# Numerical Investigation of the Effect of Hydrodynamic Mixing on Droplet Nucleation and Growth

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Aerosol flows are relevant in several applications of practical importance. These include soot formation in flames, material synthesis in flow reactors, crystallization and precipitation in the chemical and pharmaceutical industries, spray combustion and various environmental applications.

The understanding of aerosol systems in spatially homogeneous configurations has reached a mature stage, but in practice, aerosol processes and particles formation take place in highly inhomogeneous turbulent flows. By nature of turbulence, the flow is characterized by a wide range of length and time scales in the momentum, temperature, and concentration fields. Aerosol processes, such as nucleation, droplet growth by condensation (heterogeneous nucleation) and coagulation, are strongly non-linear and depend on the local vapor concentration and temperature. Moreover, aerosol processes depend on residence times and history effects. Thus, the study of aerosol flows is challenging and very little previous work exists on this topic.

In the current study, the dynamics of the nucleation and growth of di-butyl-phthalate (DBP) droplets are simulated in a counterflow configuration, i.e. a laboratory laminar stagnation flow. This experiment is chosen in order to introduce a tractable hydrodynamic residence time interacting with the time scales of aerosol processes. A counterflow flow setup consists of two opposed nozzles blowing streams towards each other. One stream is cold nitrogen and the other is hot nitrogen saturated with DBP vapor (saturation ratio $S = 1$). Near the stagnation plane (where cooling by mixing takes place), nano-size droplets of DBP nucleate and grow due to heterogeneous nucleation.

The flow field is simulated using a stream-function formulation. The GDE of the particle size distribution (PSD) is integrated to obtain transport equations for moments. The Quadrature Method of Moments (QMOM) is used for closure. Moments are transported using a second-order upwind scheme in space and an adaptive variable-order scheme in time. Homogeneous nucleation is described by classical Becker-Döring theory and heterogeneous nucleation is modelled using the generalized Mason's formula.

A wide range of hydrodynamic residence times is investigated (residence time is defined as the the ratio of the distance separating the two nozzles to the inlet velocity $L/u_0$). Two regimes are identified as shown in Figure 1. At short residence times, vapor consumption is neglected and increasing the residence time produces more particles (higher average number density). We refere to this regime as the nucleation regime. After a critical residence time is exceeded, vapor consumption becomes important. In this regime (the condensation regime) increasing the residence time consumes more vapor and thus produces less average particle number density.

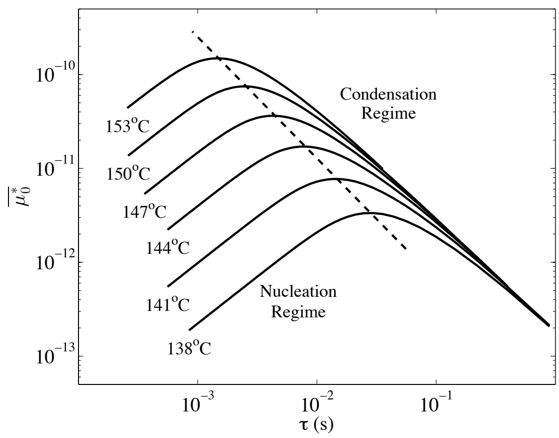


Figure 1: Dimensionless average number density ($\overline{\mu_0^*} = \int \mu_0(x)dx/\mu_r$) vs. the residence time ($\tau = L/u_0$), where $\mu_0(x)$ is the number density and $\mu_r$ is maximum possible number density. $L$ is half the separation between the two nozzles and $u_0$ is the velocity at the inlets. The cold inlet is fixed at 0°C. Curves are labeled with the value of the temperature of the hot stream. The dashed line connects the maximum values, separating the nucleation and the condensation regimes.

In the nucleation regime, the average volume fraction grows at a constant rate with residence time. Once the condensation regime is reached, the average volume fraction reaches a saturation level and the rate at which it increases starts to vanish.

Coagulation was shown to have a negligible effect on the number density distribution in both regimes under the considered conditions.

These conclusions agree with the experimental observations by Okuyama *et al.* (1987).

Okuyama, K., Kousaka, Y., Warren, D., Flagan, R., and Seinfeld, J. (1987) Homogeneous nucleation by continuous mixing of high temperature vapor with room temperature gas. *Aerosol Sci. and Tech.*, 6(1):15-27.