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Mathematical modeling of di-ethyl-hexyl-sebacate nanoparticle formation in a free turbulent jet under high nucleation rate conditions

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ABSTRACT

Mathematical modeling of di-ethyl-hexyl-sebacate (DEHS) nanoparticle formation due to homogeneous nucleation, condensation and coagulation in a hot free turbulent jet issuing into a colder environment is performed. The Reynolds-averaged Navier–Stokes equations are used to describe the fluid flow. The aerosol dynamics is treated by transforming the general dynamic equation into moment equations which are closed by assuming a log-normal shape of the particle size distribution. The contribution of condensation and coagulation to particle formation in the case of high saturation ratios and nucleation rates is studied. The sensitivity of the model to existing approximations of the vapor saturation pressure curve and the ambient temperatures is analyzed. The influence of the main control parameters of the system, such as vapor saturation temperature and nozzle exit velocity, on the aerosol characteristics formed in the turbulent jet is investigated.

1. Introduction

In an attempt to develop a reference generator for the number size distribution function in the submicron size range Koch, Lödding and Pohlmann (2012) carried out the analysis of Brownian coagulation of liquid droplets in a continuously fed well stirred tank reactor (CSTR) which operates in a regime where the particle collision time scale is small compared to the mean residence time of the aerosol in the reactor. The feed aerosol, characterized by its number current and average particle size, is generated in the turbulent jet inside the reactor by homogeneous nucleation of a saturated stream of di-ethyl-hexyl-sebacate (DEHS) vapor and subsequent growth caused by condensation and coagulation. The hot vapor issues through the nozzle into the coaxial cool air stream. Nucleation occurs close to the nozzle whereas most of the growth should take place preferably by coagulation in the similarity regime of the jet. Coagulation and mass exchange leads to a steady state aerosol leaving the CSTR. The asymptotic size regime of the steady state size distribution is influenced by the volumetric gas flow rate through the reactor, the mass flux of the feed aerosol and to a lesser extent by its mean particle size. However, the mean particle size of the feed aerosol is still an influencing parameter, and the feed aerosol source should be operated in a regime where the mean particle size and the number current are least sensitive to the operating parameters or can easily be related

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