Fully Lagrangian Approach for polydisperse droplets

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Vortex rings and related problems
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Outline

- Background
- Basic equations (droplets)
- Application to 1D flow and preliminary results
- Application to 2D flow and preliminary results
Motivation

- Sprays are essentially polydisperse
- Droplet sizes and distribution evolve with time

![Graphs showing droplet diameters and velocities](image)

*Fig. 3*  Distribution of droplet diameters and velocities in the PFI injector spray plotted against time from SOI when (a) $r = 0$ mm and $x = 15$ mm and (b) when $r = 6$ mm and $x = 55$ mm

How to model droplet concentration evolution?

Development of fully Lagrangian approach (FLA) for polydisperse droplets taking into account change in droplet size due to interphase phase exchange

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**Standard FLA**

Lagrangian variables are the initial coordinates of the droplet positions: \( x_0, y_0, z_0 \)

| Continuity equation | \( n_d \left| J \right| = n_{d0} \) |
|---------------------|----------------------------------|
| Energy balance      | \( c_{dl} \frac{\partial T_{d}}{\partial t} = q_{d} \) |

\[ |J| \equiv \left| \text{det}(J) \right| \]
\[ J_{ij} = \frac{\partial x_i}{\partial x_{j0}} \]

\[ \frac{\partial r_d}{\partial t} = \mathbf{v}_d, \quad \frac{\partial v_d}{\partial t} = \mathbf{f}_d, \]

\[ \frac{\partial J_{ij}}{\partial t} = q_{ij}, \quad \frac{\partial q_{ij}}{\partial t} = \frac{\partial f_{id}}{\partial x_{j0}} \]

A system of ODE, initial conditions correspond to the way the dispersed phase is introduced or fed to the flow.
FLA for polydisperse admixture

Lagrangian variables are the initial coordinates of the droplet positions and the initial size:

\[ x_0, y_0, z_0, r_{d0} \]

Continuity equation formulated for the distribution of droplets over space and sizes

\[ \tilde{n}_d(t, x, r_d) |J| = \tilde{n}_{d0}, \]

Jacobian of the transformation form Eulerian to Lagrangian coordinates

\[
J = \begin{pmatrix}
J_{11} & J_{12} & J_{13} & J_{14} \\
J_{21} & J_{22} & J_{23} & J_{24} \\
J_{31} & J_{32} & J_{33} & J_{34} \\
J_{41} & J_{42} & J_{43} & J_{44}
\end{pmatrix} = \begin{pmatrix}
\frac{\partial x}{\partial x_0} & \frac{\partial x}{\partial y_0} & \frac{\partial x}{\partial z_0} & \frac{\partial x}{\partial r_{d0}} \\
\frac{\partial y}{\partial x_0} & \frac{\partial y}{\partial y_0} & \frac{\partial y}{\partial z_0} & \frac{\partial y}{\partial r_{d0}} \\
\frac{\partial z}{\partial x_0} & \frac{\partial z}{\partial y_0} & \frac{\partial z}{\partial z_0} & \frac{\partial z}{\partial r_{d0}} \\
\frac{\partial r_d}{\partial x_0} & \frac{\partial r_d}{\partial y_0} & \frac{\partial r_d}{\partial z_0} & \frac{\partial r_d}{\partial r_{d0}}
\end{pmatrix}
\]

\[ |J| \equiv |\text{det}(J)| \]
For a chosen particle trajectory, we have the following system of ODE:

\[ \frac{\partial \mathbf{x}_d}{\partial t} = \mathbf{v}_d, \quad \frac{\partial \mathbf{v}_d}{\partial t} = \mathbf{f}_d, \]

\[ c_{dl} \frac{\partial T_d}{\partial t} = q_d, \quad \frac{\partial r_d}{\partial t} = \dot{r}_d, \]

\[ \frac{\partial J_{ij}}{\partial t} = q_{ij}, \quad \frac{\partial q_{ij}}{\partial t} = \frac{\partial f_{di}}{\partial x_k} J_{kj} + \frac{\partial f_{di}}{\partial r_d} J_{Aj}, \quad i = 1, 2, 3, \quad j = 1, \ldots, 4 \]

\[ \frac{\partial J_{Aj}}{\partial t} = \frac{\partial \dot{r}_d}{\partial x_{0j}} J_{Aj}, \quad \frac{\partial J_{44}}{\partial t} = \frac{\partial \dot{r}_d}{\partial r_d} J_{44}, \quad i, j = 1, 2, 3. \]

Initial conditions correspond to the way the dispersed phase is introduced or fed to the flow.
1D flow of droplets in still hot air

Force and heat flux on the droplet:

\[ f_d = 6\pi r_d^* \mu (v^* - v_d^*) \]
\[ q_d = 4\pi r_d^* \lambda (T^* - T_d^*) \]

Assume all the heat that reaches the droplet is spent on evaporation:

\[ \dot{m} = \frac{q_d}{H} \]

Non-dimensional parameters:

\[ x(d) = \frac{x^*_d}{l_T}, \quad u(d) = \frac{u^*_d}{U}, \quad t = \frac{Ut^*}{l_{T_0}}, \quad r_d = \frac{r_d^*}{r_0}, \quad \tilde{n}_d = \frac{\tilde{n}_d^*}{n_{dt}}, \]
\[ T(T_s) = \frac{T^*(T_s^*) - T_0}{T_a - T_0}. \quad l_{T_0} = \frac{m_0U}{6\pi r_0^3 \mu}, \quad m_0 = \frac{4}{3} \pi r_0^3 \rho_d l \]

Characteristic droplet radius, \( r_0 \), droplet initial velocity \( U \) and temperature \( T_0 \), \( n_{dt} \) total initial droplet number density at \( x_0 \)
1D flow of droplets in still hot air

Assume log-normal distribution of droplet sizes at $x_0$ with mean and variance for the corresponding normal distribution $M = 0.16$ and $S = 0.4$

$$\tilde{n}_{d0} = \frac{1}{r_d} \frac{1}{S \sqrt{2\pi}} \exp \left( - \frac{(\ln r_d - M)^2}{2S^2} \right)$$
1D flow of droplets in still hot air

\[
\frac{dx_d}{dt} = u_d, \quad \frac{du_d}{dt} = -\frac{1}{r_d^2} u_d, \\
T_d = 0, \quad \frac{dr_d^2}{dt} = -\delta, \\
\frac{dJ_{11}}{dt} = q_{11}, \quad \frac{dJ_{12}}{dt} = q_{12}, \\
\frac{dq_{11}}{dt} = -\frac{1}{r_d^2} q_{11} + \frac{2}{r_d^3} u_d J_{21}, \quad \frac{dq_{12}}{dt} = -\frac{1}{r_d^2} q_{12} + \frac{2}{r_d^3} u_d J_{22}, \\
\frac{dJ_{21}}{dt} = 0, \quad \frac{dJ_{22}}{dt} = \frac{\delta}{2r_d^2} J_{22}, \\
\delta = \frac{4}{9} \frac{\lambda (T_a - T_0)}{\mu H}.
\]
1D flow of droplets in still hot air

\[ \tilde{n}_d (t, x, r_d) | J | = \tilde{n}_{d0}, \]

\[ J = \begin{pmatrix} J_{11} & J_{12} \\ J_{21} & J_{22} \end{pmatrix} = \begin{pmatrix} \partial x/\partial x_0 & \partial x/\partial r_{d0} \\ \partial r_d/\partial x_0 & \partial r_d/\partial r_{d0} \end{pmatrix} \]

Initial conditions:

\[ x = x_0, u_d = 1, T_d = 0, \tilde{n}_d = \tilde{n}_{d0}, r_d = r_{d0} \]

\[ J_{11} = 1, \quad J_{12} = 0, \quad J_{21} = 0, \quad J_{22} = 1, \quad q_{11} = 0, \quad q_{12} = 0. \]
1D flow of droplets in still hot air

The system can be solved analytically:

\[ x_d = \frac{r_{d0}^2}{\delta + 1} \left[ 1 - \left( 1 - \frac{\delta t}{r_{d0}^2} \right)^{\frac{\delta + 1}{\delta}} \right], \]

\[ u_d = \left( \frac{r_d}{r_{d0}} \right)^{2/\delta} = \left( 1 - \frac{\delta t}{r_{d0}^2} \right)^{1/\delta}, \]

\[ r_d^2 = r_{d0}^2 - \delta t, \]

\[ J11 = 1, \]

\[ J22 = \frac{r_{d0}}{r_d}, \]

\[ q11 = 0. \]

The system was solved numerically using 4th order Runge-Kutta method. Numerical solution was verified against the analytical solution.
1D flow of droplets in still hot air

\( \delta = 1 \)

Discretisation: 1 - 1, 2 - 10, 3 - 100, 4 - 1000
2D flow Poiseuille flow hot gas and droplets

Force and heat flux on the droplet:

\[ f_d = 6\pi r_d^* \mu (v^* - v_d^*) \]
\[ q_d = 4\pi r_d^* \lambda (T^* - T_d^*) \]

Assume all the heat that reaches the droplet is spent on evaporation:

\[ \dot{m} = \frac{q_d}{H} \]

Non-dimensional parameters:

\[ x(d) = \frac{x(d)}{a}, \quad u(d) = \frac{u(d)}{U_m}, \quad t = \frac{U t^*}{a}, \quad r_d = \frac{r_d^*}{r_0}, \quad \tilde{n}_d = \frac{\tilde{n}_d^*}{n_{d0}} \]

\[ l_{r0} = \frac{m_0 U_m}{6\pi r_0 \mu}, \quad m_0 = \frac{4}{3} \pi r_0^3 \rho_d, \quad T(T_s) = \frac{T^*(T_s^*) - T_0}{T_a - T_0}, \quad \delta = \frac{4}{9} \frac{\lambda (T_a - T_0)}{\mu H}, \quad \beta = \frac{a}{l_r} \]

Characteristic droplet radius, \( r_0 \), maximum air velocity \( U_m \) and temperature \( T_0 \), \( n_{d0} \), total initial droplet number density at \( x_0 \).
Assume log-normal distribution of droplet sizes at $x_0$ with mean and variance for the corresponding normal distribution $M = 0.16$ and $S = 0.4$

$$\tilde{n}_{d0} = \frac{1}{r_d S \sqrt{2\pi}} \exp \left( -\frac{(\ln r_d - M)^2}{2S^2} \right)$$
2D flow Poiseuille flow hot gas and droplets

\[
\begin{align*}
\frac{dx_d}{dt} &= u_d, & \frac{dy_d}{dt} &= v_d, & \frac{du_d}{dt} &= \frac{\beta}{r_d^2} (u - u_d), & \frac{dv_d}{dt} &= \frac{\beta}{r_d^2} (v - v_d), \\
T_d &= 0, & \frac{dr_d^2}{dt} &= -\delta, \\
\frac{dJ_{11}}{dt} &= q_{11}, & \frac{dJ_{12}}{dt} &= q_{12}, & \frac{dJ_{13}}{dt} &= q_{13}, \\
\frac{dJ_{21}}{dt} &= q_{21}, & \frac{dJ_{22}}{dt} &= q_{22}, & \frac{dJ_{23}}{dt} &= q_{23}, \\
\frac{dJ_{31}}{dt} &= 0, & \frac{dJ_{32}}{dt} &= 0, & \frac{dJ_{33}}{dt} &= \frac{\delta}{2r_d^2} J_{33},
\end{align*}
\]

\[
\begin{align*}
\frac{dq_{11}}{dt} &= \frac{\beta}{r_d^2} \left( \frac{\partial u}{\partial x} J_{11} + \frac{\partial u}{\partial y} J_{21} - q_{11} \right) - \frac{2\beta}{r_d^3} (u - u_d) J_{31}, \\
\frac{dq_{12}}{dt} &= \frac{\beta}{r_d^2} \left( \frac{\partial u}{\partial x} J_{12} + \frac{\partial u}{\partial y} J_{22} - q_{12} \right) - \frac{2\beta}{r_d^3} (u - u_d) J_{32}, \\
\frac{dq_{13}}{dt} &= \frac{\beta}{r_d^2} \left( \frac{\partial u}{\partial x} J_{13} + \frac{\partial u}{\partial y} J_{23} - q_{13} \right) - \frac{2\beta}{r_d^3} (u - u_d) J_{33}, \\
\frac{dq_{21}}{dt} &= \frac{\beta}{r_d^2} \left( \frac{\partial v}{\partial x} J_{11} + \frac{\partial v}{\partial y} J_{21} - q_{21} \right) - \frac{2\beta}{r_d^3} (v - v_d) J_{31}, \\
\frac{dq_{22}}{dt} &= \frac{\beta}{r_d^2} \left( \frac{\partial v}{\partial x} J_{12} + \frac{\partial v}{\partial y} J_{22} - q_{22} \right) - \frac{2\beta}{r_d^3} (v - v_d) J_{32}, \\
\frac{dq_{23}}{dt} &= \frac{\beta}{r_d^2} \left( \frac{\partial v}{\partial x} J_{13} + \frac{\partial v}{\partial y} J_{23} - q_{23} \right) - \frac{2\beta}{r_d^3} (v - v_d) J_{33},
\end{align*}
\]
2D flow Poiseuille flow hot gas and droplets

\[ \tilde{n}_d (t, x, r_d) \mid J = \tilde{n}_{d0}, \]

\[ J = \begin{pmatrix} J_{11} & J_{12} & J_{13} \\ J_{21} & J_{22} & J_{23} \\ J_{31} & J_{32} & J_{33} \end{pmatrix} = \begin{pmatrix} \partial x/\partial x_0 & \partial x/\partial y_0 & \partial x/\partial r_{d0} \\ \partial y/\partial x_0 & \partial y/\partial y_0 & \partial y/\partial r_{d0} \\ \partial r_{d}/\partial x_0 & \partial r_{d}/\partial y_0 & \partial r_{d}/\partial r_{d0} \end{pmatrix} \]

Initial conditions:

\[ x = x_0, \quad u_d = u_{d0}, \quad v_d = 0, \quad T_d = 0, \quad \tilde{n}_d = \tilde{n}_{d0}, \quad r_d = r_{d0} \]

\[ J_{11} = 1, \quad J_{12} = 0, \quad J_{13} = 0, \quad J_{21} = 0, \quad J_{22} = 1, \quad J_{23} = 0, \quad J_{31} = 0, \quad J_{32} = 0, \quad J_{33} = 1, \]

\[ q_{ij} = 0. \]
2D flow Poiseuille flow hot gas and droplets

The system can be solved analytically:

\[ u = 1 - y^2, \quad v = 0 \]

\[ x_d = ut + (u - u_{d0}) \frac{r_{d0}^2}{\beta + \delta} \left[ \left( 1 - \frac{\delta t}{r_{d0}^2} \right)^{\frac{\beta + \delta}{\delta}} - 1 \right], \quad \frac{\beta}{\delta} \neq -1 \]

\[ u_d = u - (u - u_{d0}) \left( 1 - \frac{\delta t}{r_{d0}^2} \right)^\frac{\beta}{\delta}, \]

\[ y_d = y_0, \quad v_d = 0, \]

\[ T_d = 0, \quad r_d^2 = r_{d0}^2 - \delta t, \]

\[ q_{11} = 0, \quad q_{21} = 0, \quad q_{22} = 0, \quad q_{23} = 0, \]

\[ J_{11} = 1, \quad J_{21} = 0, \quad J_{22} = 1, \quad J_{23} = 0, \quad J_{31} = 0, \quad J_{32} = 0, \quad J_{33} = \frac{r_{d0}}{r_d}, \]

The system was solved numerically using 4th order Runge-Kutta method.
2D flow Poiseuille flow hot gas and droplets

\( \delta = 1, \beta = 1 \)

Total number density at different \( x \) cross-sections for different discretisations

1. \( x = 0 \),
2. \( x = 0.25 \),
3. \( x = 0.5 \),
4. \( x = 0.75 \),
5. \( x = 1 \)

Total number density at different \( y \) cross-sections
2D flow Poiseuille flow hot gas and droplets

\( \delta = 1, \beta = 1 \)

Velocity distribution vs size

Number density vs size

*red* \( y = 0.5 \),
*black* \( y = 0 \)
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Thank you for your attention
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