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SOLUTION-ADAPTIVE SPACE-TIME REFINEMENT FOR MULTISPECIES AEROSOL FORMATION

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A solution-dependent strategy for the simulation of aerosol dynamics arising from nucleation in a supersaturated mixture of alcohol gases subjected to very rapid cooling is presented. We apply classical nucleation theory for the prediction of aerosol properties based on [1]. A system of equations is adopted for the total mass density, the velocity and temperature fields of the carrier phase, and the mass fractions of the various species in gaseous and liquid form, as well as the number density of aerosol droplets. The capability of the new approach is illustrated by studying aerosols from alcohol vapors containing up to five different species, for which the size distribution of the aerosol droplets as well as the chemical composition is computed at different temperatures and cooling rates.

The aerosol is subject to rapid nucleation during the initial stages. In order to capture these scales we adopt a time stepping method that adapts to the instantaneous solution. We consider control of the time-accuracy by keeping the size of the time step appropriately small during the rapid nucleation stages, while increasing the size of the time step in case the dynamics slows down after the nucleation. At some point during the time integration we obtained the numerical solution $u(t_n)$ at time t_n with time step size δt. We then proceed as follows:

- Using an explicit method, e.g., Euler forward or a Runge-Kutta method, we compute the numerical solution in the next two instants of time, i.e., $u_{\delta t}(t_{n+1})$ and $u_{\delta t}(t_{n+2})$ with $t_{n+1} = t_n + \delta t$ and $t_{n+2} = t_n + 2\delta t$.
- The solution at t_{n+2} may also be approximated using one time step of size $2\delta t$, denoted by $u_{2\delta t}(t_{n+2})$.

- Likewise, we approximate the solution at t_{n+2} by taking four time steps of size $\delta t/2$, denoted by $u_{\delta t/2}(t_{n+2})$.
- We determine $\epsilon_{2\delta t} = \|u_{2\delta t}(t_{n+2}) - u_{\delta t}(t_{n+2})\|/\|u(0)\|$ and $\epsilon_{\delta t/2} = \|u_{\delta t/2}(t_{n+2}) - u_{\delta t}(t_{n+2})\|/\|u(0)\|$.

Based on the relative differences $\epsilon_{2\delta t}$ and $\epsilon_{\delta t/2}$ we proceed with updating the size of the time step. If $\epsilon_{2\delta t} < \epsilon_{TOL}$ then the size of the time step is increased by a factor $a > 1$, i.e., $\delta t \to a\delta t$. Conversely, if $\epsilon_{\delta t/2} > \epsilon_{TOL}$ then the time step is decreased by the same factor, i.e., $\delta t \to \delta t/a$. Finally, if $\epsilon_{2\delta t} > \epsilon_{TOL}$ and $\epsilon_{\delta t/2} < \epsilon_{TOL}$ then the time step is unchanged.

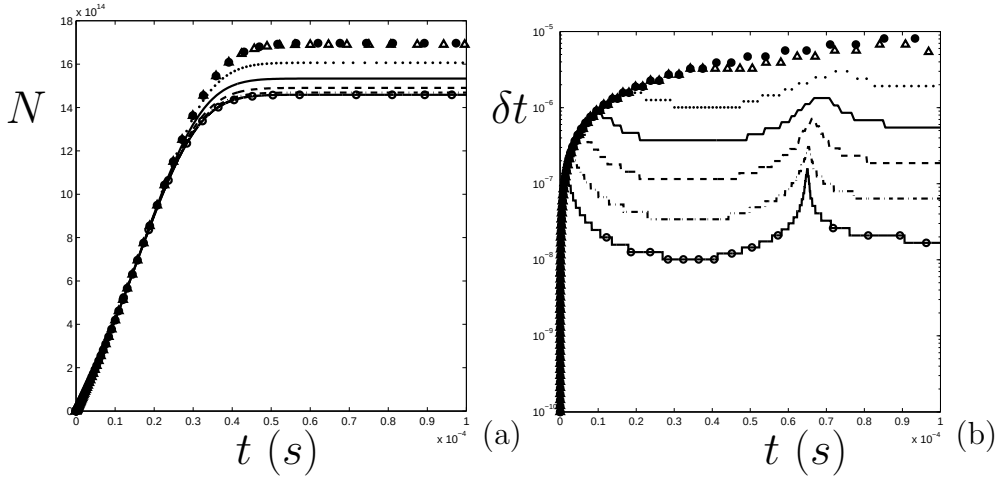

Figure 1: Number density N (per m^3) at various adaptation thresholds ϵ_{TOL} (a) and variation of the time step δt (b). Curves are labeled with ϵ_{TOL}: $\circ$ (10^{-2}), $\triangle$ (10^{-3}), dot (10^{-4}), solid (10^{-5}), dash (10^{-6}), dash-dot (10^{-7}) and solid with $\circ$ (10^{-8}). We set $\delta t_0 = 10^{-10}$ and use a time step stretching $a = 1.2$.

We illustrate the method with a cooling experiment starting at a temperature $T_1 = 275\ K$ and allow it to cool to $T_2 = 200\ K$ in a time interval of $0.01\ s$. In Figure 1(a) we present the dependence of the number density N on the adaptation threshold ϵ_{TOL}. We observe a close agreement in capturing the initial nucleation burst up to $t \approx 2 \cdot 10^{-5}\ s$ as the time step is still sufficiently small. As the nucleation burst draws to an end for $t \gtrsim 5 \cdot 10^{-5}\ s$ we notice still quite some dependency on the adaptive time stepping strategy. The asymptotic value $N(\infty)$ is seen to vary about 3% when changing the threshold from $\epsilon_{TOL} = 10^{-8}$ at which a 'converged' solution is attained to $\epsilon_{TOL} = 10^{-5}$. Current research is dedicated to an extension to the space-time framework of advection-diffusion-reaction equations in which also solution-dependent grid refinement will be applied to capture sharply localized nucleation bursts. Results of this will be presented at the conference.

REFERENCES

[1] Winkelmann, Ch., Nordlund, M., Kuczaj, A.K., Stolz, S., Geurts, B.J.: 2013. Efficient second-order time integration for single-species aerosol formation and evolution Int. J. Numer. Meth. Fluids, DOI: 10.1002/fld.3851