

NUMERICAL STUDY OF AEROSOL PARTICLE ASPIRATION INTO A THIN-WALLED TUBE ORIENTED NORMALLY TO THE FLOW

A.A. Medvedev, N.N. Trusova, S.G. Chernyi, and A.V. Sharov

*Scientific Research Institute of Aerobiology,
State Scientific Center of Virology and Biotechnology "VektorB, Novosibirsk region
Institute of Computer Technologies,
Siberian Branch of the Russian Academy of Sciences, Novosibirsk
Received February 4, 1998*

Efficiency of aerosol aspiration into a thin-walled tube from a lateral flow is calculated by numerical solution of three-dimensional Navier-Stokes equations and equations of particle motion. The results of calculation are compared with published semi-empirical equations.

1. INTRODUCTION

Contact methods associated with the necessity to sample particles into various devices are widely used in analysis of aerosols, including atmospheric aerosols. In this case, arising distortions in disperse composition of the initial aerosol can considerably exceed errors of used devices. Main sources of distortions are deflections of particle trajectories from air flow lines due to inertia, particle recoil from external surfaces of a sonde, particle sedimentation in the sampler internal path. The measure of distortion in the disperse composition of aerosol in sampling is aspiration efficiency, $A = c/c_0$, where c and c_0 are mean flow concentration of a given fraction of aerosol inside the sonde and in a non-disturbed flow, respectively.

Determination of aspiration errors for the simplest sonde, i.e., a cylindrical tube, is considered in a lot of papers (see, for instance, the review in Ref. 1). However, for many cases, in particular, for sampling into a tube oriented at an arbitrary angle to the outer flow, reliable data are yet not obtained. Such data could be used for choosing construction parameters and operation modes of samplers and for determining errors of aspiration from the turbulent atmosphere. The semi-empirical equations obtained in Refs. 1–4 on the base of experimental data do not cover the whole range of possible variation of the decisive parameters and badly agree with each other. Experimental studies of the aspiration process were performed mainly by the comparison method, when the aspiration efficiency was defined as the ratio of flow concentrations of monodisperse aerosol measured by the studied sonde and the reference one. It should be noted that this method has rather large extent of uncertainty due to different possible ways of particle behavior in contact with inner and outer surfaces of the tube: particles break, adhere to surfaces, roll, recoil, etc. Thus, the measured concentration of particles depends on physico-chemical properties of particles and the tube surfaces. The large spread in

data obtained by the comparison method is probably caused by the above-mentioned factors.

In Refs. 5–6, the process of aspiration into a tube oriented parallel to the running-on flow (coaxial sampling) was studied by the method of limit trajectories, in which particle trajectories closed at the end edges of the sonde and bounding the domain of particles entering the sonde were determined by optical methods. In this case, measured was the efficiency of outer aspiration $A_e = c_e/c_0$, where c_e is mean flow concentration of particles of a given fraction at the entrance of the sonde. It is close to full aspiration efficiency A , when influence of recoil, secondary aspiration of particles, and their sedimentation inside the tube are insignificant. If the flow direction is not parallel to the axis, the cross section of the limit-trajectory tube has a complicated shape and it is very difficult to measure its area (there are no papers on this subject yet). Besides, direct sedimentation of particles inside the tube should be taken into account in this case.

Application of numerical methods permits the effects from different factors to be taken into account. In particular, the aspiration efficiency can be calculated for the following limiting cases: all particles touching a hard wall do not fall into the sample, or particles undergo elastic repulsion off the wall. However, for accurate account for features arising in a flow, such as separations and vortexes, the model taking into account viscous effects should be used. This involves some computational difficulties in the three-dimensional case. So, numerical simulation of aspiration with use of the Navier-Stokes equations was still performed only for two-dimensional cases, such as coaxial sampling.^{7,8}

In this paper, numerical simulation of sampling into a thin-walled tube oriented normally to the outer flow is performed by use of the three-dimensional Navier-Stokes equations. Efficiency of outer and full aspiration was calculated on the assumption that all particles touching a hard wall do not fall in the sample.

2. NUMERICAL METHOD

Concentration of particles in air flow is supposed to be low and so they do not have a significant effect on air flow, which is supposed laminar, stationary, and incompressible. Aspiration process is simulated in two steps. At the first step, the field of air velocity in the vicinity of the tube and inside it is calculated by numerical solution of the Navier-Stokes equations. At the second step, trajectories of separate particles and aspiration efficiency are calculated by integration of the equations of particle motion.

The three-dimensional Navier-Stokes equations are solved by an original finite-difference method based on the conception of artificial compressibility.⁹ The calculation domain is divided into test volumes by a grid constructed in the cylindrical coordinate system, where the z -axis coincides with the axis of symmetry. Further, air velocities in grid nodes and particle trajectories are calculated in the Cartesian coordinate system.

Figure 1 presents the cross section of the calculation domain in the plane of the tube axis of symmetry and shows us the main geometrical parameters: D is the tube diameter; R_0 is radius of the outer lateral boundary; H_1 and H_2 are distances from the input edge of the tube to upper and lower boundaries of the calculation domain, respectively. The values of R_0 , H_1 , and H_2 are chosen sufficiently large, so that perturbations from the tube do not reach outer boundaries. Boundary conditions at the outer boundaries are set on the assumption that influence of viscosity upon the flow is insignificant far from the tube. At the inner and outer surfaces of the tube, velocity and pressure gradient along the normal to the wall are assumed to be zero. At the output cross section of the tube, pressure is taken so that it provides for the required flow rate through the sampler; velocity components are extrapolated onto it from the calculation domain.

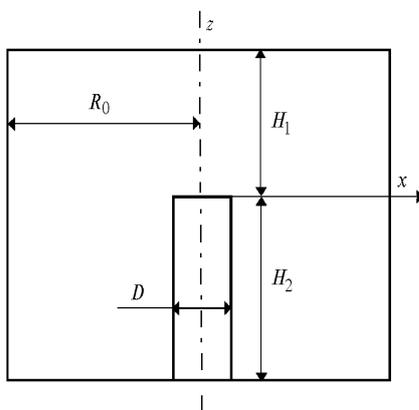


FIG. 1. Calculation domain.

Trajectories of particles are calculated by solving equations of motion written in correspondence with the Stokes law

$$m \frac{d\mathbf{u}}{dt} = \frac{3\pi\mu d_p}{C} (\mathbf{v} - \mathbf{u}), \quad (1)$$

where m and d_p are mass and diameter of a particle; \mathbf{v} is the vector of air velocity; \mathbf{u} is the vector of particle velocity; μ is air viscosity; C is the Cunningham correction for molecular sliding. Using the diameter of the tube inlet D and the outer flow velocity W as characteristic length and velocity, Eq. (1) can be written in the dimensionless form

$$\text{St} \frac{d\mathbf{u}'}{dt'} = \mathbf{v}' - \mathbf{u}', \quad (2)$$

where $\text{St} = \rho_p C d_p^2 W / 18\mu D = \tau W / D$ is the Stokes number; $\mathbf{v}' = \mathbf{v} / W$, $\mathbf{u}' = \mathbf{u} / W$, $t' = tW / D$ are air and particle dimensionless velocities and time; τ is the particle relaxation time.

Following Refs. 1–4, aspiration efficiency is considered as a function of three dimensionless variables, namely, the Stokes number St , the anisokineticity coefficient $R = W / V_0$, where V_0 is mean air velocity in the tube, and the angle α between the direction of the outer flow and the tube axis. Since the flow around the tube is not laminar, and air resistance to particle motion deviates from the Stokes law, the aspiration efficiency may depend on absolute values of particle and tube dimensions, as well as velocities of air flows. Besides, under certain conditions, the aspiration process can be affected by gravitational sedimentation of particles. These problems require further study and will be considered in our next papers.

Equation (2) can be integrated by the Runge-Kutta method of the 4th order. Start positions of trajectories are in a plane perpendicular to the velocity vector of the running-on flow. The plane is placed sufficiently far from the tube, so the flow is assumed non-disturbed. Let S_e be the area of the domain of start positions from which particles fall into the inlet of the tube, S be the area of the domain from which the particles fly into the tube at a distance of two tube diameters without touching the wall. Then the efficiency of outer aspiration is

$$A_e = \frac{c_e}{c_0} = \frac{4W S_e}{\pi D^2 V_0}. \quad (3)$$

Having substituted S_e by S in Eq. (3), we obtain the efficiency of full aspiration A .

Since the shape of the above-mentioned domains is, as demonstrated below, rather complicated, the areas S_e and S were calculated by simple summation of areas of elementary cells containing the start points

$$S = \sum_{i=1}^I \delta S_i K_i, \quad (4)$$

where δS_i is the area of the i th cell ($i = 1, \dots, I$), into which the whole domain of start positions of particles is divided. Each cell corresponds to a unique trajectory.

Here, $K_i=0$ if the particle flew by the tube or taugt the wall; $K_i=1$ if the particle fell into the inlet or at a given distance inside the tube. To save computational time and increase the accuracy of calculations, the values of S_e or S were consequently corrected by dividing cells along the boundaries of the above-mentioned domains.

3. CALCULATION RESULTS

We have calculated the efficiency of aspiration into a tube with diameter $D = 0.01$ m at the rate of the outer flow $W = 5$ m/s. The Reynolds number of a tube corresponding to these parameters is $Re = WD/\nu = 3450$, where ν is the kinetic viscosity of air. The mean rate of air exhaustion in the tube V_0 varied in the range from 1.7 to 20 m/s, and the number St varied from 0.01 to 0.4 what corresponds to particle dimensions $d_p = 2.5 \cdot 10^{-6} - 16 \cdot 10^{-6}$ m for a given values of D and W .

The values $R_0 = 18D$, $H_1 = 10D$, and $H_2 = 10D$ were fit during preliminary calculations. Their further increase has no effect on the obtained solution. Besides, calculations for sequences of grids made it possible to choose the optimum number of general grid nodes: 54 in radial direction, 47 in height of the domain (z -axis), and 20 in the angle. All the results presented below were obtained for these dimensions of the domain and grid.

Figure 2 presents separate trajectories of particles in isometry for $V_0 = 10$ m/s and Stokes number $St = 0.1$.

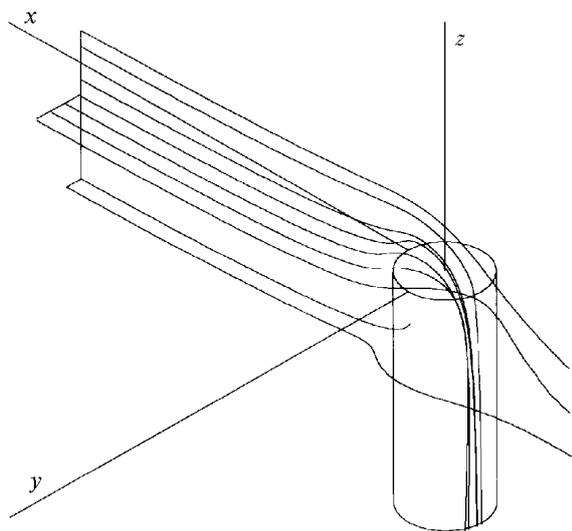


FIG. 2. Trajectories of particles.

Figure 3 presents the domain of start points from which particles fall into the input section of the tube for $V_0 = 20$ m/s and $St = 0.3$. The contour of the tube is projected onto the presented domain in order to

compare the dimensions. The attention should be paid to the narrow bands of start points at a certain distance from the cross section of the main tube of trajectories. Their appearance can be explained by the fact that, for large V_0 , particles can be sucked into the tube while turning around near its leeward side. The particles whose trajectories are closer to the inlet can “not blendB with the turn and sediment on the outer surface of the wall.

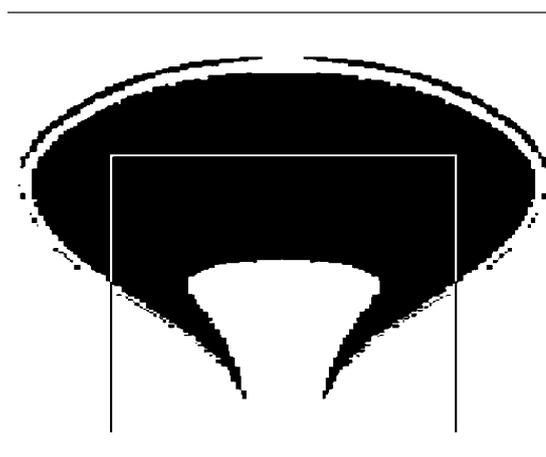


FIG. 3. Domain of start points from which particles fall into the input section of the tube.

Calculation results for the aspiration efficiency are presented in the Table.

Further, the results of calculations were compared with the following published data. The authors of Ref. 4, on the base of their own experimental data, deduced the following semiempirical relation:

$$A = 1 + 3(R \cos\alpha - 1) St \sqrt{R}, \tag{5}$$

where $0.02 \leq St \leq 0.2$; $0.5 \leq R \leq 2$; $45^\circ \leq \alpha \leq 90^\circ$, for the efficiency of aspiration into a cylindrical tube placed at an angle α to the running-on flow.

The following relation

$$A = 1 + \left[1 - \frac{1}{1 + G(\alpha) St(\cos\alpha + 4\sqrt{R} \sin\alpha)} \right] \times (R \cos\alpha - 1), \tag{6}$$

was obtained in Ref. 1. It can be simplified for $\alpha = 90^\circ$. Taking into account the value of the coefficient $G = 2.1$ obtained by the author as a result of analysis of the published experimental data, the relation has the form

$$A = 1 / (1 + 8.4 St \sqrt{R}). \tag{7}$$

TABLE I. Calculated efficiency of outer A_e and full A aspiration depending on the Stokes number St and the anisokineticity coefficient R .

St	R											
	2.9		1.7		1		0.5		0.36		0.25	
	A_e	A										
0.01	0.865	0.849	0.888	0.876	0.984	0.981	0.976	0.976	0.951	0.951	0.938	0.938
0.02	0.790	0.771	0.835	0.819	0.943	0.936	0.951	0.951	0.932	0.932	0.923	0.923
0.05	0.575	0.535	0.668	0.631	0.828	0.806	0.874	0.874	0.868	0.868	0.867	0.867
0.07	0.452	0.387	0.566	0.495	0.747	0.702	0.822	0.822	0.824	0.824	0.825	0.825
0.10	0.307	0.206	0.421	0.274	0.631	0.497	0.744	0.742	0.757	0.757	0.763	0.763
0.20	0.100	0.016	0.148	0.020	0.299	0.021	0.507	0.019	0.553	0.135	0.585	0.269
0.30	0.036	0.000	0.073	0.003	0.139	0.003	0.332	0.003	0.398	0.006	0.450	0.082
0.40	0.004	0.000	0.044	0.000	0.084	0.001	0.221	0.001	0.293	0.002	0.378	0.049

Figure 4 presents the aspiration efficiency as a function of the number St for different values of the parameter R . They are obtained by Eqs. (5) and (7) (solid lines). The values of outer aspiration efficiency calculated by the method proposed in this paper are presented by symbols. One can see that the calculated data satisfactorily agree with Eq. (5) for $R = 1.7$ and 1, i.e., for small exhaustion rates $V_0 = 3$ and 5 m/s. For $R = 0.5$ and $V_0 = 10$ m/s, agreement is considerably worse. Perhaps, this is connected with the fact that the experimental data approximated by Eq. (5) are affected by secondary aspiration, i.e., suction of particles recoiling off the outer surface of the tube. This effect is usually manifested with large air velocities at the inlet of the tube and small R when air is sucked into the tube from a wide spatial domain.

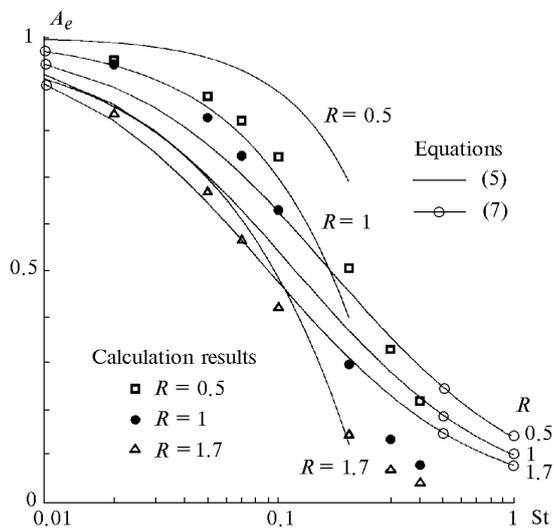


FIG. 4. Calculation results for the efficiency of outer aspiration.

In calculations, the particles that touched the tube surface were supposed lost. The results qualitatively agree with Eq. (7) which, on the one hand, is deduced on the base of a theoretical model that does not take into account the secondary aspiration. On the other hand, it includes the coefficient G obtained from a large variety of experimental data that are possibly influenced by the

secondary aspiration. Thus, taking into account the large spread of experimental data and difficulties in their interpretation, one should not expect better agreement with the results of calculations. Experimental verification of the proposed mathematical model seems to require the higher level of experiments.

4. CONCLUSION

Thus, this paper proposes the numerical method, using which the efficiency of outer and full aspiration is calculated for a thin-walled tube oriented normally to the flow. Since the results of calculations are presented as a function of dimensionless variables St and R , they can be applied for correction of results and choosing of operation modes of different sampling tubes. The proposed numerical method is applicable also for a more general case, i.e., aspiration from an arbitrarily oriented flow.

ACKNOWLEDGMENTS

This work was partially supported by the Russian Foundation for Basic Researches (Project No. 96-01-01934) and RFFR-INTAS (Project No. 95-1149).

REFERENCES

1. J.H. Vincent, *Aerosol Sampling: Science and Practice* (Wiley, New York, 1989), 385 pp.
2. A.G. Laktionov, Tr. Inst. Prikl. Geofiz., issue 7, 83-87 (1973).
3. M.D. Durham and D.A. Lindgren, J. Aerosol Sci. **11**, No. 2, 179-188 (1980).
4. S. Hangal and K. Willeke, Atmos. Environ. **24**, No. 9, 2379-2386 (1990).
5. S.P. Belyaev and L.M. Levin, Tr. Ins. Exp. Meteorol., issue 20, 3-33 (1971).
6. G.N. Lipatov, S.A. Grinshpun, G.L. Shingaryov, and A.G. Sutugin, J. Aerosol Sci. **17**, No. 5, 763-769 (1986).
7. D.J. Rader and V.A. Marple, Aerosol Sci. & Technol., No. 8, 283-299 (1988).
8. B.Y.H. Liu, Z.Q. Zhang, and T.H. Kuehn, J. Atmos. Sci. **20**, No. 3, 367-380 (1989).
9. Yu.A. Gryazin, S.G. Chernyi, S.V. Sharov, and P.A. Shashkin, Dokl. Ross. Akad. Nauk **353**, No. 4, 478-483 (1997).