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# Stochastic modelling of aerosol deposition for LES of 90° bend turbulent flow

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**Abstract**

Aerosols deposition in turbulent bend flows is a major concern that is critical to many industrial, environmental and biomedical applications. In this work, a well-resolved LES was performed to compute the deposition efficiency of aerosols in turbulent circular cross-section bend flow of Dean number $De = 4,225$. The numerical predictions were compared to the experimental work of Pui et al. [Pui, D.Y.H., Romay-Novas, F., Liu, B.Y.H., 1987. Experimental study of particle deposition in bend of circular cross-section. Aerosol Sci. Technol. 7, 301–315] and the fully-resolved LES of Breuer et al. [Breuer, M., Baytekin, H.T., Matida, E.A., 2006. Prediction of aerosol deposition in 90° bends using LES and an efficient Lagrangian tracking method. J. Aerosol Sci. 37, 1407–1428]. In the present LES, a slightly coarser but unstructured-grid numerical description was adopted, entailing that a portion of the small scales' contribution to particle dispersion to be discarded. Thus, a Langevin-type stochastic model was used to model the effect of the discarded sub-grid motion on aerosol deposition. This stochastic model was shown to perform well in previous studies [Berrouk, A.S., Laurence, D., Riley, J.J., Stock, D.E., 2007. Stochastic modelling of inertial particle dispersion by subgrid motion for LES of high Reynolds number pipe flow. J. Turbulence, 8, 50]. Good care was taken to ensure that the main dynamical features of the continuous phase were captured by the present LES. An estimation of the filtered-out kinetic energy was provided. Results of the present LES with SGS model for particles were found to compare well with the experimental work and the fully-resolved LES (near-wall DNS) of Breuer for all the range of the Stokes number considered, $0.001 < St < 1.5$. Influence of the SGS model for particles was visible for the deposition efficiency of aerosols with Stokes number $St < 0.3$.

*Keywords:* LES; Aerosols deposition; Bend; Sub-grid; Stochastic

## 1. Introduction

Deposition of aerosols in turbulent bend flows is encountered in many industrial, environmental and biomedical applications of practical interest. Experimental and numerical studies of inertial deposition in curved pipes have been motivated by interest in calculating the deposition of inhaled particles in human airways. The aim is to help providing more effective treatment of lung diseases, better protection against toxic airborne pollutants, and improvement in routes of systemic drug administration (Finlay, 2001). Other applications consist of systems for sampling aerosol particles from atmosphere or industrial process streams that commonly occur in bends of piping systems. A significant loss of particles can take place in a bend as a result of inertial deposition. To obtain accurate data, it is important to correct for the losses of particles in bends as well as other parts of

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## Nomenclature

*Roman letters*

| | |
|---|---|
| $\bar{p}$ | Filtered pressure field |
| $\bar{S}_{ij}$ | Resolved rate of strain tensor |
| $\bar{u}_i$ | Filtered fluid velocity |
| $\tilde{k}_{SGS}$ | Modified SGS kinetic energy |
| $k_{SGS}$ | SGS kinetic energy |
| $A_{s,i}$ | Drift vector |
| $B_{s,ij}$ | Diffusion matrix |
| $C_0^*$ | Diffusion coefficient |
| $C_0$ | Kolmogorov constant |
| $C_D$ | Drag coefficient |
| $C_n$ | Cunningham slip correction factor |
| $C_s$ | Smagorinsky constant |
| $d_p$ | Particle diameter |
| $De$ | Dean number $De = Re/\sqrt{R_0}$ |
| $k_{SGS}$ | SGS kinetic energy |
| $N_p^{after\ bend}$ | Number of particles that exit the bend |
| $N_p^{bend}$ | Number of particles that deposit in the bend |
| $R_0$ | Curvature ratio $R_0 = R_b/R$ |
| $R_b$ | Radius of curvature of the bend |
| $Re_\tau$ | Friction Reynolds number |
| $Re_p$ | Particle Reynolds number |
| $T^*_{SGS}$ | Fluid sub-grid time scale with inertia and CT effects included |
| $T_{E,SGS}$ | Eulerian sub-grid time scale |
| $T_E$ | Eulerian time scale |
| $T_{L,SGS}$ | Lagrangian sub-grid time scale |
| $T_L$ | Lagrangian time scale |
| $U_0$ | Mean velocity |
| $u_\tau$ | Friction or shear velocity |
| $u_p$ | Particle velocity |
| $u_r$ | Mean slip velocity between fluid and inertial particles |
| $u_s$ | Velocity of the fluid seen |
| $u_i$ | Fluid fluctuating turbulent velocity |
| $W_i$ | Wiener process |
| $x_i$ | Cartesian coordinate system directions |
| $x_p$ | Particle position |
| $y^+$ | Dimensionless distance from the wall |
| $g$ | Gravity force |
| $h$ | Grid spacing |
| $I$ | Inner radius of the curved bend |
| $k$ | Total Kinetic energy |
| $O$ | Outer radius of the curved bend |
| $R$ | Tube radius |
| Re | Flow Reynolds number: $Re = u_b D/\nu$ |
| St | Stokes number $St = \tau_p/T$ |
| $T$ | Integral time scale $T = R/U_0$ |
| $t$ | Time |

*Greek letters*

| | |
|---|---|
| $\beta$ | Ratio between the Lagrangian and the Eulerian time scales |
| $\Delta t$ | Time step |
| $\Delta$ | Filter width |
| $\delta_{ij}$ | Kornecker Delta |
| $\epsilon_r$ | Dissipation rate of the SGS kinetic energy |
| $\eta_p$ | Deposition efficiency |
| $\nu$ | Kinematic fluid viscosity |
| $\nu_{SGS}$ | Sub-grid scale eddy viscosit. |
| $\rho_f$ | Fluid density |
| $\rho_p$ | Particle density |
| $\tau_{ij}$ | Sub-grid stress tensor |
| $\tau_p$ | Particle response time |
| $\tau_w$ | Wall shear stress $\tau_w = \rho_f u_\tau^2$ |

*Acronyms*

| | |
|---|---|
| CT | Cross Trajectory |
| DNS | Direct Numerical Simulation |
| LES | Large Eddy Simulation |
| RANS | Reynolds-Averaged Navier-Stokes |
| SDE | Stochastic Differential Equation |
| SGS | Sub-Grid Scale |
| SM | Stochastic Model |

the sampling system. This is a major concern for High-Tech industries such as semiconductor manufacturing. For the oil and gas industry, predicting inertial particle deposition and the accompanying erosion phenomena is crucial to avoiding extremely expensive component repair, replacement or failure, and by consequence expensive system shutdown.

For many of these applications, a Direct Numerical Simulation (DNS) is not practical with today's computers while the Reynolds-Averaged Navier-Stokes approach (RANS) is facing many limitations (Lakehal, 2002). Thus, Large Eddy Simulation (LES) has emerged as a promising tool to address these types of problems and its use has increased over the years.

Large eddy simulation is essentially an under-resolved simulation of the complex turbulence phenomenon that uses a model to account for the lack of small scale resolution. In LES, the conflicting requirements of complexity reduction while maintaining accurate predictions are achieved by coarsening the numerical description through spatial filtering on one hand and using a sub-grid stress (SGS) modelling on the other hand. In the filtering process the instantaneous information concerning the dynamics of the small scales is washed out.

In LES of dispersed turbulent multiphase flows, it has been common that tracking inertial particles in turbulent flows is carried out using only the filtered velocity field, considering as negligible any transport by the sub-grid