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Critical trajectories for aerosol particles: Their determination for impaction in fibrous filters and in oscillating bubbles

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ABSTRACT

Critical trajectories for aerosol particles in a gas flow are the ones which divide an aerosol flux into different parts, for example aerosol which is, and is not deposited. They can exist in all gas flows in which aerosol motion is governed by gas velocity rather than by diffusion and we describe two mathematical methods for their calculation. For deposition by impaction on a filter fibre it is necessary to solve the differential equations for particle motion and an efficient iterative procedure is used to obtain the critical trajectories.

Jonas and Schütz (1988) have shown that aerosol impaction is an important mechanism for the removal of aerosol from an oscillating sodium vapour bubble formed during a hypothetical core disruptive accident in a fast reactor. For these one-dimensional oscillations, when the gas velocity within a bubble is a linear function of position, we extend their work by calculating critical trajectories directly from the integral equation describing a depositing particle for two models with different initial conditions. With initially entrained uniform aerosol, the percentage impacted is independent of the inclusion of gravity in the calculations as long as regions empty of aerosol do not appear in the bubbles. Numerical results are obtained for a wide range of amplitudes of bubble oscillations and aerosol in the size range 1-30 μm. In agreement with Jonas and Schütz, we find that a considerable fraction of the aerosol at larger sizes is removed by impaction. The theory is also shown to apply to other types of bubble oscillation including those of a spherical bubble.

1. Introduction

Critical trajectories for aerosol particles which divide different outcomes for the particles can exist in all gas flows in which aerosol motion is governed by gas velocity rather than by diffusion, namely for all except small particles at low velocities. They are important in many flows leading to aerosol deposition, aerosol impaction, and aerosol selection, and, for filtration, their importance was recognised by Davies (1973). Their calculation enables the parameters of the flow and particle characteristics for particular outcomes to be found without calculating large numbers of aerosol trajectories, and would have applications to large scale calculations of aerosol motion involving rebound (Tu et al., 2004) and for aerosol entering and passing into the human respiratory system (Lai et al., 2008, 2013). The determination of particle trajectories by solution of their equation of motion in a given flow field was discussed by Davies (1973), and here we describe a very efficient method for reaching the limiting critical trajectory for impaction in a fibrous filter by a process of iteration. We also describe a direct method for their determination applicable to impaction in an oscillating gas bubble inside a liquid in which the equations in a time-dependent velocity field can be transformed into an integral equation.

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In both cases the flow field in which the particles move must be known or calculable, and we assume that the particles are subject to Stokes′ drag in conditions such that the Stokes number, $\mathrm{St} \geq 1$ so that diffusion can be neglected in describing the particle motion.

In our previous work on filtration (Dunnett & Clement, 2006, 2009, 2012), the boundary element method was used to calculate the flow field for aerosol particles incident on a fibre. The deposition mechanisms examined for a growing deposit were diffusion (Dunnett & Clement, 2006) and also interception (Dunnett & Clement, 2009, 2012). The aim of calculating limiting critical trajectories in the same flow field is to extend this work to deposition by impaction where these trajectories are ones for which particles just touch the growing deposit surface. Once these limiting trajectories are known, it is possible to determine the deposition pattern within a filter and the filter efficiency as deposit is collected. The iterative method described in Section 2 to determine these trajectories is based on Newton′s method used to determine zeros of a function. We find that it is very efficient and only a few iterations are necessary to determine a critical trajectory.

A large bubble consisting mainly of sodium vapour could be formed during a hypothetical core disruptive accident (HCDA) in a liquid-metal-cooled fast breeder reactor (LMFBR). This bubble would initially be under the surface of the sodium, but could transport radioactive aerosol from the core to give a 'primary or HMA bubble source term' in the inner reactor containment. The possible magnitude of this source term has been the subject of simulant experiments (Berthoud et al., 1988), and impaction and washout mechanisms have been identified as contributing substantial amounts to removal of aerosol from the bubble (Jonas & Schütz, 1988). In this paper, we contribute to the theory needed to quantify the removal rates, in particular by showing how aerosol removal by impaction may be efficiently calculated for certain realistic types of bubble oscillation.

Aerosol trajectories in a time-dependent gas velocity field can be calculated from the equation of motion of a particle in the field. In Section 3, we describe how critical trajectories which impact into walls at specified times can be calculated for fields which are linear in position, but arbitrary functions of time. Such fields naturally describe gas flows required to keep the pressure uniform for a wide class of rapid bubble oscillations. These include the one-dimensional motion considered by Jonas & Schütz (1988) which is described here.

The equation of motion for a spherical aerosol particle is taken from Jonas & Schütz (1988), and the thermodynamic functions needed to perform calculations in high temperature sodium vapour are summarised in Appendix A. The calculations are restricted to the Stokes drag regime for aerosol up to 30 μm in radius.

Equations with, and without, gravity included are considered to see when results for impaction should correspond. Remarkably, the impaction percentage from an initially uniform entrained aerosol is unchanged if none of the gas space becomes empty of aerosol.

The basic theory is described in Section 3 and involves formally integrating the equation of motion so that initial and final boundary conditions are incorporated into the resulting integral equation. For linear velocity fields, the integral equation is linear, so that final positions along trajectories can be scaled from initial positions. This process makes it easy to identify critical trajectories and directly calculate percentages of aerosol impacted, and the proportions of the cavity which are empty and filled with aerosol of a given size at any time.

In Section 4, we show that a similar theory applies to the calculation of deposition in radial oscillations of a spherical bubble to calculate percentages of aerosol deposited by impaction. Some extensions of the theory to more complex bubble oscillations are also considered.

The calculations described in Section 5 were originally made in unpublished work by Robin Clement in the 1990s. Two models were introduced to represent limiting cases for aerosol inside an oscillating bubble. In the first model (I) the aerosol is initially entrained at the maximum gas velocity and in the second model (II) entrained at the minimum (zero) velocity. As initial conditions in bubbles formed in possible accidents might not be well specified, these models would bracket all possibilities. This uncertainty was not considered by Jonas & Schütz (1988).

It is not easy to integrate numerically the integral equation for the whole range of parameters considered because rapidly varying exponential functions are involved. A numerical scheme that has proved to be satisfactory is described in Appendix B. The results for calculations using both models are given in Section 5. For model 1, where no empty regions appear in the bubble, results for the percentage of aerosol impacted are given as functions of aerosol size, oscillation amplitude, and time during an oscillation. In model II, where empty regions do appear, results for their percentage size are also given.

Finally, in the conclusions in Section 6, we summarize the results obtained and point out some other possible applications of the theory including deposition in aerosol passage to the lung.

2. Critical trajectories for impaction on a fibre

In the case of aerosol filtration with particles such that the Stokes number, $\mathrm{St} > 1$, inertial impaction will be the main mechanism of capture. The Stokes number is given by $\mathrm{St} = d_\mathrm{p}^2 \rho_\mathrm{p} U_0 C/(8\mu d_\mathrm{f})$; d_p and d_f are the particle and fibre diameters, respectively, ρ_p the particle density, C the Cunningham correction factor, and μ the air viscosity.

The critical trajectories separate those particles that will impact the filter from those that do not, and are tangential to the fibre surface at impact, see Fig. 1. Away from the fibre particles are initially moving with the flow in the x direction with velocity $u = U_0$ and the problem of finding the critical trajectory reduces to that of finding the distance from the axis, y_0, for a trajectory to reach the appropriate tangential boundary condition on the fibre surface. This reduces to solving the differential equations for a trajectory which satisfy a particular boundary condition. The equations for a trajectory in a two-dimensional