Modeling aerosol scavenging by drops: from microphysical CFD simulations to a global collection kernel

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Scavenging aerosol particles by droplets is an efficient way of removing hazardous particles from gases. Therefore, predicting removal rates by means of a realistic collection kernel is a purpose in several research fields like environment, industrial or atmospheric science. An effective scavenging kernel must take into consideration several coupled collection mechanisms such as Brownian scavenging, phoretic and electrostatic forces leading to capture and inertial impaction/interception which depend on the flow regime around the drop. Examining Wang *et al* (1978) collection kernel K_W (describing scavenging situations where only Brownian, phoretic and electrostatic mechanism take place), and Mohebbi *et al* (2003) scavenging kernel (predicting exclusively inertial capture) shows the lack of universality of scavenging kernels but also the lack of precise numerical or experimental reference data enabling a more general correlation for the scavenging kernel to be derived. We propose to improve available reference data using numerical scavenging experiments: simulations of particles-laden flows (particle diameter $d_p \in [1nm; 100\mu m]$) around a water drop of diameter $d_d \in [78; 598]\ \mu m$ at moderate Reynolds number ($Re \in [1; 100]$) are achieved. A global collection kernel is then derived from these new scavenging efficiencies.

The microphysical modeling is achieved in two steps. First, the continuous phase motion is simulated in non-dimensional form by a finite volume method, taking into account the shear stress continuity at the droplet's interface. Then, the discrete phase is modeled using Lagrangian stochastic tracking method with large time steps (one way coupling): the explicit integration scheme (Mohaupt *et al* (2011)) is used to predict position and velocity of particles taking into account flows velocities, particle's deviation due to inertia and Brownian motion. Status of particles at the end of the simulation (i.e. captured or not) is computed to acquire collection efficiencies for each scavenging situation.

Data thus obtained are used to set up a new collection kernel by upgrading K_W which depends, among other parameters, on a mean ventilation coefficient f_p implemented to take into consideration the asymmetry of the aerosol concentration field around the drop due to the flow regime. Similarly, the concentration field of inertial particles is asymmetric because of the deviation of those aerosols from streamlines. Replacing f_p by $f_p' = f_p * F + G$ (f_p being the Beard (1974) correlation for non-inertial particles) into K_W extends its prediction capabilities. In this expression, F and G are given by (1) and (2):

$$F = \left(1 + 2Re^{1/2}St\right)^2 \qquad (1)$$

$$G = f_p'^{inf}\left(\frac{1}{\pi}\operatorname{atan}\left(2.5\log\left(\frac{St}{0.54Re^{-0.225}}\right)\right) + \frac{1}{2}\right)^4 \qquad (2)$$

with $f_p'^{inf} = \frac{(d_d+d_p)^2 \mu_a Re}{8{d_d}^2 D_{B_p}\rho_a}$ (infinite inertia situation) and where St is the Stokes number of the particle, μ_a (resp. ρ_a) the dynamic viscosity (resp. density) of the air and D_{B_p} the Brownian particle diffusivity.

This correlation allows efficient and computational cheap predictions of scavenging efficiencies depending on Brownian motion, phoretic and electrostatic forces and inertial impaction/interception as shown in Table 1.

Table 1: Deviation between references values (Grover *et al* (1977) and Wang *et al* (1978)) and predicted values of collection kernels for $d_p \in [1\ nm; 20\ \mu m]$ and relative humidities $\in [50; 100]\%$. RMSE: Root Mean Square Error, R²: Coefficient of Determination.

Reynolds number	RMSE	R²
1	0,07	0,99
4	0,14	0,97
10	0,13	0,98
30	0,12	0,98
100	0,19	0,96
Mean value	0,13	0,98

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