Particle Reynolds stress model for wall turbulence with inertial particle clustering

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Abstract. The modification of Zaichik particle Reynolds stress transport model for turbulent particle-laden flows is developed taking into account the clustering phenomenon of inertial particles. The main novelty is the new boundary condition for the particle Reynolds stress, which is posed at some distance from the wall in the viscous sublayer and is consistent with the power-law singularity of particle concentration at the wall. The modified model avoids the spurious bifurcation of the solution, which observed for non-modified Zaichik model with the near-equilibrium wall boundary condition.

1. Introduction
The clustering of inertial particles in near-wall turbulent particle-laden flows has a significant effect on the processes of heat transfer and dispersion of particles. It also poses the challenges for the Eulerian/Eulerian two-fluid modeling of particulate flows, because of the breakdown of the continuity of the dispersed phase. The near-equilibrium assumptions having to be used in the closure of transport equation for the statistical moments of particle velocity become invalid when the particle relaxation time is of the order of (or greater than) turbulence timescale.

The influence of non-equilibrium effects on particle motion in wall-bounded turbulence has some special features. The drastic increase in the turbulence timescale with the distance from the wall creates the situation when the particle relaxation time can be larger than the turbulence timescale only in a thin near-wall region. It can improve the predictive ability of the Eulerian/Eulerian two-fluid models in wall-bounded turbulent flows for a wider range of particle Stokes numbers that one could ever have anticipated. In this paper, we consider the modification of the second-moment closure model for particle Reynolds stress developed by Zaichik [1] through the novel boundary condition at the wall. Although this model includes the near-equilibrium gradient diffusion model for the third moment of particle velocity, this modification taking into account the results of asymptotic theory for inertial particle accumulation in wall turbulence [2] can improve the predictive ability of a model for highly inertial particles to some extent.

2. Second-moment closure model of particle-laden turbulence
The turbulent flow in a plane channel laden with small inertial particles is considered. The particle motion obeys the following equation \( \dot{v}_{pi} = (v - v_{pi}) / \tau \), where the particle relaxation time \( \tau \) is assumed to be constant and independent of the particle relative velocity. In this case, the particle motion in wall-normal direction can be decoupled from the motion in other directions, so that the calculation of the statistical moments of particle velocity becomes a one-dimensional mathematical problem.
2.1. Near-equilibrium second-moment closure for particle turbulence

For the case of elastic rebound of particles from the wall, the following transport equations for the wall-normal particle velocity moments can be written as

\[
\frac{d\langle v_p^2 \rangle}{dy} + \left(\langle v_p^2 \rangle + g_v \langle v^3 \rangle\right) \frac{d\ln \Phi}{dy} = 0, \quad \frac{d\langle v_p^3 \rangle}{dy} + \langle v_p^2 \rangle \frac{d\ln \Phi}{dy} = \frac{2}{\tau} (f_v \langle v_p^2 \rangle - \langle v_p^3 \rangle) \tag{1}
\]

where \( \Phi \) is the particle concentration, \( f_v = (1 + \tau/T_{lp})^{-1} \), \( g_v = f_v T_{lp}/\tau \) [1], \( T_{lp} \) is the Lagrangian timescale of fluid velocity fluctuations along the particle trajectory and the relation \( \langle v_p^3 \rangle = 0 \) is taken into account.

The Lagrangian timescale of fluid velocity fluctuations along the particle trajectory is calculated using the Wang and Stock model for the homogeneous isotropic turbulence [3]

\[
T_{lp} = \left[1 - \frac{0.644}{(1 + \tau/T_E)^{0.41(1+0.001\tau/T_E)}}\right] T_E, \quad T_E = \frac{T_L}{0.356}, \tag{2}
\]

where \( T_L \) is the Lagrangian timescale of fluid turbulence.

The near-equilibrium approximation for the third moment \( \langle v_p^3 \rangle \) can be derived by the Chapman-Enskog method [4,5] or by the truncation of the transport equation for the higher-order moments of particle velocity [1] and has the form

\[
\langle v_p^3 \rangle = -D_p \frac{d\langle v_p^3 \rangle}{dy}, \tag{3}
\]

where \( D_p = \langle v_p^2 \rangle + f_v \langle v^3 \rangle T_{lp} \) is the particle turbulent diffusion coefficient.

From (1)-(3) the following equation for the second moment of the particle velocity can be derived

\[
\tau \frac{d}{dy} \left( D_p \frac{d\langle v_p^2 \rangle}{dy} \right) - \left( \frac{d\langle v^2 \rangle}{dy} \right)^2 + 2(f_v \langle v_p^2 \rangle - \langle v_p^3 \rangle) = 0. \tag{4}
\]

The boundary conditions at the wall and at the centerline according to the near-equilibrium model [1] can be written as

\[
\frac{d\langle v_p^2 \rangle}{dy} = 0, \text{ at } y = 0, \quad \frac{d\langle v_p^2 \rangle}{dy} = 0, \text{ at } y = h \tag{5}
\]

where \( h \) is the channel half-width.

2.2. Particle concentration and second moment of particle velocity near-wall asymptotics at large Stokes numbers

The asymptotic analysis of the kinetic equation for the probability distribution function of particle velocity in the vicinity of the wall (\( y \to 0 \)) has shown the division of particles in two groups: ballistic and diffusional particles at Stokes numbers \( \tau/T_{lp} \) of the order of 1 and greater [2]. The velocity statistics of diffusional particles are in equilibrium with the local fluid turbulence \( \langle v_p^2 \rangle_{\text{diff}} = f_v \langle v^2 \rangle \), so that they are slow because of the decay of fluid velocity close to the wall

\[
\langle v_p^2 \rangle - y^4, \quad \langle v_p^2 \rangle_{\text{diff}} \sim y^4 \text{ if } y \to 0 \tag{6}
\]
The second moment of the velocity of diffusional particles can be found from the following near-equilibrium relation

\[ \langle v_p^2 \rangle_{\text{diff}} = f_\tau \langle v_f^2 \rangle \]  

(7)

The concentration of diffusional particles is calculated after the substitution of (7) into (1)

\[ \Phi \sim \langle v_f^2 \rangle \sim \frac{1}{n_\nu} \sim y^{\frac{4\tau}{n_\nu}} \tau, \]  

(8)

and has a power-law singularity at the wall [2].

Since the fast ballistic particles give a regular contribution to the particle concentration, the expression (8) gives the leading-order term of the particle concentration expansion near the wall. In [2] it has been shown that the second moment of particle velocity obeys the power law

\[ \langle v_p^2 \rangle \sim y^{\frac{4\tau}{n_\nu}} \tau, \]  

(9)

which is greater than the equilibrium expression (6) at \( y \to 0 \).

### 2.3. Irregular behavior of the particle Reynolds stress in the near-equilibrium model

According to (9), for highly inertial particles with the large Stokes numbers, the particle Reynolds stress is much greater than the equilibrium expression (6) at \( y \to 0 \). The solution with a similar property exists for the near-equilibrium model (4), as was shown in [6]. Indeed, if one neglects the fluid Reynolds stress \( \langle v_f^2 \rangle \) in a vicinity of the wall, then the equation (4) has the simple solution [1,6]

\[ \langle v_p^2 \rangle = \left\{ \begin{array}{ll}
0 & \text{when } 0 < y < y_0(\tau), \\
\left( \frac{y - y_0(\tau)}{\tau} \right)^2 & \text{when } y > y_0(\tau), \text{if } \tau \leq \tau_c
\end{array} \right. \]  

(10)

\[ \langle v_p^2 \rangle = \langle v_p^2 \rangle_w + \left( \frac{y}{\tau} \right)^2, \text{if } \tau \geq \tau_c, \]  

(11)

where \( y_0(\tau) \) is some decreasing function of \( \tau \), \( \langle v_p^2 \rangle_w \) is the value of particle Reynolds stress at the wall, which is equal to zero providing \( \tau \leq \tau_c \), where the critical value of particle relaxation time is determined by a condition \( y_0(\tau_c) = 0 \).

In [1,6] it was shown that bifurcation of the solution of (4) occurs when \( \tau = \tau_c \) such that the value \( \langle v_p^2 \rangle_w \) being zero at \( \tau \leq \tau_c \) becomes non-zero when \( \tau \geq \tau_c \). This bifurcation is spurious as it is corroborated neither numerical nor experimental data. As it is seen from (10),(11), the particle Reynolds stress has irregular behavior in the near-wall region with the discontinuity of the second-order derivative of the second moment of particle velocity.

### 2.4. Wall function for the second moment of particle velocity

It can be easily shown that out-of-equilibrium expression (9) is not consistent with the equation (4), which has the near-equilibrium asymptotic (8) near the wall. To improve the performance of the near-equilibrium model (4), we suggest the use of the method of wall functions known from the CFD practice. In this method, the boundary conditions are posed not on the wall but at some distance from the wall, usually, on the first node of the computational grid, and have the form of the matching conditions with some near-wall asymptotic expressions. Below we impose the following boundary condition for the equation (4) at the distance \( y = y_1 \), which follows from (1), (8).
The following algorithm of calculation of the particle concentration and the second-order moment of particle velocity can be proposed. First, the second-order moment is obtained in the region \( y_1 \leq y \leq h \) by solving the ordinary differential equation (4) with boundary conditions (12) and (5) (at the center of a channel). In the region \( 0 \leq y \leq y_1 \), the second-order moment is subsequently reconstructed using (9)

\[
\frac{d \langle v_p^2 \rangle}{dy} = -\langle v_p^2 \rangle + g_\tau \frac{d \ln \Phi}{dy} = \frac{4\tau}{\tau + T_{\eta p}} \langle v_p^2 \rangle + g_\tau \frac{\langle v_p^2 \rangle}{y_1}, \text{ at } y = y_1 \tag{12}
\]

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\[
\langle v_p^2 \rangle = \langle v_p^2 \rangle_{y_1} \left( \frac{y}{y_1} \right)^{\frac{4\tau}{\tau + T_{\eta p}}} \tag{13}
\]

At the second stage, the particle concentration is calculated by integrating (1).

3. Results and discussion

The turbulent particle-laden flow in a plane channel was simulated using the model (4) with two variants of boundary conditions. The first variant that we refer to as the Zaichik model utilizes the near-equilibrium boundary conditions (5). In the second variant, which will be referred to as the modified Zaichik model, the boundary conditions (5),(12) are used at point \( y_1 = 1 \) (here and throughout the paper, the wall units are used for the representation of all variables). The wall-normal fluid Reynolds stress \( \langle v_f^2 \rangle \) is taken from the DNS data of Soldati and Marchioli [7] for \( Re = h = 155 \). The Lagrangian timescale of fluid turbulence is calculated by the expression \( T_\tau = \sqrt{5^2 + (0.42(y_1 - 0.5y^2/h))^2} \) fitting the DNS data [8].

Figure 1. The r.m.s. of wall-normal particle velocity for different Stokes numbers.
The profiles of particle Reynolds stress across the channel are shown in Figure 1 for different Stokes numbers, which is defined here as the particle relaxation time in wall units ($St = \tau$). In addition to the DNS data of A. Soldati and C. Marchioli for $St=1$, 5 and 25 and particle-to-fluid density ratio $\rho = 770$ [7], the results of DNS [9] for $St=117$ and $\rho = 2040$ are shown. In this case, the Schiller-Nauman correction to the particle drag force was utilized in a simplified form, assuming the mean particle Reynolds number is constant and equal to 2. The good agreement between both models and DNS data is observed for particles with medium inertia for $St < 25$, when these curves do not depart notably from the equilibrium relation (7) (dash-dot line), while for highly inertial particles with $St = 117$ the modified Zaichik model gives more realistic prediction of particle Reynolds stress than non-modified model, although some discrepancies can be seen in the near-wall region.

The profiles of particle concentration divided by its value at the channel center are shown in Figure 2. As it can be seen, while for $St < 25$ both models demonstrate satisfactory agreement with the DNS data, for high-inertia particles the particle concentration by Zaichik model disagrees qualitatively with the DNS data, as it does not describe the particles pile-up near the wall observed in the DNS data. The modified Zaichik model predicts the particle accumulation at the wall, as it is seen from Fig.2. It should be noted that the DNS data [9] for particle concentration suffer from the unsteadiness caused by the insufficient simulation timespan to sample the particle concentration statistics, which makes impossible the direct comparison of the steady solutions with these data.

The major advantage of modified Zaichik models is the regular behavior of the solution at arbitrary Stokes numbers in contrast to the near-equilibrium Zaichik model, which exhibits bifurcation of solution at some critical Stokes number. For the considered plane channel flow the critical value of the particle relaxation time has proved to be $\tau_{cr} = 48.5$. At this Stokes number, the numerical solution of the equation (4) encounters the problems with numerical convergence (cf. [10]). Figure 3 shows the profile of the intensity of wall-normal particle velocity, on which the spurious oscillations are observed in the vicinity of the wall. It can be clearly seen that the near-wall profile of particle Reynolds stress is well fitted by the expression (10) in the region $y_0 < y < 1$, where $y_0 = 0.01$, while in the region $0 < y < y_0$, the solution tends to the near-equilibrium expression (7).

![Figure 1. The particle concentration for different Stokes numbers.](image)
Conclusion

The modified second-moment closure model of Zaichik for particle Reynolds stress transport in turbulent particle-laden flows is developed, which takes into account the power-law singularity of particle concentration at the wall related with the phenomenon of clustering of inertial particles. The main novelty is the new boundary condition for the particle Reynolds stress, which is posed at some distance from the wall within the viscous sublayer as in the method of wall functions widely used in CFD. This boundary conditions take into account the power-law singularity of particle concentration at the wall and make it possible to avoid the spurious bifurcation of the solution observed for the near-equilibrium model.

The comparison of the profiles of wall-normal particle Reynolds stress predicted by the modified Zaichik model with the DNS data for the turbulent channel flow has shown that the modified model gives more realistic results for highly inertial particles with St~100, especially in the near-wall region. Although the notable discrepancy is still observed at large Stokes numbers attributed to the near-equilibrium closure for the transport of third moments of particle velocity, the developed model can be used as more robust Eulerian-Eulerian two-fluid model for engineering calculations of particle-laden flows.

Acknowledgments

The work is partly supported by the Russian Foundation for Basic Research grant (19-08-00781). The used analytical methods and numerical algorithms are developed under the state contract with IT SB RAS.

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Figure 3. The r.m.s. of wall-normal particle velocity for St=48.5.