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Stochastic modeling of the multiple rebound effects for particle–rough wall collisions

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The statistical behavior of colliding spherical particles onto rough walls is investigated by simulating deterministic rebounds onto two geometric rough walls with different collision angles. The first wall is generated from Gaussian distribution of wall roughness angles, whereas the other consists in a Gaussian distribution of the wall roughness heights and positions. The distribution of wall roughness angles experienced by the incident particles at the first rebound matches the effective probability distribution function (PDF) given by Sommerfeld and Huber [Sommerfeld, M., Huber, N., 1999. Experimental analysis and modelling of particle–wall collisions. Int. J. Multiphase Flow 25, 1457–1489]. The probability of the particles to make multiple rebounds according to the first rebound angle is characterized. As shown by the probability distribution function of the effective particle rebound angles, the multiple rebounds appear to be crucial for the global behavior of the particles moving away from the near-wall region, especially for the particles hitting the wall with primary collision angles very close to zero (referred to as grazing incident angles or particles). The multiple rebound effects lead to a zero probability for the particles to rebound with a grazing angle after the final collision onto the rough wall, contrary to the results obtained with the "Shadow Effect Model". With a special emphasis on the description of the rebound mechanisms shown by the simulation results obtained with deterministic rebounds, a new Lagrangian stochastic model based on only one rebound but incorporating the effects of multiple rebounds, is proposed for the particle–rough wall interaction. The model is validated by comparing the PDF of the effective rebound angle with available measurements.

1. Introduction and background

Disperse multiphase flow problems involving the particle–wall interactions arise in many processes of practical importance. The relevance of these interactions has been extensively investigated. For example, aerodynamic drag and lift forces acting on a finite-sized rigid spherical particle moving in the vicinity of a wall are correlated to the separation distance from the wall, according to the measurement (Muthanna et al., 2005) and the theoretical investigations (see e.g. Zeng et al., 2007). Moreover, the rebounds onto the wall are frequent for inertial particles whose response time is larger than characteristic time scales of fluid phase. These collisions, besides the change of the velocity direction, induce the loss of the momentum, the rotation of the particle and sometimes particle fractures. For such particles, the understanding of these rebound processes is of fundamental importance, in order to compute realistic trajectories from the equations of motion. To gain a basic understanding of the controlling mechanisms, many Lagrangian and Eulerian researches have been dedicated to the particles bouncing onto smooth walls (see e.g. Ottjes, 1978; Oesterlé, 1991; Sakiz and Simonin, 1999; Alipchenkov et al., 2001). However, according to Tsuji et al. (1987), inelastic collisions of spherical particles onto a plane wall result in many particles sliding along the wall after a number of collisions, contrary to experiments.

In practice, the walls are rough and their effects on the dispersed phase depend on the ratio between the particle diameters and the sizes of the asperities. Recent measurements in horizontal and vertical turbulent two-phase channel flows from Kussin and Sommerfeld (2002) and Benson et al. (2005) have shown that wall roughness has a strong effect on the dispersed phase properties. Kussin and Sommerfeld (2002) showed that the wall roughness enhances the transverse dispersion of the particles and their fluctuating velocities throughout the channel. Their measurements indicated that the wall roughness also causes a conspicuous reduction of the particle transport velocity. Except the analogous results on the wall roughness effects reported by Kussin and Sommerfeld (2002), the reduction of the particle transport velocity showed in the experiments of Benson et al. (2005) with the fully rough walls compared to the corresponding result for the smooth wall is around 40%.

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In the light of these measurements, the interaction between the particles and the wall roughness must be taken into account in numerical simulations. However, the problem remains the accurate modeling of the physical mechanisms that arise during the interactions.

The most natural approach consists in a deterministic modeling of the rough wall. The underlying idea of this modeling is the prior representation of the rough wall structure. Although the wall geometry is deterministic, its modeling is performed using stochastic approaches. In this way, by assuming no correlation between the position of the incident particle and the wall roughness structure, Matsumoto and Saito (1970a,b) consider a periodic location of the asperities and a uniform distribution of the roughness heights. The rough wall structure is modeled as the following sine function:

$$y = A_r \sin\left(\frac{2\pi}{L_r}x + \alpha\right) \tag{1}$$

in which α is the phase of the roughness treated randomly according to a uniform distribution in $[0, 2\pi]$. A_r and L_r are the amplitude and the cycle of the wall roughness, respectively.

Comparisons between numerical simulations and measurements showed reasonable agreement for both mean velocity and concentration of the dispersed phase in the channel. However, Sommerfeld (1992) pointed out that the walls in the experiments must be regarded as smooth, because the measurements were conducted in a channel made of glass plates. For these reasons, the experiments demonstrate the effect of slight non-spherical particles instead of the wall roughness.

The two-dimensional geometrical rough wall model proposed by Frank et al. (1993) is based on the random distribution of height and location of the rough wall asperities. The rough wall surface is schematically described from a juxtaposition of polygonal elements whose vertex coordinates s_n and z_n are provided from a random uniform distribution over $\left[\frac{1}{2}\overline{S}, \frac{3}{2}\overline{S}\right]$ and $[-z_{\max}, z_{\max}]$, respectively. The model parameters $z_{\max}$ and $\overline{S}$, which must be determined by a prior microscopic examination of the wall material specimens, are functions of the diameter of particles d_p and of the mean values of the length scale and the amplitude of the wall surface roughness. Numerical predictions of the particle mean velocities in gas-particle horizontal channel flow showed a good agreement with measurements for large inertial particles, whereas they were overestimated for the smaller diameters. The discrepancies were attributed to the effects of three-dimensional roughness, which may play an important role in the loss of kinetic energy during rebounds.

Despite the importance of the three-dimensional structure of the wall roughness, the realistic two-dimensional stochastic roughness structure proposed by Tsirkunov and Panfilov (1998) consists, by using the cubic spline, in the connection of a finite number N of random points $(x_i, y_i)_{1\leqslant i\leqslant N}$ satisfying:

$$\begin{cases} x_1 = 0 \\ x_i = x_{i-1} + h + \xi & (i = 2, 3, \ldots, N) \\ y_i = \eta & (i = 1, 2, \ldots, N) \end{cases} \tag{2}$$

where $2h$ is the mean cycle of the roughness, and the random values ξ and η are sampled from Gaussian distribution with a zero mean value and standard deviations $\Delta\xi$ and $\Delta\eta$, respectively. $\Delta\eta$ defines the mean height of the asperities of a surface or the mean roughness depth. The parameters $h, \Delta\xi$ and $\Delta\eta$ should be determined from measurements.

To validate this model, Tsirkunov and Panfilov (1998) investigated the rebound process with three different rough walls: a sine-shaped profile, the above model (2) and a sample of measured profile, on which 10^5 particles have been thrown for a given collision angle. The particles were allowed to make multiple rebounds onto the rough wall in order to leave the rough wall structure. The scattering of the particles after rebound onto each of the rough walls is compared with the case of smooth wall. With the sine-shaped profile, a narrow dispersion over the direction of particle velocity is obtained. By contrast, a spread similar distribution of rebound angle was observed for the other two wall cases. This result indicates that the modeling of the roughness structure by sine-shaped is inadequate. The second important result is the probability density function of the rebound angle of the particles that reveals a zero probability to rebound with an angle very close to zero (referred to as grazing angle or particle, in the following). Indeed, as long as the particle rebounds with a grazing angle, it would encounter another asperity, resulting most probably in a large rebound angle which would ensure that the particle leaves the near-wall region.

Granted the deterministic modeling of the rough wall is very precise to investigate the mechanisms arising during the particle–rough wall interactions, however such an approach turns out too cumbersome for practical computations because of the determination of collision location onto the geometrical wall whenever a rebound occurs.

Another more practical description of particle–rough wall interactions consists in the stochastic modeling. In this approach, it is not needed to construct the rough wall structure. However, one attempts to model the effect of the roughness on the colliding particle onto the wall. The basic idea assumes whenever the particle reaches the rough wall, it contacts a smooth "virtual" inclined wall with a randomly chosen angle γ (see Fig. 1). This "virtual wall" modeling approach first introduced by Tsuji et al. (1987) implicitly assumes that the roughness height is negligible. Their "*Abnormal bouncing model*" based on the "virtual wall" concept that would enable spherical particles to bounce on the wall, even in the case of inelastic rebounds, provides the inclined virtual wall angle γ by the following empirical formulation for a given incident angle α^-:

$$\gamma = \begin{cases} c R^k \delta_0(\beta - \alpha^-) & \text{if } \alpha^- \leqslant \beta \\ 0 & \text{otherwise} \end{cases} \tag{3}$$

where R is a random number between $]0, 1]$, $\beta = 7^\circ$, $c = 5$, $k = 4$ and δ_0 is empirically obtained as a function of Froude number (Fr) by:

$$\delta_0 = \frac{2.3}{Fr} - \frac{91}{Fr^2} + \frac{1231}{Fr^3}, \quad Fr = \frac{\bar{u}}{\sqrt{gh}} \tag{4}$$

in which $\bar{u}$ is the mean fluid velocity and h the channel height.

This model implies that only the particles that reach the wall with an incident angle smaller than the empirical limit angle β, experience the wall roughness effects. Furthermore, the empirical

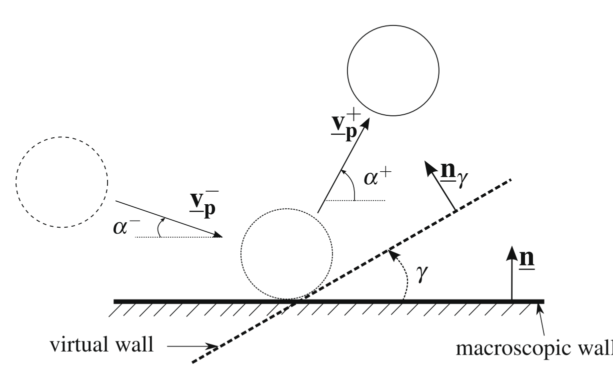

Fig. 1. Illustration of the rebound of a spherical particle onto the inclined smooth virtual wall.

formulation of δ_0 is intrinsically attached to horizontal flows. Accordingly, the recent use of the "Abnormal bouncing model" by Fukagata et al. (2001) to analyze the redistribution effects of momentum by wall roughness on dispersed phase, in the framework of Lagrangian simulations of the vertical turbulent channel flow of gas-particle, led them to treat it as a parameter. They showed that the probability distribution function of the wall roughness γ arising from "Abnormal bouncing model" is expressed by:

$$P(\gamma) = \begin{cases} \frac{[c\delta_0(\beta-\alpha^-)]^{-\frac{1}{k}}}{k}\gamma^{\left(\frac{1}{k}-1\right)}, & 0 < \gamma < c\delta_0(\beta - \alpha^-) \\ 0, & \text{otherwise} \end{cases} \tag{5}$$

This formulation indicates a high probability of the choice of acute roughness angles.

Although the "Abnormal bouncing model" expresses a perspective effect of the rough wall in terms of the collision angle, its major drawback is its incapability of reproducing wall roughness effects for incident angles larger than $\beta = 7^\circ$. Basically, there is no physical argument that could defend the restriction of wall roughness effects for this incident angle domain. Moreover, the fact that an incident particle may not hit a negative roughness angle makes this model questionable. Actually, with a coarse approximation of an asperity of the wall by a triangular shape whose the base represents the macroscopic wall, there is no physical reason that the probability for an incident particle to reach the descendant side (characterized by negative angles) is null, and equals 1 for the ascendant side. Another unpractical aspect of the use of "Abnormal bouncing model" remains that the empirical values $c,\ k$ and δ_0 can be changed according to the case. Obviously, the use of the model by Fukagata et al. (2001) to predict the particle phase properties in rough channel yields discrepancies between the measurement and the results, even by modifying roughness and rebound parameters.

The "*Virtual wall*" concept also constitutes the support of the model of Sommerfeld (1992). However to improve the model, he suggests:

- a random choice of the inclined virtual wall angle γ for all collision angle α^-,
- the wall roughness angle γ is chosen with respect to a probabilistic distribution law (uniform, Gaussian with zero mean and a given standard deviation $\Delta\gamma$) in $[-\gamma_{max}, \gamma_{max}]$.

The first point assumes wall roughness effects for all particle trajectories while the second one allows the random choice of negative angles. The maximum roughness angle γ_{max} is obtained in terms of the particle diameter and the most important parameters of the rough wall, i.e. the mean roughness depth and the mean cycle of roughness. In this model, the perspective effect of the rough wall experienced by the incident particle is ignored, contrary to the "Abnormal bouncing model". That obviously leads to some rebound issues for both the small collision angles and the negative sampled wall roughness angles: the incident particle crosses the wall after rebound. In other words, the particle goes out of flow domain. To overcome this problem, the solution adopted by Sommerfeld (1992) consists in the change from $\gamma < 0$ to an effective roughness angle $\gamma_{eff} = -\gamma > 0$. This means that the sampling of the wall roughness angle for these small collision angles is performed according to another stochastic law which is far from a Gaussian. Therefore, the distribution of the wall roughness angle experienced by the colliding particles onto the rough wall (referred to as incident effect) for a certain range of the collision angles is of a crucial aspect to describe the rebound process.

Furthermore, the measurement of the distribution of the physical wall roughness angle by Schade and Hädrich (1998) and Sommerfeld and Huber (1999) validates the Gaussian shape approximation. However, Schade and Hädrich (1998) pointed out that the effective probability density function (PDF) of the roughness angle "*seen*" by the particles should be a modification of the distribution of the physical wall roughness angle by an incident effect.

According to Sommerfeld and Huber (1999), there exists a so-called "*shadow effect*" for the small collision angles which results in the combination of the incident and rebound effects. The first one occurs before particle–wall collision and is due to a perspective of the physical rough wall for a given incident particle, while the second effect that arises after the particle–wall collision is due to the assumption that the particle should return in the flow. From the first effect, Sommerfeld and Huber (1999) show that the effective probability distribution function of the wall roughness inclination seen by the incident particles is as follows:

$$P_{eff}(\alpha^-, \Delta\gamma, \gamma) = \frac{\sin(\alpha^- + \gamma)}{\sin\alpha^-} P_g(\Delta\gamma, \gamma)\xi(\alpha^-, \Delta\gamma) \tag{6}$$

$\xi(\alpha^-, \Delta\gamma)$ ensures the normalization of the PDF for the given collision angle α^-. $P_g(\Delta\gamma, \gamma)$ is the unconditional normal distribution defined by:

$$P_g(\Delta\gamma, \gamma) = \frac{1}{\sqrt{2\pi\Delta\gamma^2}} \exp\left(-\frac{\gamma^2}{2\Delta\gamma^2}\right) \tag{7}$$

The procedure proposed by Sommerfeld and Huber (1999) to account for "*shadow effect*" in Lagrangian particle simulations is as follows:

- the roughness angle is sampled from the normal distribution function (7),
- if a negative roughness angle with an absolute value larger than α^- is sampled, an unphysical collision results, namely the particle comes from behind the wall and hence a new value is sampled for γ,
- if the collision leads to the rebound velocity directed towards the wall, a new roughness angle has to be sampled.

According to Konan et al. (2006), the PDF of wall roughness resulting from this procedure might be expressed by:

$$P^\star_{eff}(\gamma|\underline{\mathbf{v}}_\mathbf{p}^-) = \lambda\left(\underline{\mathbf{v}}_\mathbf{p}^-\right) H\left(-\underline{\mathbf{v}}_\mathbf{p}^- \cdot \underline{\mathbf{n}}_\gamma\right) H\left(\underline{\Phi}_\gamma\left(\underline{\mathbf{v}}_\mathbf{p}^-\right) \cdot \underline{\mathbf{n}}\right) P_g(\Delta\gamma, \gamma) \tag{8}$$

where the application $\underline{\Phi}_\gamma$ from the set of the incident velocities ($\underline{\mathbf{v}}_\mathbf{p}^-$, such as $\underline{\mathbf{v}}_\mathbf{p}^- \cdot \underline{\mathbf{n}} < 0$) towards the set of the rebound velocities is defined by the particle rebound law on a smooth inclined wall of angle γ. The normalization coefficient λ of the PDF is given by:

$$\lambda\left(\underline{\mathbf{v}}_\mathbf{p}^-\right) = \left[\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} H\left(-\underline{\mathbf{v}}_\mathbf{p}^- \cdot \underline{\mathbf{n}}_\gamma\right) H\left(\underline{\Phi}_\gamma\left(\underline{\mathbf{v}}_\mathbf{p}^-\right) \cdot \underline{\mathbf{n}}\right) P_g(\Delta\gamma, \gamma) d\gamma\right]^{-1} \tag{9}$$

The first Heaviside function of Eq. (8) conditions the realisability of virtual wall angle by ensuring that the incident particle comes from the flow and hits the virtual wall: $\underline{\mathbf{v}}_\mathbf{p}^- \cdot \underline{\mathbf{n}}_\gamma < 0$. The second one states that rebounded particle returns into the flow after collision: $\underline{\Phi}_\gamma(\underline{\mathbf{v}}_\mathbf{p}^-) \cdot \underline{\mathbf{n}} > 0$.

As it is shown by the model (8), the procedure proposed by Sommerfeld and Huber (1999) rather leads to a random sampling of the wall roughness angle from a truncated normal distribution. Therefore, the procedure does not accurately account for the incident effect, since the wall roughness is not sampled from the effective PDF (6). However, it has been applied with relative success by comparison with experiments in RANS/Lagrangian simulations (see e.g. Laìn et al., 2002). It enabled to investigate the influence of the 3D wall roughness on the particle velocity variance, turbulent transport, and the concentration of the particles in a vertical turbulent channel flow in the framework of LES/DPS simulations at low Reynolds number (Squires and Simonin, 2006). Moreover, it has been used by Konan et al. (2006) in the derivation of Eulerian rough wall boundary conditions in the framework of continuum approach. However, they pointed out the many grazing particles generated by the "shadow effect model". This is expressed by a significant probability for the particles to rebound with an angle close to zero. Especially, when the incident collision angle is small, it emerges a significant probability that the colliding particle rebounds with a zero wall-normal velocity (Konan et al., 2007; Sommerfeld and Huber, 1999). Because of the grazing particles, crucial closure problems in the derivation of Eulerian rough wall boundary conditions occurred (Konan et al., 2006). According to Konan et al. (2007), the underestimation of the wall-normal velocity variance arisen in their LES/DPS simulations with the "shadow effect model", is the consequence of the absence of mechanisms that would allow the grazing particles to return in the flow. Furthermore, Tsirkunov and Panfilov (1998) have shown that the probability density to rebound with null angle tends towards zero for the very small collision angle. They argued that the major drawback in Sommerfeld's (1992) stochastic model is the impossibility of the multiple rebounds. Basically, a particle could not indefinitely move along the wall, since it might hit another asperity of the rough wall. Most probably, that would ensure its moving away from the near-wall region. But such an eventuality is unimaginable with the "Shadow Effect Model" because the analysis that led to its proposition ignores the roughness heights.

It emerges from all these investigations that the "shadow effect" procedure suggested by Sommerfeld and Huber (1999) cannot correctly reproduce the incident effect experienced by the particles during the collision step especially for small collision angle, and it describes partially the mechanisms that ensure the rebound of the particles. Therefore, we might wonder:

- what is the real wall roughness angle distribution "*seen*" by an incident particle?
- what is the effective behavior of a particle undergoing the collision process with the rough wall?

The present paper investigates a statistical analysis on the mechanisms that occur during particle–rough wall collisions. Answers to both foregoing questions are given by performing deterministic rebounds of particles onto two different two-dimensional rough wall geometries. The mechanisms showed by the results are discussed and used as support of the derivation of "*Rough Wall Multi-Collision model*", a new Lagrangian procedure of particles–rough wall interaction treatment. Finally, a comparison between Sommerfeld and Huber (1999) measurements of probability density function of rebound angles and the results of simulations with the "*Shadow Effect model*" and the "*Rough Wall Multi-Collision model*" is given.

2. Statistical study of the rebound of particles on geometrical rough walls

2.1. Setup of the particle deterministic rebounds on the geometrical walls

Despite the three-dimensional aspect of the wall roughness and its most probably crucial influence in the description of the rebound mechanisms of the particles onto the rough walls, we considered the wall roughness as two-dimensional.

We simulated two roughness geometries. The first (referred to as wall N°1) is consistent with Sommerfeld's (1992) approach with the Gaussian distribution of the roughness angles. The simulation of the wall is performed by connecting, by segments of a line, a finite number N of points $(x_i, y_i)_{1\leqslant i\leqslant N}$ generated according to:

$$\begin{cases} x_1 = 0, \quad y_1 = 0 \\ x_{i+1} = x_i + \Delta x & (i = 2, N) \\ y_{i+1} = y_i + \Delta x \cdot \tan\gamma_i & (i = 2, N) \end{cases} \tag{10}$$

where Δx is a sampling distance whose modification leads to a simple homothetic transformation of the simulated wall. γ_i denotes the ith wall roughness angle sampled from the unconditional normal distribution (7) for a given wall roughness standard deviation $\Delta\gamma$.

In this first model, the distribution of the positions and heights of the asperities are not directly investigated. For the second wall (referred to as wall N°2), we used the roughness structure proposed by Tsirkunov and Panfilov (1998) (2) that accounts for the random distribution of both positions and heights.

Two rough walls are assumed *statistically similar* if exactly the same distribution of the wall roughness angle is found for an incident particle of diameter d_p that hits both walls with a vertical angle $\frac{\pi}{2}$.

In order to compare statistics resulting from deterministic rebounds onto both wall types for a given wall roughness standard deviations, we defined the corresponding parameters h, $\Delta\xi$ and $\Delta\eta$ of the model of Tsirkunov and Panfilov (1998). The procedure to assess these parameters is empirical and starts by arbitrary choice for them to simulate the rough wall. The next step consists in throwing thousands of particles onto that simulated wall for an incident angle equal to $\frac{\pi}{2}$. The parameters are modified until the expected standard deviation of the wall roughness distribution is obtained.

To simulate the two standard deviations $\Delta\gamma = 2.5^\circ$ and $\Delta\gamma = 5^\circ$, the two diameters of the particles used are $d_p = 500\ \mu\text{m}$ and $d_p = 100\ \mu\text{m}$, respectively. We simulated only one rough wall N°2, with the parameters $h = 12.8\ \mu\text{m}$, $\Delta\xi = 0.0\ \mu\text{m}$ and $\Delta\eta = 0.808\ \mu\text{m}$ that exactly correspond to each couple of parameters $(\Delta\gamma = 5^\circ,\ d_p = 100\ \mu\text{m})$ and $(\Delta\gamma = 2.5^\circ,\ d_p = 500\ \mu\text{m})$. Fig. 2(a) and (b) presents two *statistically similar* rough walls with the wall roughness standard deviation $\Delta\gamma = 2.5^\circ$.

Deterministic rebounds of the particles onto these walls are carried out by throwing many particles on them for a given incident angle α^-. The initial position (x_p, y_p) of the particles is such that x_p is randomly chosen between the wall bounds whereas y_p should be greater than the greatest height of the wall roughness. Moreover, after a rebound if the particle continues to move towards the wall (Fig. 3(a)) or rebounds with a grazing angle

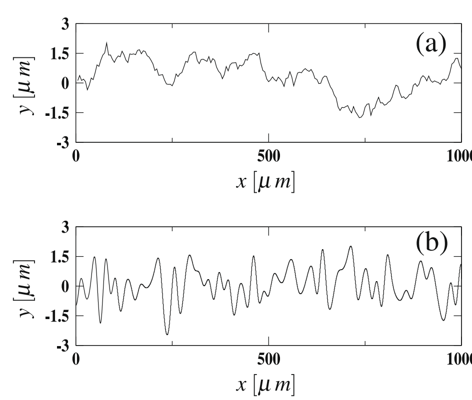

Fig. 2. Simulated profiles of the wall roughness structure. (a) Gaussian distribution of the wall roughness angles with $\Delta\gamma = 2.5^\circ$ (referred to as wall N°1). (b) Gaussian distribution of both roughness height and position (referred to as wall N°2) with $h = 12.8\ \mu\text{m}$, $\Delta\xi = 0.0\ \mu\text{m}$ and $\Delta\eta = 0.808\ \mu\text{m}$.

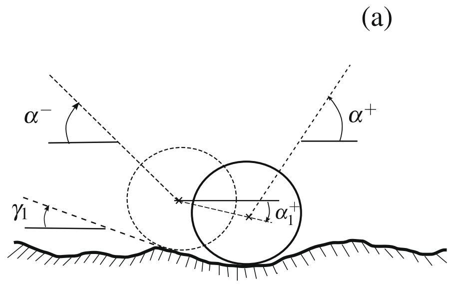

Fig. 3. Illustration of the multiple rebounds. (a) The particle continues to move towards the wall after the first rebound. (b) The particle rebounds with a positive angle after the first rebound. The wall roughness positions are spread out to clearly exhibit the rebound possibilities in terms of the first rebound angle α_1^+.

(Fig. 3(b)), the particles are enabled to make multiple rebounds in order to leave the wall region. In other words, while the particles may hit the wall another time, the new collision point and the rebound velocities are computed until their complete moving away from the wall. The pertinence of this assumption will be discussed. Furthermore to better grasp the mechanisms, fully elastic rebounds are considered and the rebound velocities are then given by: $\left(u_p^+ = u_p^-,\ v_p^+ = -v_p^-\right)$. The superscripts $(-)$ and (+) denote the particle properties before and after rebound, respectively. Three collision angles: $\alpha^- = 2.5^\circ,\ 12.5^\circ$ and 32.5° that typically express small (or grazing), medium and large collision angle are studied.

2.2. Statistical analysis of simulation results

2.2.1. Distribution function of the wall roughness angles

According to the measurements of Sommerfeld and Huber (1999), the distribution of the wall roughness angles can be approximated by a normal distribution function. However, the distribution of the wall roughness experienced by a colliding particle in terms of its attack angle onto the rough wall might be considered as an open problem. Actually, even though Sommerfeld and Huber (1999) have shown from both geometrical and mathematical arguments that the effective distribution function of the wall roughness seen by the particle is modeled by (6) and (7), neither measurements nor numerical experiments validate this theoretical formulation. Furthermore, it is obvious that the distribution of wall roughness angle experienced by the particle differs according to the collision angle, and it might spread or restrict to a certain domain of roughness angles for large or small collision angles. That is simply a perspective effect.

Fig. 4(a)–(f) presents the distribution of the wall roughness seen by the incident particle just at the first collision on the wall, for the three incident cases and the two standard deviations of wall roughness. The first interesting result is that the distributions obtained with all simulated cases and both geometrical wall models are nearly identical despite the difference in the generation of the rough walls. This indicates that the statistical behavior of the particles is independent of the wall model during the first collision step. Moreover, comparisons between the distribution of the wall roughness angles drawn from deterministic rebounds and the effective distribution (6) and (7) show excellent agreement, even for the small collision angle. Secondly, the results do not show a truncated Gaussian shape of the wall roughness distribution as it occurs in the framework of the "Shadow Effect Model" (Sommerfeld and Huber, 1999) with the small collision angles.

2.2.2. Stochastic characterization of the multiple rebounds

Fig. 3(a) and (b) shows, in terms of rebound angle α_1^+ resulting from the first collision of the particle, that the particle may reach again the wall, whether it continues to move towards the wall or it rebounds with a grazing angle. Actually, when the particle continues to move towards the wall, this means that the first rebound angle α_1^+ is negative, and consequently the particle will inevitably reach the wall. This is illustrated in Fig. 5 by the constant shape of the curve for $\alpha_1^+ < 0$ indicating a probability equal to 1 to make another rebound. The second part highlighted by Fig. 5 shows that with a positive rebound angle, there exists a decreasing probability for the particle to make another rebound when the rebound angle increases. The probability to make another rebound when $\alpha_1^+ > 0$, emphasized in Fig. 5, decreases exponentially with the increase of the rebound angle α_1^+. Therefore, the probability depicts in Fig. 5 describes the conditioned probability $P^\star\left(n > 1|\alpha_1^+, \alpha^-\right)$ on both the first rebound angle α_1^+ and the collision angle α^- that more than one rebound happens. Furthermore, it appears that this probability to have another rebound slightly depends on the collision angle α^- onto the wall.

To conclude, the particle has a non-zero probability to make another rebound, even if the rebound angle is greater than zero.

2.2.3. Probability density function of the rebound angles

The particle rebound angle distribution function is one of the most important characteristics for the statistical description of the behavior of the particles after collision onto the wall. In Fig. 6(a)–(f), we plotted three types of rebound angle PDF of the particles that:

(1) experience one and only one rebound and leave the wall region,
(2) make more than one rebound before their moving away from the wall,
(3) all the particles gathered under both (1) and (2).
This last rebound angle distribution function will be referred to as the *final rebound angle PDF of the particles* in the following.

A first conspicuous result exhibited in the figures is that the final rebound angle PDF exactly matches the PDF of the rebound angle of particles that make just one rebound. Furthermore, the rebound angle PDF of particles that make more than one rebound is shifted with respect to both other PDF when the collision angle increases. Note that in the case with $\Delta\gamma = 2.5^\circ$ and $\alpha^- = 32.5^\circ$, the particles experienced just one rebound (refer to Fig. 6(c)). For a collision angle close to the wall standard deviation, the PDF of item (2) is approximately equal to those of (1) and (3); whereas for a larger collision angle, likely because of the decrease of the number of multiple rebounds, a more pronounced difference between the PDF (2) and (1) or (3) is observed. To clearly account for what is occurring, the probability to make multiple rebounds as a function of the collision angle α^- is plotted in Fig. 7. The behavior of this probability demonstrates that an increase of the incident angle leads to a reduction of the number of multiple rebounds. Thus, it

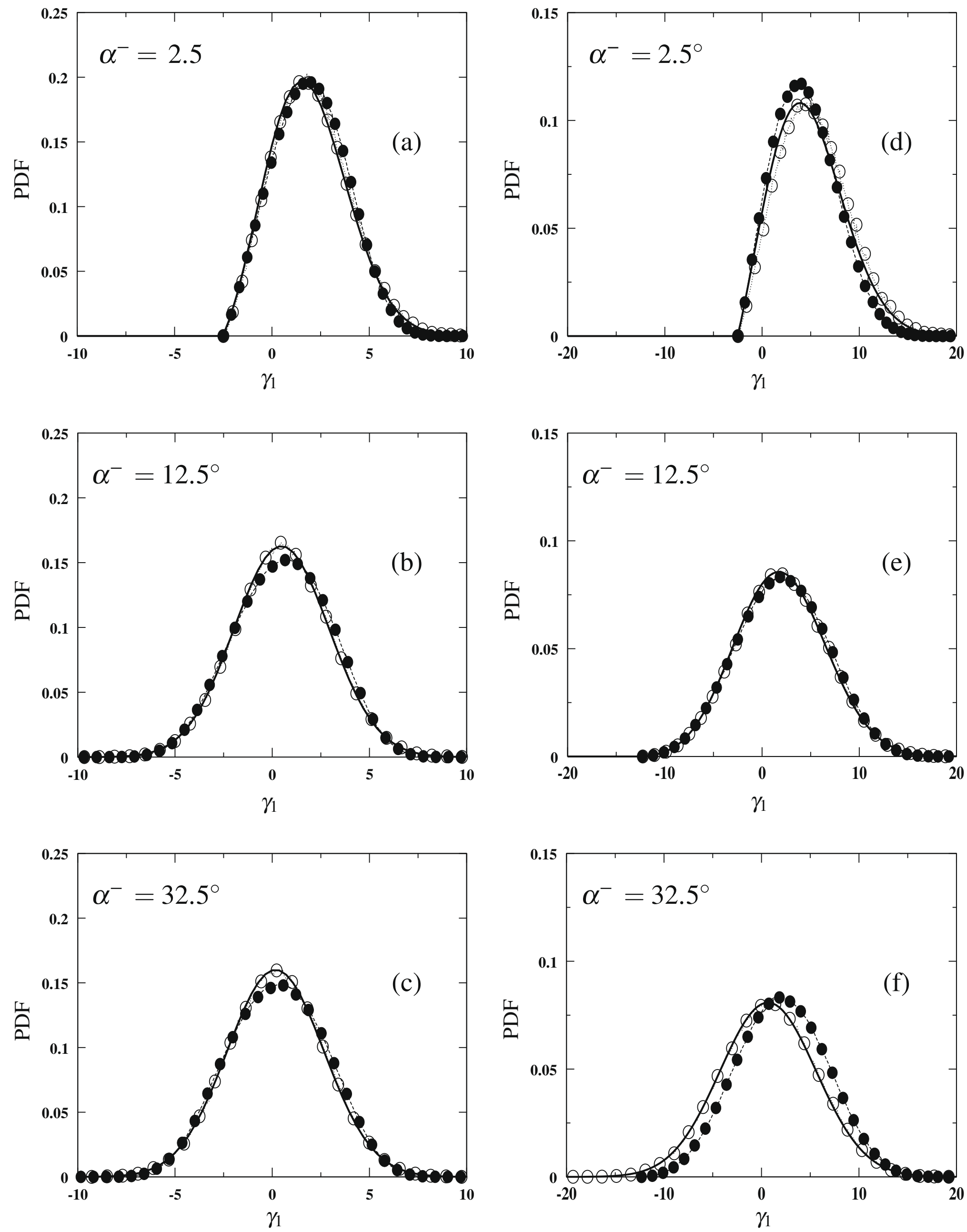

Fig. 4. Probability distribution function of the wall roughness angle (γ_1) at the first collision onto the rough wall for a given collision angle α^- and the wall roughness standard deviation ($\Delta\gamma = 2.5^\circ$: (a)–(c) and $\Delta\gamma = 5.0^\circ$: (d)–(f)). Empty and filled symbols denote the distributions obtained from wall N°1 and N°2, respectively. The solid line plots the effective distribution (6) and (7) of Sommerfeld and Huber (1999).

emerges from these statistics that the percentage of particles that experience several rebounds remains smaller than 10% with a maximum value for an incident angle about $2\Delta\gamma$. This percentage strongly decreases when the collision angle increases. For instance, less than 1% of the particles experience several rebounds with collision angle greater than $5\Delta\gamma$. In the case of Fig. 6(c) where the impact angle is about $\alpha^- = 32.5^\circ$ and the standard deviation of the wall roughness angles is $\Delta\gamma = 2.5^\circ$, any second rebound was happened. The small amount of the multiple rebounds shown for all the cases results in a weak weight in the PDF of the rebound angle for all particles. Accordingly, the PDF of the rebound angle for all particles is identical to that for particles experiencing just one rebound (see Fig. 6). On balance, it appears that the multiple rebounds have a weak effect when the collision angle is large, whereas they are crucial in the description of the rebound process of the grazing incident particles.

Another important result showed by these rebound angle PDFs is that the probability for the particles to rebound with a grazing angle is zero, contrary to the "*Shadow Effect Model*".

3. Stochastic Lagrangian modeling of particles–rough wall interactions with multiple rebound effects

3.1. Basic approximation

The above mentioned deterministic rebounds of particles onto the geometrical rough walls pointed out two fundamental steps during the rebound process: incidence and reflection. It emerged

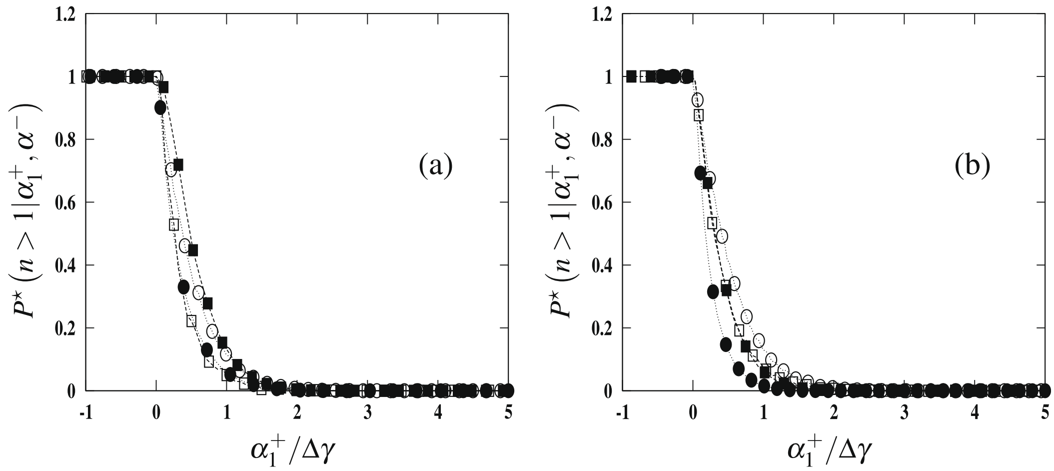

Fig. 5. Probability to make more than one rebound in terms of the first rebound angle α_1^+. The wall roughness standard deviations in cases (a) and (b) are $\Delta\gamma = 2.5°$ and $\Delta\gamma = 5.0°$, respectively. The symbols ○ and □ represent the collision angles $\alpha^- = 2.5°$ and $\alpha^- = 12.5°$. Empty and filled symbols refer to wall N°1 and wall N°2, respectively.

that the distribution function of the final rebound angle is nearly identical to those that make only one rebound. This leads us to assume that a particle experiences only one effective virtual rebound, in the framework of the present modeling. Furthermore, the inclined virtual wall approach on which the particle collides is resumed. Therefore, the description of the particle–rough wall interactions sums up into the accurate modeling of incident effect in order to provide the virtual wall angle in terms of the incidence and reproduce more closely multiple rebound effects through a unique rebound model.

3.1.1. Analysis of the incident effect

The incident effect is characterized by a perspective of the physical rough wall "*seen*" by a colliding particle onto the wall. In the framework of the stochastic modeling of the wall roughness effect, this might be expressed by a modification of the distribution of the physical wall roughness angles for each incident particle. For example with the "Shadow Effect Model", even though the resulting truncated Gaussian distribution of wall roughness angles is the result of a joint description of the incidence and the rebound of the particle on the rough wall, this modeling highlights an underlying incident effect. Actually, by defining the conditional standard deviation of wall roughness angle on the incidence α^- such that: $[\sigma(\gamma|\alpha^-)]^2 = \langle\gamma^2|\alpha^-\rangle - \langle\gamma|\alpha^-\rangle^2$, where $\langle\gamma^2|\alpha^-\rangle = \int_{-\pi/2}^{\pi/2}\gamma^2 P^{\star}_{eff}(\gamma|\alpha^-)d\gamma$ and $\langle\gamma|\alpha^-\rangle = \int_{-\pi/2}^{\pi/2}\gamma P^{\star}_{eff}(\gamma|\alpha^-)d\gamma$ with the wall roughness conditioned PDF $P^{\star}_{eff}(\gamma|\alpha^-)$ given by (8). One shows, in the case of the fully elastic rebounds, that for grazing incident particles (defined by an incidence $\alpha^- \to 0, \pi$) the conditional standard deviation $\sigma(\gamma|\alpha^-)$ tends to $\Delta\gamma\sqrt{1-\frac{2}{\pi}}$. The distribution of the wall roughness is then reduced to around 60% of the Gaussian distribution of physical wall angles. For vertical incidences with $\alpha^- \to \pi/2$, the conditioned standard deviation $\sigma(\gamma|\alpha^-)$ tends to $\Delta\gamma$. This means that the distribution of the wall roughness expands with the increase of the particle collision angle, and beyond a certain collision angle the shadow effect does not exist anymore.

Such an incident effect occurs in the "Abnormal bouncing model" (Tsuji et al., 1987), although no physical evidence can support it.

The particle collisions onto the deterministic rough walls showed that the wall roughness angle distribution "seen" by an incident particle at the first rebound is exactly modeled by the effective distribution of Sommerfeld and Huber (1999). Because the basic point of this new modeling is that the particle makes only one rebound, the wall roughness should systematically be sampled from the effective distribution of Sommerfeld and Huber (1999).

3.1.2. Analysis of the rebound effect

The rebound effect should be considered as the realisability condition of the rebound. It requires that the particle exits the near-wall region for all collision angles. This implies the condition $\underline{\mathbf{v}}_{\mathbf{p}}^+ \cdot \underline{\mathbf{n}} > 0$ (where $\underline{\mathbf{v}}_{\mathbf{p}}^+$ and $\underline{\mathbf{n}}$ denote the rebound velocity and the macroscopic wall unit vector directed towards the flow, respectively), that the particle returns in the flow after rebound is a necessary one. However, it is far from sufficient since the eventuality of multiple rebounds might be crucial in the description of the collision process for a certain number of rebounds, especially for those that occur with a grazing rebound angle. Therefore in the framework of the present modeling, in which it is assumed that the particle goes towards the flow after making only one effective rebound, a necessary and sufficient condition of the realisability of the particle rebound should integrate both the "natural" condition $\underline{\mathbf{v}}_{\mathbf{p}}^+ \cdot \underline{\mathbf{n}} > 0$ and the probability to make one and only one rebound.

The proposed rebound effect model is mathematically supported by the following proof. Let R be the probability that a given incident particle with a collision angle α^- leaves the macroscopic wall with a rebound angle α^+ after rebound. Considering that the particle might hit the wall many times before exiting the near-wall region, if we denote with $Q(\alpha^+, n|\alpha^-)$ the conditional probability that the incident particle hitting the wall with an angle α^- leaves the wall region with a rebound angle α^+ after n rebounds, R takes the following form:

$$R(\alpha^+|\alpha^-) = \sum_{n=1}^{\infty} Q(\alpha^+, n|\alpha^-) \tag{11}$$

Furthermore, by considering for a given collision angle α^- both the following events: "*make only one rebound*" and "*make two rebounds at least*" whose probabilities are, respectively, $Q(\alpha^+, n=1|\alpha^-)$ and $Q(\alpha^+, n>1|\alpha^-)$, the probability (11) may be expressed as:

$$R(\alpha^+|\alpha^-) = Q(\alpha^+, n=1|\alpha^-) + Q(\alpha^+, n>1|\alpha^-) \tag{12}$$

It emerges that the modeling of the multiple rebound effects can be summed up to those of both the foregoing complementary events.

A multiple rebound process necessarily assumes that the particle has already rebounded once, and first with an angle α_1^+. Therefore, by defining $Q(\alpha^+, n|\alpha_1^+, \alpha^-)$ conditional probability on both the first rebound angle α_1^+ and the collision angle α^-, that the colliding particle leaves the wall region with α^+ after n rebounds; and introducing in addition the transition probability $R_1(\alpha_1^+|\alpha^-)$ that the incident particle rebounds the first time onto an inclined smooth

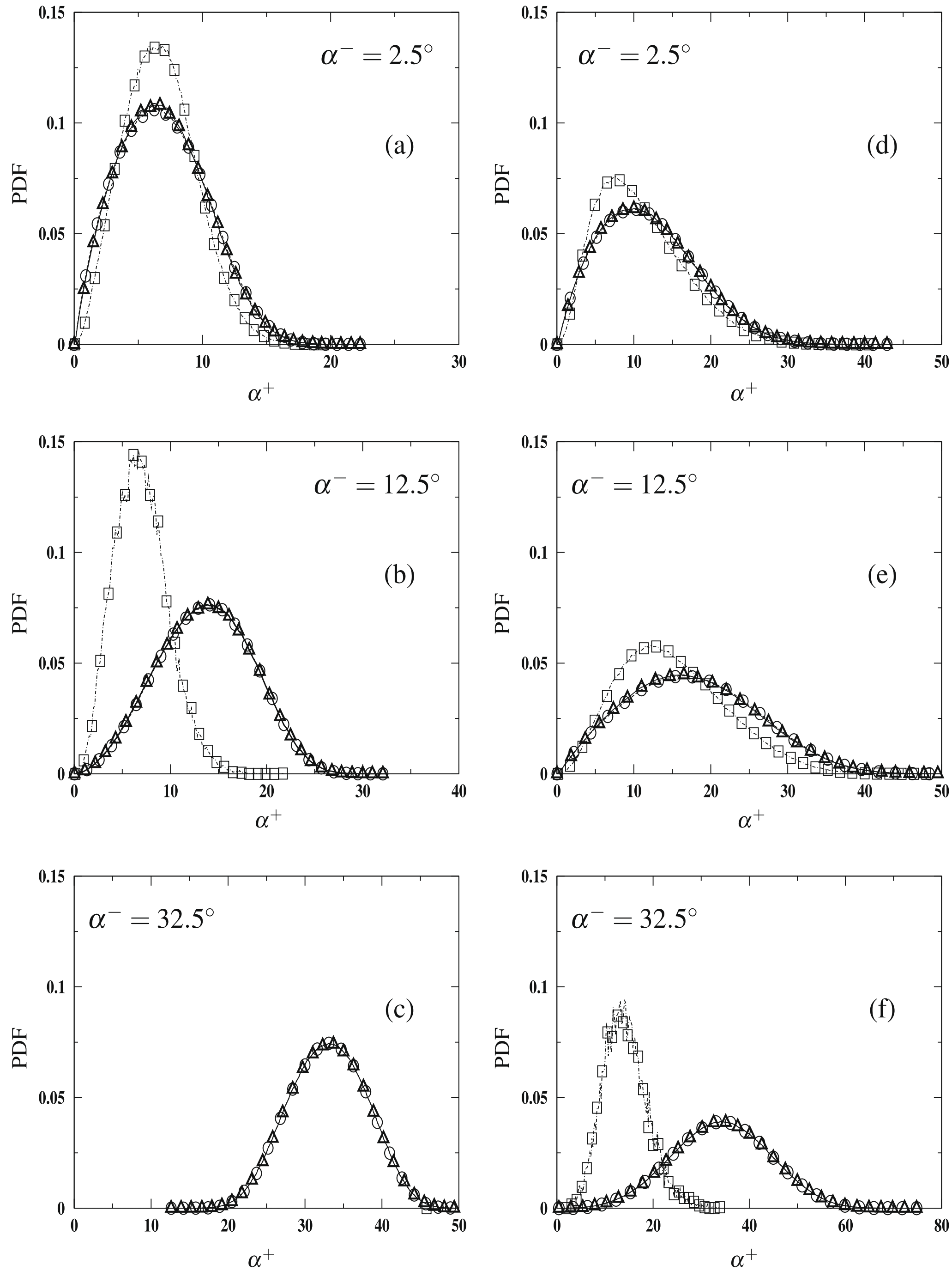

Fig. 6. PDFs of the rebound angle conditioned on both the number n of rebounds and the collision angle α^- (wall N°1). (a)–(c) and (d)–(f) represent rough walls with $\Delta\gamma = 2.5^\circ$ and $\Delta\gamma = 5.0^\circ$, respectively. △ refers to the rebound angle PDF of all the particles leaving the wall region whatever the number of rebounds: $R(\alpha^+|\alpha^-)$. ○ is the rebound angle PDF of the particles experiencing just one rebound: $Q(\alpha^+|n=1,\alpha^-)$, whereas □ denotes the PDF for the particles that make more than one rebound: $Q(\alpha^+|n>1,\alpha^-)$.

wall with $\alpha^+ = \alpha_1^+$, we may write that the conditional probability $Q(\alpha^+, n|\alpha^-)$ is:

$$Q(\alpha^+, n|\alpha^-) = \int_{-\pi/2}^{\pi/2} Q(\alpha^+, n|\alpha_1^+, \alpha^-) R_1(\alpha_1^+|\alpha^-)\, d\alpha_1^+ \tag{13}$$

According to Konan et al. (2006), the probability $R_1(\alpha_1^+|\alpha^-)$ is modeled by:

$$R_1(\alpha_1^+|\alpha^-) = \int_{-\pi/2}^{\pi/2} \delta(\alpha_1^+ - \phi_{\alpha^-}(\gamma)) P_{eff}(\gamma|\alpha^-) d\gamma \tag{14}$$

where ϕ_{α^-} is a function of wall roughness angle γ that derives from the rebound laws on a smooth inclined wall for a given collision angle α^-. Note that P_{eff} is the wall roughness angle PDF referred by Sommerfeld and Huber (1999) in which the random sample should be performed according to Section 3.1.1.

Moreover, introducing the probability $P^\star(n|\alpha_1^+, \alpha^-)$ that the particle makes n rebounds before exiting the wall region, conditioned on both the first rebound angle α_1^+ and the incident angle α^-, we may express the probability $Q(\alpha^+, n|\alpha_1^+, \alpha^-)$ as follows:

$$Q(\alpha^+, n|\alpha_1^+, \alpha^-) = Q(\alpha^+|n, \alpha_1^+, \alpha^-) P^\star(n|\alpha_1^+, \alpha^-) \tag{15}$$

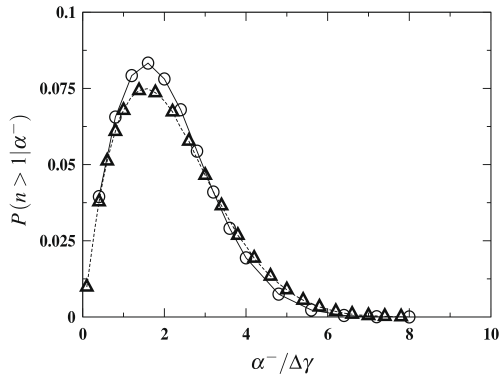

Fig. 7. Probability to make more than one rebound according to the collision angle α^-. ○ and △ refer to the wall roughness standard deviation $\Delta\gamma = 2.5^\circ$ and $\Delta\gamma = 5.0^\circ$, respectively (wall N°1).

Finally, from (13) and (15), the probability $Q(\alpha^+, n=1|\alpha^-)$ that the incident particle makes one and only one rebound before leaving the wall region satisfies:

$$Q(\alpha^+, n=1|\alpha^-) = \int_{-\pi/2}^{\pi/2} Q\left(\alpha^+|n=1, \alpha_1^+, \alpha^-\right) P^\star\left(n=1|\alpha_1^+, \alpha^-\right) R_1\left(\alpha_1^+|\alpha^-\right) d\alpha_1^+ \quad (16)$$

Furthermore, the probability $Q(\alpha^+|n=1, \alpha_1^+, \alpha^-)$ obviously equals $\delta(\alpha^+ - \alpha_1^+)$, since it defines the probability conditioned on just one rebound while at the same time the rebound angle is already set to α_1^+. Hence:

$$Q(\alpha^+, n=1|\alpha^-) = P^\star(n=1|\alpha^+, \alpha^-) R_1(\alpha^+|\alpha^-) \quad (17)$$

The second probability $Q(\alpha^+, n>1|\alpha^-)$ of the modeling (12) that the particle leaves the wall at least after two rebounds can be modeled similarly by introducing the probability $P(n>1|\alpha^-)$ to make over one rebound for a given collision angle α^-. In other words:

$$Q(\alpha^+, n>1|\alpha^-) = Q(\alpha^+|n>1, \alpha^-) P(n>1|\alpha^-) \quad (18)$$

Furthermore,

$$P(n>1|\alpha^-) = 1 - P(n=1|\alpha^-) \quad (19)$$

where by definition:

$$P(n=1|\alpha^-) = \int_{-\pi/2}^{\pi/2} P^\star(n=1|\alpha^+, \alpha^-) R_1(\alpha^+|\alpha^-)\, d\alpha^+ \quad (20)$$

Substituting (17) and (18) into (12), the exact formulation of the rebound effect reduces to:

$$R(\alpha^+|\alpha^-) = P^\star(n=1|\alpha^+, \alpha^-) R_1(\alpha^+|\alpha^-) + Q(\alpha^+|n>1, \alpha^-) P(n>1|\alpha^-) \quad (21)$$

At this stage, the explicit forms of both probabilities $P^\star(n=1|\alpha^+, \alpha^-)$ and $Q(\alpha^+|n>1, \alpha^-)$ are still unknown, therefore closure assumptions are needed to achieve the modeling of the rebound effect.

First, we assume that the probability $P^\star(n=1|\alpha^+, \alpha^-)$, is very weakly conditioned on the incident angle α^- for a given first rebound angle α^+. Therefore, we can write that:

$$P^\star(n=1|\alpha^+, \alpha^-) \approx P^\star(n=1|\alpha^+) \quad (22)$$

This assumption is clearly supported by the results of the deterministic rebounds of the particles on the geometrical walls (as shown by Fig. 5).

The second assumption concerns the PDF of the rebound angle α^+ of the particles that experience multiple rebounds $Q(\alpha^+|n>1, \alpha^-)$. This probability is assumed to be nearly equal to the one of the particles that experience only one collision $Q(\alpha^+|n=1, \alpha^-)$. Therefore:

$$Q(\alpha^+|n>1, \alpha^-) \simeq Q(\alpha^+|n=1, \alpha^-) = \frac{Q(\alpha^+, n=1|\alpha^-)}{P(n=1|\alpha^-)} \quad (23)$$

This assumption seems especially strong in the case of large collision angles, however it looks suitable for smaller collision angles (refer to the discussion of Section 2.2.3). Due to the weak effect of the multiple rebounds in the case of large collision angles, this assumption should not induce a significant inaccuracy.

Substituting (17), (19), (22) and (23) in (21), the modeling of the multiple rebound effects through the unique effective rebound becomes:

$$R(\alpha^+|\alpha^-) = \frac{P^\star(n=1|\alpha^+) R_1(\alpha^+|\alpha^-)}{P(n=1|\alpha^-)} \quad (24)$$

With the above assumptions, the generated absolute error in the rebound effect model (24) expresses as follows:

$$\delta R(\alpha^+|\alpha^-) = P(n>1|\alpha^-)[Q(\alpha^+|n>1, \alpha^-) - Q(\alpha^+|n=1, \alpha^-)] \quad (25)$$

This error remains small as shown by the results of the deterministic rebounds of particles on the geometrical rough wall (refer to Fig. 6).

3.2. Validation of the modeling of the rebound effect

Validation and setup of the proposed rebound effect model (24) through a stochastic process requires an accurate analytic formulation of the probability $P^\star(n=1|\alpha^+)$ to make only one rebound conditioned on the rebound angle α^+.

3.2.1. Analytical formulation of the probability to make only one rebound

In the framework of the "Shadow effect model", because the return of the particle towards the flow after collision onto the virtual wall is just conditioned by a rebound velocity $\underline{\mathbf{v}}_\mathbf{p}^+$ such that: $\underline{\mathbf{v}}_\mathbf{p}^+ \cdot \underline{\mathbf{n}} > 0$, the probability can simply be described by a Heaviside function:

$$P^\star(n=1|\alpha^+) = \begin{cases} 1 & \text{if } \alpha^+ > 0 \\ 0 & \text{otherwise} \end{cases} \quad (26)$$

in which α^+ denotes the rebound angle of the particle.

However, the shape of this probability is contradicted by the previous deterministic collision simulations that show another shape with three fundamental domains in terms of the rebound angle. A first domain indicates a null probability to make just one rebound: this is typically related to the cases of the rebound particles that continue to move towards the rough wall after a collision. Such particles would obviously make another rebound before exiting the near-wall region. The second domain for which this probability presents a significant slope is about the grazing rebound angles. It expresses a non-zero probability for such rebounded particles to collide again with the asperities of the wall. Beyond a certain rebound angle (the third domain) the probability for the particle to experience only one collision onto the wall is about one.

It appears that the shape of the probability to make only one rebound showed by the deterministic rebounds is accurately reproduced by the following analytical formulation (see Fig. 8):

$$P^\star(n=1|\alpha^+) = \begin{cases} \tanh\left(\beta \frac{\alpha^+}{\Delta\gamma}\right) & \text{if } \alpha^+ \geqslant 0 \\ 0 & \text{if } \alpha^+ \leqslant 0 \end{cases} \quad (27)$$

with $\beta \simeq \frac{3}{2}$.

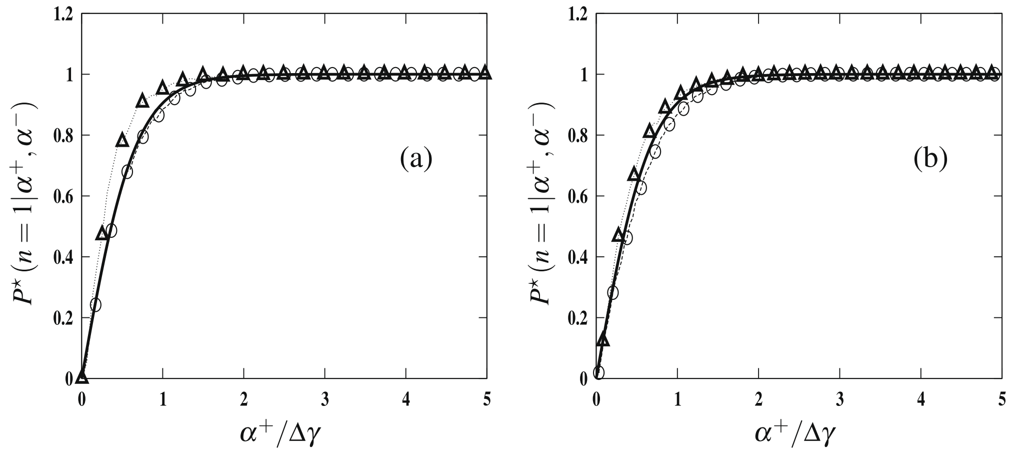

Fig. 8. Validation of the analytical formulation (solid line) of the probability to make only one rebound. Two collision cases onto the wall N°1 are shown by ○: $\alpha^- = 2.5°$ and △: $\alpha^- = 12.5°$. (a) and (b) define the wall roughness standard deviations $\Delta\gamma = 2.5°$ and $\Delta\gamma = 5.0°$, respectively.

Finally, we can note that the main difference between the proposed new rebound effect and the one expressed through the "Shadow effect model" (Sommerfeld and Huber, 1999) is that the "Shadow effect model" admits as absolute event the fact that the particle leaves the near-wall region provided that the rebound angle is positive, without another possible mechanism which would ensure that the particles move away from the wall, especially the grazing rebounded particles (Fig. 9). Therefore, in the "Shadow effect model", even if the random wall roughness angle was supplied according the "effective PDF", the problem of grazing particles after rebound should always arise.

3.2.2. Validation: case of fully elastic rebounds

To validate the rebound effect described by (24) and (27), we first assumed fully elastic collisions with 2*D* wall roughness effects with $\underline{\mathbf{n}}_\gamma = (-\sin\gamma, \cos\gamma, 0)$, and whereby we can easily formulate analytically the transition probability $R_1(\alpha^+|\alpha^-)$ (14), because of the very simple definition of ϕ_{α^-}. In the frame of fully elastic rebounds, the rebound angle α^+ conditional on the wall roughness angle γ is given by $\phi_{\alpha^-}(\gamma) = 2\gamma + \alpha^-$. Thus, substituting ϕ_{α^-} in (14), the probability $R(\alpha^+|\alpha^-)$ becomes:

$$R(\alpha^+|\alpha^-) = \frac{\Theta(\alpha^+,\alpha^-)}{\int_0^{\frac{\pi}{2}} \Theta(\alpha^+,\alpha^-) d\alpha^+} \tag{28}$$

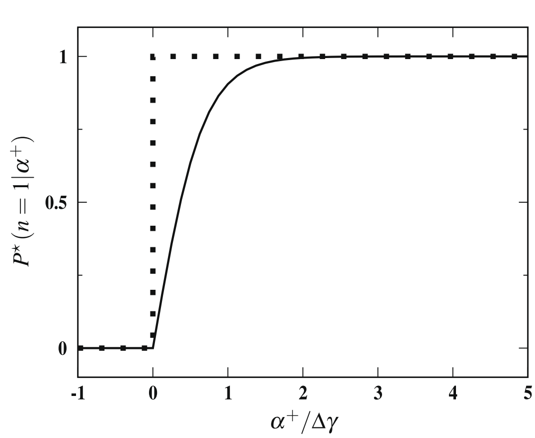

Fig. 9. Illustration of the difference between the probability to make only one rebound with the "Shadow effect model" (dotted line) (26) and with the new modeling approach (solid line) (27).

where

$$\Theta(\alpha^+,\alpha^-) = \tanh\left(\frac{3}{2}\frac{\alpha^+}{\Delta\gamma}\right)\sin\left(\frac{\alpha^+ + \alpha^-}{2}\right)\exp\left[-\frac{(\alpha^+ - \alpha^-)^2}{8\Delta\gamma^2}\right] \tag{29}$$

Fig. 10(a) and (b) shows comparisons of the PDF of the rebound angles between deterministic elastic rebounds of particles onto geometrical rough walls and analytic formulations (28) and (29) for two wall roughness standard deviations $\Delta\gamma = 2.5°$ and $\Delta\gamma = 5.0°$, and for three incident angles: $\alpha^- = 2.5°$, $\alpha^- = 12.5°$ and $\alpha^- = 32.5°$. One can notice in these figures that for the small, medium and high collision angles, the stochastic modeling of the multiple rebound effects (24) and (27) accurately predicts the rebound angle distribution. Furthermore, these results show that the model leads to a zero probability to rebound with grazing angle, for any collision angle onto the rough wall.

3.3. Stochastic Lagrangian procedure of the "Rough Wall Multi-Collisions Model"

The idea of the virtual wall on which the incident particle bounces to simulate wall roughness effects is resumed in the present stochastic model. However the incident particle clearly performs only one rebound, but the proposed rebound effect reproduces multiple rebound effects. Typically, if a sampled wall roughness angle leads to an high probability to make another rebound, it is systematically rejected and another wall roughness angle is sampled. The procedure used to take into account the mechanisms described in Sections 3.1.1 and 3.1.2 is the following:

(1) *Incident shadow effect*: the wall roughness γ is sampled from the effective distribution function (30) (Sommerfeld and Huber, 1999):

$$P_{eff}(\gamma|\underline{\mathbf{c}}_\mathbf{p}^-) = \begin{cases} \frac{1}{\sqrt{2\pi\Delta\gamma^2}} \frac{\underline{\mathbf{v}}_\mathbf{p}^- \cdot \underline{\mathbf{n}}_\gamma}{\underline{\mathbf{v}}_\mathbf{p}^- \cdot \underline{\mathbf{n}}} \exp\left(-\frac{\gamma^2}{2\Delta\gamma^2}\right)\xi(\underline{\mathbf{v}}_\mathbf{p}^-, \Delta\gamma) & \text{if } \underline{\mathbf{v}}_\mathbf{p}^- \cdot \underline{\mathbf{n}}_\gamma \leqslant 0 \\ 0 & \text{if } \underline{\mathbf{v}}_\mathbf{p}^- \cdot \underline{\mathbf{n}}_\gamma \geqslant 0 \end{cases} \tag{30}$$

where $\underline{\mathbf{v}}_\mathbf{p}^-$ is the particle incident velocity, $\underline{\mathbf{n}}$ and $\underline{\mathbf{n}}_\gamma$ are, respectively, unit normal vectors that define the macroscopic wall and the virtual wall inclined at angle γ (Fig. 1). $\xi(\underline{\mathbf{v}}_\mathbf{p}^-, \Delta\gamma)$ ensures the normalization of the PDF. Because the particle should come from the flow, the condition $\underline{\mathbf{v}}_\mathbf{p}^- \cdot \underline{\mathbf{n}} < \mathbf{0}$ should be expected for any colliding particles. Note that the sampling of the wall roughness angle according to the PDF (30) could be achieved from a rejection method.

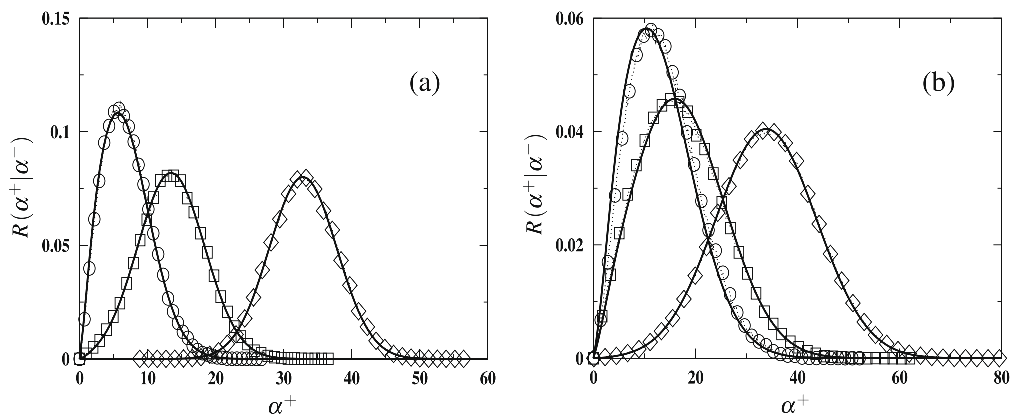

Fig. 10. Validation of the rebound effect modeling (24) and (27) (solid line) by comparison with deterministic rebound results (symbols) in the case of fully elastic collision (28) onto the wall N°1. Symbols ○, □ and ◊ denote, respectively $\alpha^- = 2.5°$, $\alpha^- = 12.5°$ and $\alpha^- = 32.5°$ while (a) and (b) represent the rough wall cases with standard deviations $\Delta\gamma = 2.5°$ and $\Delta\gamma = 5.0°$, respectively.

(2) *Classical rebound law*: the rebound velocity and the rebound angle α^+ corresponding to the foregoing sampled wall roughness angle γ are assessed from a classical sliding or non-sliding rebound law of particles colliding onto a smooth wall inclined of an angle γ.
(3) "*Grazing rebound effect*": assessment of the probability $P^\star(n = 1|\alpha^+)$ to make only one rebound in terms of the rebound angle α^+ from (27) and:
- if $\alpha^+ \leqslant 0 : P^\star(n = 1|\alpha^+) = 0$ then a new wall roughness angle must be sampled: resume of step (1);
- if $\alpha^+ > 0 : P^\star(n = 1|\alpha^+) > 0$ then another number $s \in [0, 1]$ is randomly chosen according to an uniform distribution and the decision of keeping the sampled wall roughness angle is dictated by the following items:
  - if $s \in]0, P^\star(n = 1|\alpha^+)]$ then the wall roughness angle is kept and rebound is ended,
  - if $s \in [P^\star(n = 1|\alpha^+), 1]$ then a new wall roughness angle must be sampled: resume of step (1).

When $P^\star(n = 1|\alpha^+) > 0$, the procedure of keeping the wall roughness angle γ provided by (1), is summarized by Fig. 11.

4. Applications

This section focuses on the application of both stochastic models ("Shadow Effect Model" and "Rough Wall Multi-Collisions Model") to simulate inelastic rebounds of spherical particles onto rough walls. The results are compared with the measurements conducted by Sommerfeld and Huber (1999). The simulation method is exactly the same used by Sommerfeld and Huber (1999) to validate "Shadow Effect Model". Accordingly, the simulations of the rebounds onto the rough wall are achieved from the distributions of both the streamwise velocity and the angular velocity of the incident particles onto the wall. We assumed a Gaussian shape for each of these distributions. According to the measurements, the mean velocity of the incident particles is 5.91 m s^{-1} with a rms of 1.16 m s^{-1}. Since experimental data on the angular velocity are not available, the estimation of the mean and rms values is performed according to the method suggested by Sommerfeld and Huber (1999). Thus, the mean and the rms value are taken to be equal to 16,336 rad s^{-1} and 5655 rad s^{-1}, respectively. The measured wall roughness standard deviation is about $\Delta\gamma = 3.8°$. The method to account for the restitution (e_w) and the friction (μ_w) coefficients at the wall is the one of Sommerfeld and Huber (1999) that in the framework of collisions of spherical particles onto a smooth horizontal wall is expressed by:

$$e_w(\alpha^-) = \begin{cases} \frac{e_h - 1}{\alpha_e}\alpha^- + 1 & \text{if } \alpha^- \in [0, \alpha_e] \\ e_h & \text{if } \alpha^- \geqslant \alpha_e \end{cases} \quad (31)$$

and

$$\mu_w(\alpha^-) = \begin{cases} \frac{\mu_h - \mu_0}{\alpha_\mu}\alpha^- + \mu_0 & \text{if } \alpha^- \in [0, \alpha_\mu] \\ \mu_h & \text{if } \alpha^- \geqslant \alpha_\mu \end{cases} \quad (32)$$

where e_h, μ_h and μ_0 are the rebound coefficients. The angles α_e and α_μ that appear in (31) and (32) are obtained from experiments. Denoting the particle properties before and after rebound by the superscripts (−) and (+), respectively, the rebound velocities are:

$$\begin{cases} u_p^+ = u_p^- - \mu_w(1 + e_w)\varepsilon v_p^- \\ v_p^+ = -e_w v_p^- \\ \omega_p^+ = \omega_p^- + 5\mu_w(1 + e_w)\varepsilon \frac{v_p^+}{d_p} \\ \varepsilon = sign\left(u_p^- - \frac{d_p}{2}\omega_p^-\right) \end{cases} \quad (33)$$

According to available measurements, the rebounds of glass bead particles with diameter $d_p = 500$ μm onto the stainless steel wall are simulated for three different incident angles 5°, 15° and 25°, with the rebound coefficients: $e_h = 0.7$, $\mu_h = 0.15$, $\mu_0 = 0.4$, $\alpha_e = 22.0°$ and $\alpha_\mu = 20.0°$. A total of 10^7 incident trajectories is simulated for each incident angle.

It should be noted that in order to remain consistent with the stochastic simulation procedures of the wall roughness effects, in which the incident particle bounces onto a smooth wall inclined

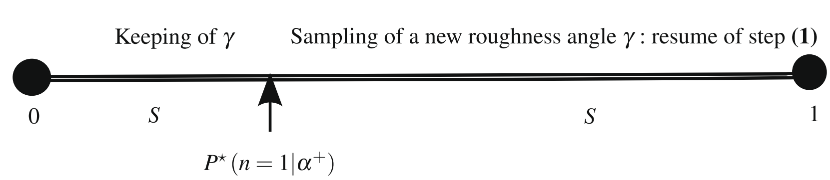

Fig. 11. Summary of the procedure used to keep the sampled wall roughness angle γ at step (3).

of an angle γ, the global collision angle onto that smooth wall is taken to be equal to $\alpha^- + \gamma$ instead of α^- in (31) and (32).

Since, we set the incident angles of the particles, the analysis of the behavior after the rebound is restricted to the distribution of the rebound angles.

To prove that both incident and rebound mechanisms must be correctly accounted for in order to accurately describe the particles–rough wall interactions, we introduced the ''Advanced Shadow Effect Model'' which corresponds to the ''Shadow Effect Model'' procedure with the wall roughness sampled randomly according to the effective distribution function (30), instead of the normal distribution.

Fig. 12 shows the distribution of rebound angles for each of the incident angles (5°, 15° and 25°) simulated with the three models. The results are compared with the measurements. It appears a good agreement between the distributions simulated with the ''Rough Wall Multi-Collision Model'' and the measurements for the three incident angles. That is characterized by a zero probability to rebound with a grazing rebound angle even for grazing incident particles. This good agreement highlights the importance of multiple rebound effects, especially for the grazing incident particles onto the wall.

Rebound angle distribution functions simulated with the ''Shadow Effect Model'' show an identical shape profiles with a significant probability for the rebound angles close to zero while the incident angle is relatively small (refer to Fig. 12(a) and (b)). Actually, for incident angles smaller than 15°, the particle has a high probability to rebound with a grazing angle. This effect becomes more pronounced when the colliding angle is $\alpha^- = 5°$. Such a spurious effect might lead to some important discrepancies in the prediction of particulate phase properties in channel flows, where the particles tend to reach the wall with a small incident angle (Sommerfeld, 1992; Konan et al., 2007). In that situation, most of them could remain grazing and this would lead to the accumulation of particles in the near-wall region, contrary to what is observed in experiments with rough wall.

The same non-zero probability for particles to rebound with a grazing angle when they reach the wall with a small collision angle does not vanish when using the ''Advanced Shadow Effect Model''. It can be observed in Fig. 12(a) and (b) that it decreased compared to those with the standard procedure of the ''Shadow Effect Model''. Therefore, with the smaller collision angles, both the ''Shadow Effect Model'' and the ''Advanced Shadow Effect Model'' are not able to correctly predict the distribution of the rebound angles. This demonstrates that the ''natural'' condition of the rebound expressed just by a positive dot product of the rebound velocity and the wall normal unit vector ($\underline{\mathbf{v}}_\mathbf{p}^+ \cdot \underline{\mathbf{n}} > 0$) is not sufficient to simulate accurately the wall roughness effects for small collision angles.

On the other hand, the good agreement showed by Fig. 12(c) for the three models with measurements indicate a correct prediction of the statistical rebound behavior of the particles when they collide the wall with a large angle. This identical result between the three models is expected, since in the case of the large collision angles the number of multiple rebounds was found from deterministic rebounds to be smaller than 1%, which then results in a weak effect of the multiple rebounds.

5. Conclusion

Measurements in literature show that wall roughness has a conspicuous effect on the properties of the dispersed phases in

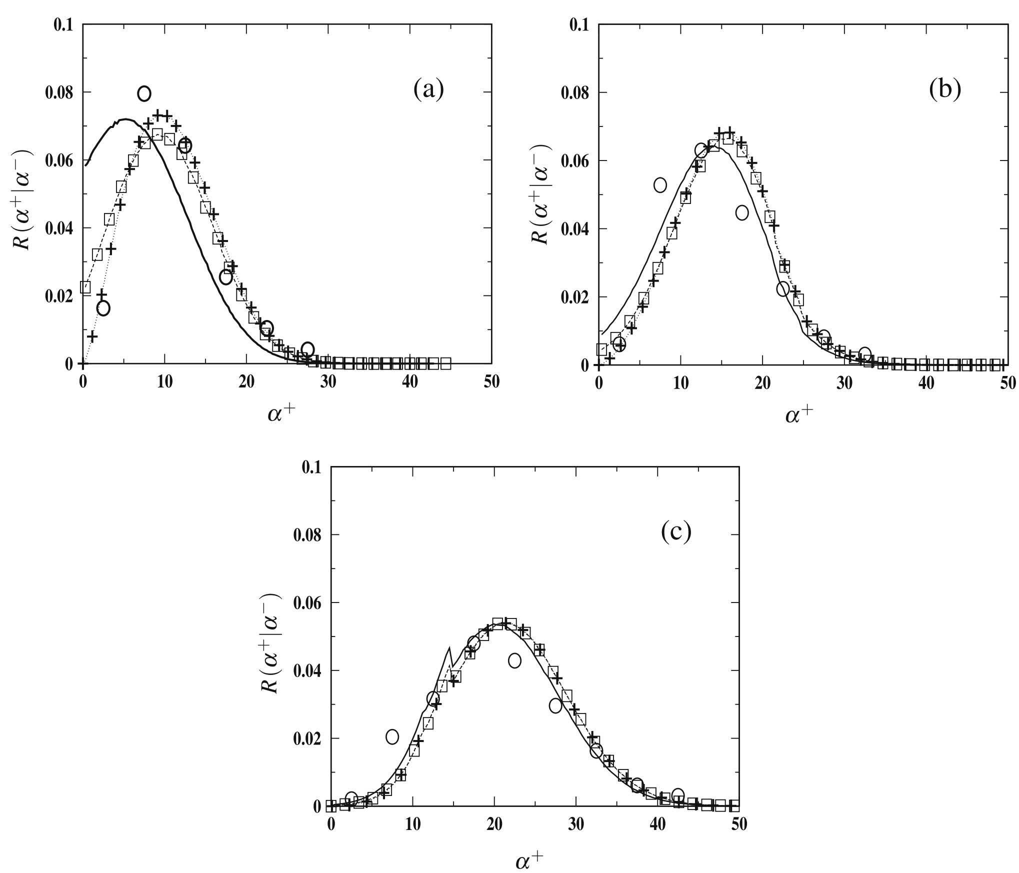

Fig. 12. Comparison between the measured PDF of the rebound angles by Sommerfeld and Huber (1999) (○) and the simulations performed from the stochastic models. Solid line: ''Shadow Effect Model'', □: ''Advanced Shadow Effect Model'' and +: ''Rough Wall Multi-Collision Model''. Cases are defined by a particle diameter $d_p = 500$ µm, a wall rough standard deviation $\Delta\gamma = 3.8°$ and the collision angles (a) $\alpha^- = 5.0°$, (b) $\alpha^- = 15.0°$ and (c) $\alpha^- = 25.0°$.

turbulent flows. In this work, a brief review of the behavior of both the geometrical representation of the wall and the stochastic description of particles–rough wall interactions is presented. As the "*Shadow Effect Model*" of Sommerfeld and Huber (1999) appeared as the most advanced and practical stochastic process to account for the wall roughness effects on the particulate phases, a special emphasis was given to exhibit the particle–rough wall interaction mechanisms expressed through its formulation.

Furthermore, as it was shown in both the derivation of Eulerian rough wall boundary conditions and the Lagrangian simulations in channel flows with rough walls, by Konan et al. (2006, 2007), the "*Shadow Effect Model*" leads to a non-zero probability for the colliding particles to remain grazing after the rebound. Especially, the model leads to a significant probability that the particles reaching the wall with a small collision angle remain grazing, thus indicating a strong likelihood to rebound with a null wall-normal velocity, contrary to observations.

Motivated by the inability of the "*Shadow Effect Model*" to properly account for the wall roughness effects for the particles that hit the wall with a grazing angle, deterministic rebounds of spherical particles onto geometrical two-dimensional walls are carried out to statistically investigate the behavior of the particles interacting with rough walls. The simulations showed three important results: (1) the wall roughness angle distribution experienced by an incident particle at the first rebound is exactly defined by the *effective* distribution function given by Sommerfeld and Huber (1999), (2) the particle has a non-zero probability to make another rebound, even if the rebound angle is greater than zero, and (3) the final rebound angle distribution function of the particles is nearly identical to those that make only one rebound.

The three points showed in our investigation on deterministic rebounds are used to derive the "*Rough Wall Multi-Collisions Model*", a stochastic process which models particles–rough wall interactions through a unique rebound approach and reproduces the effects of multiple rebounds through the probability to make only one rebound.

Moreover, in order to assess the assumptions that support the "*Rough Wall Multi-Collisions Model*", we finally simulated the inelastic rebound step of the spherical particles onto the rough wall in the experiment of Sommerfeld and Huber (1999) in a narrow channel with rough walls. Excellent agreement was obtained between the simulated rebound PDF with the "*Rough Wall Multi-Collisions Model*" and the measurements for small, medium and large collision angles. Non-zero probability for the particles to remain grazing is found with the "*Shadow Effect Model*", contrary to experiments. These results indicate that the accurate treatment of the wall roughness effects in a stochastic approach requires both a precise modeling of the incident effect, and a correct rebound process able to describe mechanisms that ensure that particles leave the wall region, such as multiple rebounds.

Because of the three-dimensional aspect of the rough wall structure, the mechanisms of multiple collisions may be significantly modified, especially for the collisions that happen with large impact angles onto the rough wall. However, for the collisions that occur with very small angles (which are dominating the multiple rebound effects), the main findings about the statistical behavior of such colliding particles should not significantly change. The methodology developed in this manuscript to investigate the statistical behavior of particles onto the two-dimensional rough wall can be resumed to account for the collisions of the spherical particles onto the three-dimensional features of wall roughness.

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