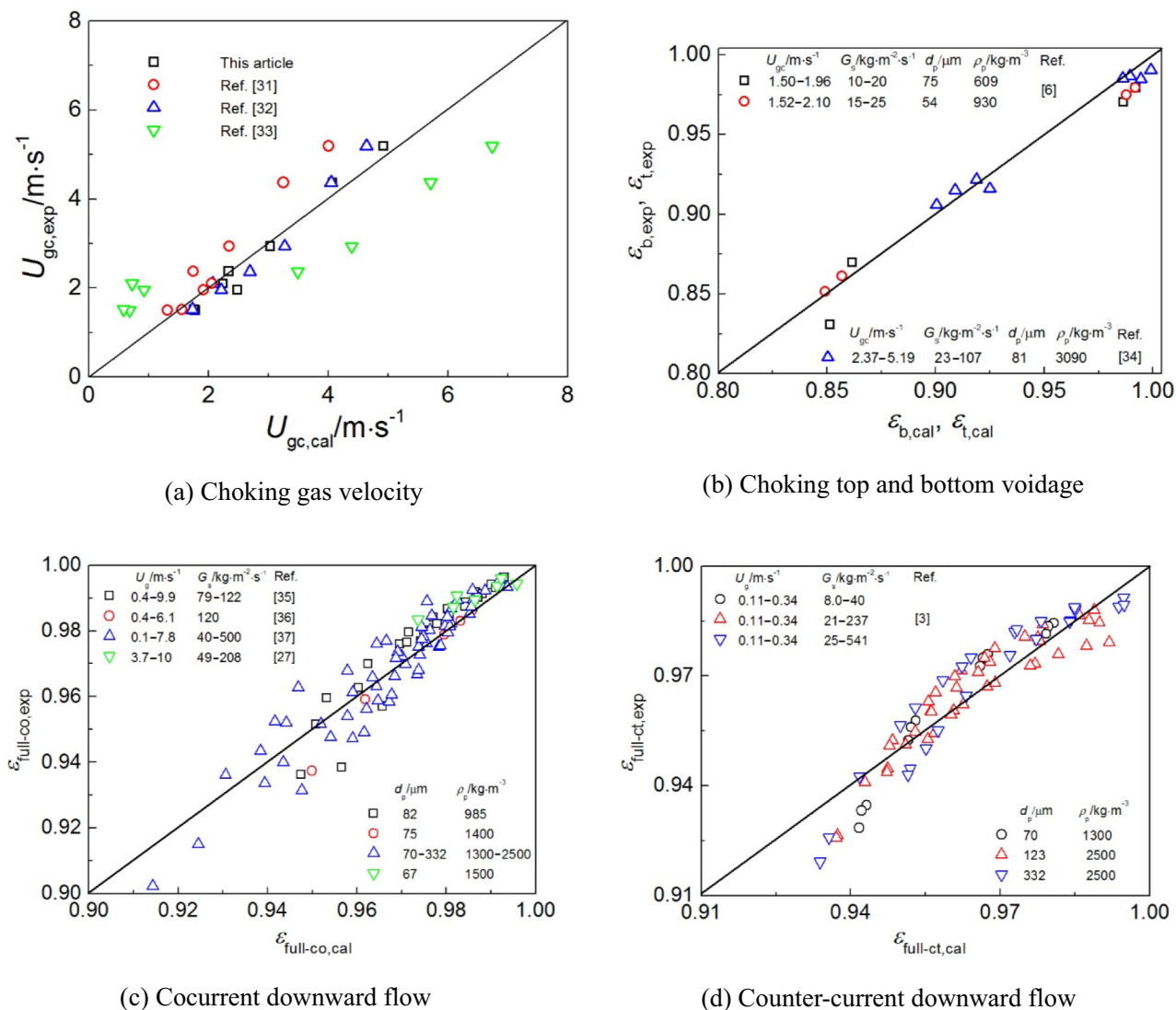


Fig. 6. Comparison between correlation prediction and experimental data for (a) choking gas velocity, (b) choking top and bottom voidage, (c) cocurrent downward flow and (d) counter-current downward flow.

experimental data are generally consistent under the various operation conditions, demonstrating their applicability.

As shown in Fig. 6(c) and (d), the predicted voidage in the fully developed cocurrent and counter-current downward flow are generally consistent with the measured data. However, it seems that the experimental data in the counter-current downward flow show a C-shaped profile. This may be because the experimental data were obtained in a very narrow range of gas velocity ($U_g \leq 0.34 \text{ m} \cdot \text{s}^{-1}$). Since these regressed correlations were developed in a wide range of operating conditions, they can be used to estimate the hydrodynamic parameters to facilitate the engineering application of the EMMS-based phase diagram.

5. Conclusions

The EMMS model and its extensions were used to simulate gas–solid fluidization systems under different operation modes as well as different flow regimes of cocurrent upward flow.

Utilizing the simulation results, the phase diagram of gas–solid generalized fluidization of Geldart A and B particles was drawn accurately, since the particle clustering phenomenon was considered in the EMMS-based simulation. The EMMS-based phase diagram not only

predicts the detailed flooding zone in the counter-current downward flow, but also illustrates the bubbling/turbulent transition line and the choking area in the cocurrent upward flow.

For the convenience of engineering design and scale-up of gas–solid generalized fluidization systems, the simulation results were further correlated in the form of dimensionless numbers to incorporate the influences of both operating conditions and material properties on some critical hydrodynamic parameters. The dimensionless correlations were also validated by comparing with a large amount of experimental data in this article.

Nomenclature

Ar	Archimedes number
D_t	reactor diameter, m
d_p	particle diameter, m
G	gravitational acceleration, $\text{m} \cdot \text{s}^{-2}$
G_s	solids flux, $\text{kg} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$
H_t	reactor height, m
K	coarse-grain ratio
Re_p	Reynolds number
U_c	turbulent transition velocity, $\text{m} \cdot \text{s}^{-1}$
U_d	normalized superficial solid velocity

U_g	superficial gas velocity, $\text{m}\cdot\text{s}^{-1}$
U_g^*	normalized superficial gas velocity
U_{gc}	choking gas velocity, $\text{m}\cdot\text{s}^{-1}$
U_{gf}	flooding gas velocity, $\text{m}\cdot\text{s}^{-1}$
$U_{gf,s}$	gas velocity at the onset of flooding, $\text{m}\cdot\text{s}^{-1}$
$U_{gf,e}$	gas velocity at the end of flooding, $\text{m}\cdot\text{s}^{-1}$
U_p	superficial particle velocity, $\text{m}\cdot\text{s}^{-1}$
U_{pg}	Ratio of solid to gas velocity
U_t	particle terminal velocity, $\text{m}\cdot\text{s}^{-1}$
U_{tr}	fast fluidization transition velocity, $\text{m}\cdot\text{s}^{-1}$
ε	voidage
ε_b	choking bottom voidage
ε_{CGP}	internal voidage of CGP
ε_{full}	voidage in fully developed region of downer
$\varepsilon_{full-co}$	voidage in the fully developed region of cocurrent downward flow
$\varepsilon_{full-ct}$	voidage in the fully developed region of counter-current downward flow
ε_t	choking top voidage
ρ_f	gas density, $\text{kg}\cdot\text{m}^{-3}$
ρ_p	particle density, $\text{kg}\cdot\text{m}^{-3}$
ρ_{pf}	Ratio of particle to fluid density
μ_f	fluid viscosity, $\text{kg}\cdot\text{m}^{-1}\cdot\text{s}^{-1}$

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Original EMMS model and its extension models

Table A1

Constitutive equations for the original EMMS model

Equations	Mathematical expression
Force balance for dilute phase	$\frac{3}{4}C_{df}\frac{1-\varepsilon_f}{d_p}\rho_f U_{st}^2 - (1-\varepsilon_f)(\rho_p - \rho_f)g = 0$
Force balance for dense phase	$\frac{3}{4}C_{dc}\frac{1-\varepsilon_c}{d_p}\rho_f U_{sc}^2 f + \frac{3}{4}C_{di}\frac{f}{d_{ci}}\rho_f U_{si}^2 - f(1-\varepsilon_c)(\rho_p - \rho_f)g = 0$
Pressure balance	$C_{df}\frac{1-\varepsilon_f}{d_p}\rho_f U_{st}^2 + \frac{f}{1-f}C_{di}\frac{1}{d_{ci}}\rho_f U_{si}^2 - C_{dc}\frac{1-\varepsilon_c}{d_p}\rho_f U_{sc}^2 = 0$
Mass balance for the gas	$U_g - U_f(1-f) - U_{cf} = 0$
Mass balance for the particles	$U_p - U_{pf}(1-f) - U_{pc}f = 0$
Cluster equation	$d_{cl} = g d_p \left(\frac{U_p}{1-\varepsilon_{max}} - \left(U_{mf} + \frac{\varepsilon_{mf} U_p}{1-\varepsilon_{mf}} \right) \right) / \left(N_{st} \frac{\rho_p}{\rho_b - \rho_f} - \left(U_{mf} + \frac{\varepsilon_{mf} U_p}{1-\varepsilon_{mf}} \right) g \right)$
Stability condition	$N_{st} = \frac{\rho_p - \rho_f}{\rho_f} g \left\{ U_g + (f U_c - U_g) \frac{(\varepsilon_f - \varepsilon_c) f^2}{1-\varepsilon_f + (\varepsilon_f - \varepsilon_c) f} \right\} \rightarrow \min$

Table A2

Constitutive equations for the EMMS bubbling model

Equations	Mathematical expression
Force balance for bubble phase	$\frac{3}{4} C_{Di} \frac{\rho_b}{d_b} f_b U_{si}^2 - f_b (\rho_e - \rho_g) g = 0$
Force balance for emulsion phase	$\frac{3}{4} C_{De} \frac{\rho_g}{d_p} (1 - f_b) (1 - \varepsilon_e) U_{se}^2 + \frac{3}{4} C_{Di} \frac{\rho_b}{d_b} f_b U_{si}^2 - (1 - f_b) (1 - \varepsilon_e) (\rho_p - \rho_g) g = 0$
Mass balance for the gas	$U_g - U_{ge} (1 - f_b) - U_{bf} = 0$
Mass balance for the particles	$U_p - U_{pe} (1 - f_b) = 0$
Stability condition	$N_{st} = \frac{\rho_b - \rho_g}{\rho_p} \frac{1 - 2f_b}{1 - f_b} g U_{ge} + \frac{\rho_b - \rho_g}{\rho_p} \frac{f_b^2}{1 - f_b} g U_b + \frac{3}{4} \frac{f_b}{H_b (1 - \varepsilon_s)} K g d_b U_g \rightarrow \min$

Table A3

Constitutive equations for the EMMS cocurrent downer model

Equations	Mathematical expression
Force balance for dilute phase	$\frac{3}{4} C_{Df,z} \frac{(1 - f_z)(1 - \varepsilon_{f,z})}{d_p} \rho_g U_{sf,z}^2 \pm (1 - f_z)(1 - \varepsilon_{f,z}) (\rho_p - \rho_g) (a_{f,z} - g) \pm \tau_{wpl,z} = 0$
Force balance for dilute phase	$\frac{3}{4} C_{Dc,z} \frac{f_z(1 - \varepsilon_{c,z})}{d_p} \rho_g U_{sc,z}^2 + \frac{3}{4} C_{Di,z} \frac{f_z}{d_{d,z}} \rho_g U_{si,z}^2 \pm f_z(1 - \varepsilon_{c,z}) (\rho_p - \rho_g) (a_{c,z} - g) \pm \tau_{wpc,z} = 0$
Pressure balance	$C_{Df,z} \frac{1 - \varepsilon_{f,z}}{d_p} \rho_g U_{sf,z}^2 + \frac{f_z}{1 - f_z} C_{Di,z} \frac{1}{d_{d,z}} \rho_g U_{si,z}^2 - C_{Dc,z} \frac{1 - \varepsilon_{c,z}}{d_p} \rho_g U_{sc,z}^2 = 0$
Mass balance for the gas	$U_g - f_z U_{c,z} - (1 - f_z) U_{f,z} = 0$
Mass balance for the particles	$U_p - f_z U_{pc,z} - (1 - f_z) U_{pf,z} = 0$
Height calculation	$\Delta H_z = \left(\frac{1}{1 - \varepsilon_z} + \frac{1}{1 - \varepsilon_{z-1}} \right) \left(\frac{U_{pc,z}}{1 - \varepsilon_{c,z}} - \frac{U_{pf,z-1}}{1 - \varepsilon_{f,z-1}} \right) \frac{U_p}{a_{c,z} + a_{f,z-1}}$
Stability condition	$N_{gs0,z} = 1 + \frac{A f_z^2 (1 - f_z) U_{f,z}}{B U_g} \rightarrow \min$ $A = (1 - \varepsilon_{f,z}) (a_{f,z} - g) - (1 - \varepsilon_{c,z}) (a_{c,z} - g) + \frac{(\varepsilon_z - \varepsilon_{f,z})}{f_z (1 - \varepsilon_z) (\rho_p - \rho_g)} \tau_{wpl,z}$ $B = (1 - f_z) (1 - \varepsilon_{f,z}) (a_{f,z} - g) + f_z (1 - \varepsilon_{c,z}) (a_{c,z} - g) + \frac{\tau_{wpc,z}}{\rho_p - \rho_g}$

Table A4

Constitutive equations for the EMMS counter-current downer model

Equations	Mathematical expression
Force balance for dilute phase	$\frac{3}{4} C_{Df,z} \frac{(1 - f_z)(1 - \varepsilon_{f,z})}{d_p} \rho_g U_{sf,z}^2 - (1 - f_z)(1 - \varepsilon_{f,z}) (\rho_p - \rho_g) (a_{f,z} + g) + \tau_{wpl,z} = 0$
Force balance for dilute phase	$\frac{3}{4} C_{Dc,z} \frac{f_z(1 - \varepsilon_{c,z})}{d_p} \rho_g U_{sc,z}^2 + \frac{3}{4} C_{Di,z} \frac{f_z}{d_{d,z}} \rho_g U_{si,z}^2 - f_z (1 - \varepsilon_{c,z}) (\rho_p - \rho_g) (a_{c,z} + g) + \tau_{wpc,z} = 0$
Pressure balance	$C_{Df,z} \frac{1 - \varepsilon_{f,z}}{d_p} \rho_g U_{sf,z}^2 + \frac{f_z}{1 - f_z} C_{Di,z} \frac{1}{d_{d,z}} \rho_g U_{si,z}^2 - C_{Dc,z} \frac{1 - \varepsilon_{c,z}}{d_p} \rho_g U_{sc,z}^2 = 0$
Mass balance for the gas	$U_g - f_z U_{c,z} - (1 - f_z) U_{f,z} = 0$
Mass balance for the particles	$U_p - f_z U_{pc,z} - (1 - f_z) U_{pf,z} = 0$
Height calculation	$\Delta H_z = \left(\frac{1}{1 - \varepsilon_z} + \frac{1}{1 - \varepsilon_{z-1}} \right) \left(\frac{U_{pc,z}}{1 - \varepsilon_{c,z}} - \frac{U_{pf,z-1}}{1 - \varepsilon_{f,z-1}} \right) \frac{U_p}{a_{c,z} + a_{f,z-1}}$
Stability condition	$N_{gs0,z} = 1 + \frac{A f_z^2 (1 - f_z) U_{f,z}}{B U_g} \rightarrow \min$ $A = (1 - \varepsilon_{f,z}) (a_{f,z} + g) - (1 - \varepsilon_{c,z}) (a_{c,z} + g) - \frac{(\varepsilon_z - \varepsilon_{f,z})}{f_z (1 - \varepsilon_z) (\rho_p - \rho_g)} \tau_{wpl,z}$ $B = (1 - f_z) (1 - \varepsilon_{f,z}) (a_{f,z} + g) + f_z (1 - \varepsilon_{c,z}) (a_{c,z} + g) - \frac{\tau_{wpc,z}}{\rho_p - \rho_g}$