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Application of the characteristics-based sectional method to spatially varying aerosol formation and transport

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ABSTRACT

The characteristics-based ssolution. It is easy to verify thatectional method (CBSM) offers an Eulerian description of an internally mixed aerosol. It was shown to be robust and capable of exact preservation of lower order moments, allowing for highly skewed sectional droplet size distributions. In this paper we apply CBSM to a spatially varying flow, by incorporating the fractional step method. In this way an accurate time integration of the spatial terms in the transport equations for the velocity, mass fractions and sectional droplet concentrations is achieved. Integrating CBSM into the compressible PISO (Pressure-Implicit with Splitting of Operators) algorithm allows for phase change and corresponding changes in pressure. We apply CBSM to a lid-driven cavity flow. First, the steady state isothermal flow solution is validated against published data. Next, by releasing a saturated vapor into the cavity while cooling the walls, we simulate the formation of aerosol. The accuracy of the solution is studied, as well as the performance of the CBSM scheme in the spatially varying context. The solution of the velocity is shown to be accurate, even at CFL (Courant–Friedrichs–Lewy) numbers of unity. The feasibility of the developed method is demonstrated in a 3D complex geometry studying the aerosol generation via nucleation of hot vapors cooled by a dilution stream of cold air in a double-mixing tee system. The sectional approach delivers detailed information about the aerosol formation and size distribution of the droplets in the domain.

1. Introduction

In aerosol science a common way of mathematically describing the dispersed phase is by adopting a continuous size distribution, expressing the concentration of droplets with a certain size or composition in space and time. Such a description, without the expensive necessity of tracking each individual particle, allows to investigate size-dependent aerosol processes, such as filtration, deposition, drift and light refraction. A popular method of finding a numerical approximation to the size distribution is the sectional approach (Gelbard, Tambour, & Seinfeld, 1980), in which the size domain is split up into discrete sections, each containing droplets within a pre-defined size range. The evolution of the size distribution is then governed by a manageable number of balance equations for each section.

In Frederix, Stanic, Kuczaj, Nordlund, and Geurts, (2016) CBSM was proposed and illustrated in spatially homogeneous

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Nomenclature

Δt	time step size
Δx	cell size
β	coagulation kernel
δ	Dirac delta function
κ	mixture thermal conductivity
$\kappa_l^\star$	pure constituent liquid thermal conductivity
$\kappa_v^\star$	pure constituent vapor thermal conductivity
μ	mixture viscosity
∇	nabla operator
∂_t	partial time derivative
∂_z	partial droplet size derivative
$\psi^\star$	vapor compressibility ratio
ρ	mixture mass density
$\rho^\star$	pure constituent liquid mass density
σ	droplet surface tension
σ_g	geometric standard deviation
τ	rate of strain tensor
θ	weight for θ-scheme
$\mathbf{A}$	discrete pressure equation coefficient matrix
$\mathbf{b}$	discrete pressure equation source vector
CFL	Courant–Friedrichs–Lewy number
CMD	count median diameter
c_p	mixture heat capacity at constant pressure
D	pipe diameter
d	droplet diameter
$D^\star$	diffusion coefficient
d_c	count mean diameter
d_g	geometric mean diameter
d_{HC}	Hatch–Choate theoretical count mean diameter
D_t	material time derivative
E	Kelvin effect factor
e	convergence measure
$\mathbf{I}$	identity tensor
I	size dependent condensation rate
i	section index subscript
j	species index subscript
J_{coa}	coagulation rate
J_{nuc}	nucleation rate
k	iteration index superscript
k_B	Boltzmann constant
L	size of the cavity
M	number of species
m	time level index superscript
N	droplet number concentration
n	droplet size distribution function
N_c	number of computational volumes
N_P	number of iterations
$\mathbf{p}$	discrete pressure vector
P	number of sections
p	pressure
Q	molar mean molecular weight
Re	Reynolds number
r_P	PISO pressure equation residual
S	vapor-to-liquid mass transfer rate
S_{cond}	vapor-to-liquid condensation mass transfer rate
S_{nuc}	vapor-to-liquid nucleation mass transfer rate
S^s	vapor saturation ratio
T	temperature
t	time
$\mathbf{u}$	mixture velocity
U	velocity magnitude
$\mathbf{u}_c$	species-independent diffusive correction velocity
$\mathbf{v}$	diffusive vapor velocity
V_m	molecular volume
$\mathbf{x}$	position vector
X	vapor mole fraction
Y	vapor mass fraction
y	sectional interface droplet mass
Y^s	vapor equilibrium mass fraction
Z	liquid mass fraction
z	droplet mass
z_{nuc}	critical cluster size of nucleation

conditions of aerosol formation. The current paper extends this development and presents the corresponding method with which aerosol dynamics can be simulated in heterogeneous situations. This completes the necessary step toward a method that can be applied to realistic conditions of multiphase flow and phase changes. Such application is shown for aerosol formation in a 2D cavity and in a 3D double-mixing tee configuration.

The CBSM uses the condensational characteristics in the size domain to solve for nucleation and subsequent condensational growth of droplets. CBSM is based on the sectional formulation of Kumar and Ramkrishna (1996), in which each section contains a pre-specified representative size around which droplets are 'sampled'. By distributing nucleated, grown or coagulated droplets over adjacent sections, one can analytically preserve a pre-selected number of moments of the size distribution. This is essential to conserve number and mass density, or other moments of the distribution. A second advantage which was introduced by CBSM is that, by using an analytic solution for condensational growth through tracking the characteristics of condensation, a robust algorithm is formulated not suffering from a severe time step restriction. Third, CBSM was shown to work on a highly skewed distribution of sections, e.g., a logarithmic distribution, which allows to span many orders of magnitude in the size domain at acceptable costs. To capture nucleation accurately, this was shown to be essential. Finally, through exact moment preservation CBSM may be constructed such that non-negativity of the size distribution solution is guaranteed.

Hitherto, CBSM was only applied to a spatially homogeneous setting, in which the General Dynamic Equation (GDE) (Friedlander, 2000) for the size distribution reduces to one dimension, i.e., the size coordinate. This simplifies the presentation significantly, as one is only concerned with the size space, not physical space. Also, we did not consider any coupling of the aerosol processes to the fluid flow. In practice, however, condensation and evaporation will have an effect on pressure, velocity and temperature, indicating that CBSM must be embedded in an algorithm to solve for the dynamics of the flow. In this paper we apply CBSM to a spatially inhomogeneous setting, in which the aerosol mixture is subject to species convection and diffusion. This poses two challenges. First, we would like to retain CBSM's previously mentioned main strengths in the inhomogeneous setting. Second,