Calculation of the drag coefficient of micro and nanoparticles

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Abstract. A numerical simulation of the flow of air around micro or nanoparticles was carried out. The results of calculating the drag coefficient for various diameters of the free-stream Mach number are presented. For particles with a diameter of 10 and 100 μm, the influence of flow turbulence was taken into account. The calculated dependences obtained are compared with empirical formulas.

1. Introduction

When constructing a physical and mathematical model of the flow, it is necessary to accurately predict the local flow characteristics that arise when the gas medium interacts with the particle. In the interaction of shock and detonation waves with particles, the accuracy of predicting the rate relaxation of particles depends on the accuracy of setting such a flow parameter as the drag coefficient. The correctness of the results directly depends on the chosen model of the interaction of the flow and the particle at the boundary of two phases.

A number of works are devoted to the study of the interaction of flows with particles at the micro level. In [1] the problem of the flow around a system of bodies (cylinders or spheres) was solved by numerical methods. The flow regimes are described; a parametric analysis of the phenomenon under study is carried out. Based on the obtained data, a map of the modes of flow around the shock wave near the bodies is compiled, depending on the Mach number of the incoming flow and the distance between the bodies.

In [2] a numerical simulation of the interaction of a shock wave with a system of stationary particles located along the flow and perpendicular to it was carried out. The dependence of the particle drag coefficient on the Mach number of the flow behind the shock wave is found. It is shown that in the case when the particles are perpendicular to the flow, the flow regime has a negligible effect on the drag coefficient, and in the case when the particles are located along the flow their mutual influence remains at a large distance.

In article [3] a numerical simulation of the flow of a two-phase mixture of gas and submicron metal particles onto an obstacle with a needle located in front of it was carried out. The structure of the separated flow is studied and various approximation formulas (Milliken, Hendersen, etc.) are compared for the law of resistance of spherical particles.

In [4] physical and mathematical models were proposed for describing the processes of propagation, damping, and suppression of detonation in hydrogen-oxygen, methane-oxygen, and
silane-air mixtures with inert micro- and nanoparticles. The resistance coefficient is specified using the empirical Cunningham formula.

The aim of this work is a numerical study of the influence of the free-stream Mach number and the Reynolds number through the particle diameter on their drag coefficient.

2. Formulation of the problem
Figure 1 presents a diagram of the simulated area. Air was chosen as the test gas at a temperature $T_{st} = 300$ K and an initial pressure $P_{st} = 100$ kPa. The particle diameter and Mach number varied: $d$ – from 10 nm to 100 μm; $M$ – from 1.1 to 3.

![Figure 1. Scheme of the simulation.](image)

The problem was solved in a two-dimensional axisymmetric formulation in the ANSYS Fluent calculation package. The Favre-averaged Navier-Stokes equations supplemented by the SST ($k-\omega$) model of turbulence or the model of laminar flow, depending on the Reynolds number, were used as a mathematical model. For approximation in time, an implicit second-order scheme was used, and for approximation in space of inviscid flows, a third-order accuracy AUSM splitting scheme was used.

3. Calculations results
The drag coefficient $C_d$ was adopted as the main simulation result. This coefficient was also calculated using the empirical Henderson formulas [5] and using the approximation formula [6] with the Cunningham correction taken from the review paper [7]. The obtained values were compared with each other.

For particles with a diameter of 10 μm and 100 μm, the calculations were performed in two versions: with a turbulence model and a laminar flow model. This was done to identify the effect of the model used on the calculation results. For these diameters, the Reynolds number is quite significant which allows us to use the turbulence model ($k-\omega$ in the SST version of the Mentor). The calculation results for a particle with the diameter of 100 μm are presented in Figure 2.

The resulting $C_d$ values for various flow models (laminar and turbulent flow) are somewhat different. The turbulent flow model gives large values of the drag coefficient; however, this difference decreases with increasing Mach number. The numerical data are overestimated in comparison with the results of calculations using the Cunningham correction. For Henderson's formula, more complete agreement is observed as the Mach number increases.

For a particle with the diameter of 10 μm a similar trend is observed, see Figure 3. However, the difference between the values of the drag coefficient obtained from numerical calculations for laminar and turbulent flow is not so significant. For Mach numbers $M > 1.5$ this difference is negligible.
Figure 2. The dependence of the resistance coefficient on the Mach number for $d = 100 \mu m$. The results of numerical modeling and calculations by approximation dependencies.

Figure 3. The dependence of the resistance coefficient on the Mach number for $d = 10 \mu m$. The results of numerical modeling and calculations by approximation dependencies.

For particles with a diameter of $d = 10 \text{ nm} - 1 \mu m$ calculations were carried out only using the laminar flow model, since precisely at this Reynolds number this mode is observed. Figure 4 presents the calculation results for a particle with a diameter of $d = 1 \mu m$.

As can be seen from Figure 4, obtained as a result of numerical simulation, the values of $c_d$ qualitatively repeat the approximation dependences. However, these values are overestimated in comparison with calculations using the Cunningham correction and underestimated in comparison with the curve obtained by the Henderson formula.

As for the previous cases, obtained as a result of numerical simulation, the values of the resistance coefficient for $d = 100 \text{ nm}$ qualitatively repeat the approximation dependences, see Figure 5. The numerical data show overestimated values in comparison with empirical formulas.
Figure 4. The dependence of the resistance coefficient on the Mach number for $d = 1 \mu m$. The results of numerical modeling and calculations by approximation dependencies.

Figure 5. The dependence of the resistance coefficient on the Mach number for $d = 100 \text{ nm}$. The results of numerical modeling and calculations by approximation dependencies.

For $d = 10 \text{ nm}$ the discrepancy between numerical and empirical data increases, see Figure 6. Such a discrepancy is associated with the realization of the free-molecular flow regime at which the Knudsen number $Kn \sim 10$ which violates the continuity hypothesis and leads to the necessity of taking into account correction factors in the boundary conditions on the particle.

4. Conclusions
Using numerical methods the dependences of the drag coefficient of particles of various diameters on the Mach number of the incoming flow are obtained.

The obtained values are compared with empirical dependences, which showed the need to take correction factors into account, especially for nanoscale particles.

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Figure 6. The dependence of the resistance coefficient on the Mach number for $d = 10$ nm. The results of numerical modeling and calculations by approximation dependencies.

Nomenclature

$T_s$ – static temperature;

$P_s$ – static pressure;

$d$ – diameter of the particle;

$M$ – free stream Mach number

$Cd$ – particle drag coefficient

$Kn$ – Knudsen number

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