Commun. Comput. Phys.
doi: 10.4208/cicp.180714.200415a

Vol. **18**, No. 3, pp. 723-756
September 2015

Modelling and Numerics for Respiratory Aerosols

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Received 18 July 2014; Accepted (in revised version) 20 April 2015

Abstract. In this work, we present a model for an aerosol (air/particle mixture) in the respiratory system. It consists of the incompressible Navier-Stokes equations for the air and the Vlasov equation for the particles in a fixed or moving domain, coupled through a drag force. We propose a discretization of the model, investigate stability properties of the numerical code and sensitivity to parameter perturbation. We also focus on the influence of the aerosol on the airflow.

AMS subject classifications: 65M60, 35Q30, 35Q83, 35Q92

Key words: Aerosols, Navier-Stokes-Vlasov system, discretization, finite-element method, particle-in-cell method, stability properties.

1 Introduction

The evolution of droplets or particles in a surrounding fluid is a phenomenon encountered in several areas, ranging from medicine (aerosol therapy) to motor industry (transport and combustion of petrol). In the particular case of aerosol therapy, *in vivo* observations of drug delivery in the airways induce several difficulties. For instance, aerosol deposition maps require heavy experimental protocols, which cannot be easily repeated, and the obtained measurements may not be accurate enough.

Consequently, the choice of physically relevant models, and thereafter the design of stable, efficient numerical methods allow *in silico* experiments which can provide a wide range of results for various physical situations and parameters (type of aerosols, surrounding fluids, pathological state$\cdots$).

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Several kinds of modelling are available to describe the aerosol motion in a fluid. Two of them are discussed quite in detail in [31]: one can consider individual particles on the one hand, or a collection of particles on the other hand.

Two-phase models consider the collection of droplets or particles as a fluid and study the evolution, for instance, of aerosol concentration in the ambient fluid. Those models are most certainly adapted in the case when the volume fraction occupied by the dispersed phase is not negligible with respect to the volume fraction occupied by the surrounding fluid [7, 17, 34, 36]. Unfortunately, such models do not allow an accurate description of particle deposition. This is why we shall only focus on spray models in which the discrete aspect of the dispersed phase is kept.

Following particles as individuals is the other classical strategy, see [9, 15, 16, 39, 47] for instance. Nevertheless, describing the behaviour of such a (very) large number of particles may lead to both technical and numerical difficulties if one tries to keep track of each individual trajectory. For instance, the *Atomiser pocket aeroneb GO* from DTF[†] Corporation has the following characteristics: airflow rate of 0.3 mL/min, average (in mass) diameter equal to 3.6 μm. Hence, this nebulizer allows the injection of 10^{10} particles in one minute.

In this context of very numerous particles, and since the volume occupied by the aerosol remains negligible in the human airways, the formalism of statistical physics and kinetic theory is an especially well-adapted modelling approach. This type of coupling was first introduced by O'Rourke [40] or Williams [44] and is now quite often used to model aerosol transport in the lung, see [10, 13, 27]. As for the interaction between the aerosol and the surrounding fluid, following a nomenclature introduced by O'Rourke (see also [22]), we assume the spray to be *thin*. This means that

- the aerosol volume fraction in the mixture remains negligible;
- there are no interactions between the aerosol particles;
- the aerosol can have an effect on the fluid, as a response to the drag force exerted by the fluid on the particles.

Note that, for two-phase models as well as ODE ones, the aerosol retroaction on the fluid is seldom taken into account, to the best of our knowledge. In the same context of aerosol kinetic modelling we consider hereafter, article [27] presents a study of aerosol transport in the trachea where the retroaction is taken into account.

The aerosol is then described by a distribution function which satisfies a Vlasov-type equation. The fluid is assumed to be homogeneous, Newtonian, incompressible, and can be described using the Navier-Stokes equations, see [28] for instance. The physical domain can be either fixed or time-dependent.

The aerosol and fluid are coupled through two terms: the particle acceleration, depending on the relative velocity of the particle in the fluid, and the retroaction force

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[†] See `http://www.dtf.fr`