University of Brighton

Advanced Engineering Centre

Vortex rings and related problems
24th August 2018, Brighton

Fully Lagrangian Approach for polydisperse droplets

Oyuna Rybdylova

EPSRC Engineering and Physical Sciences Research Council

Outline

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

Motivation

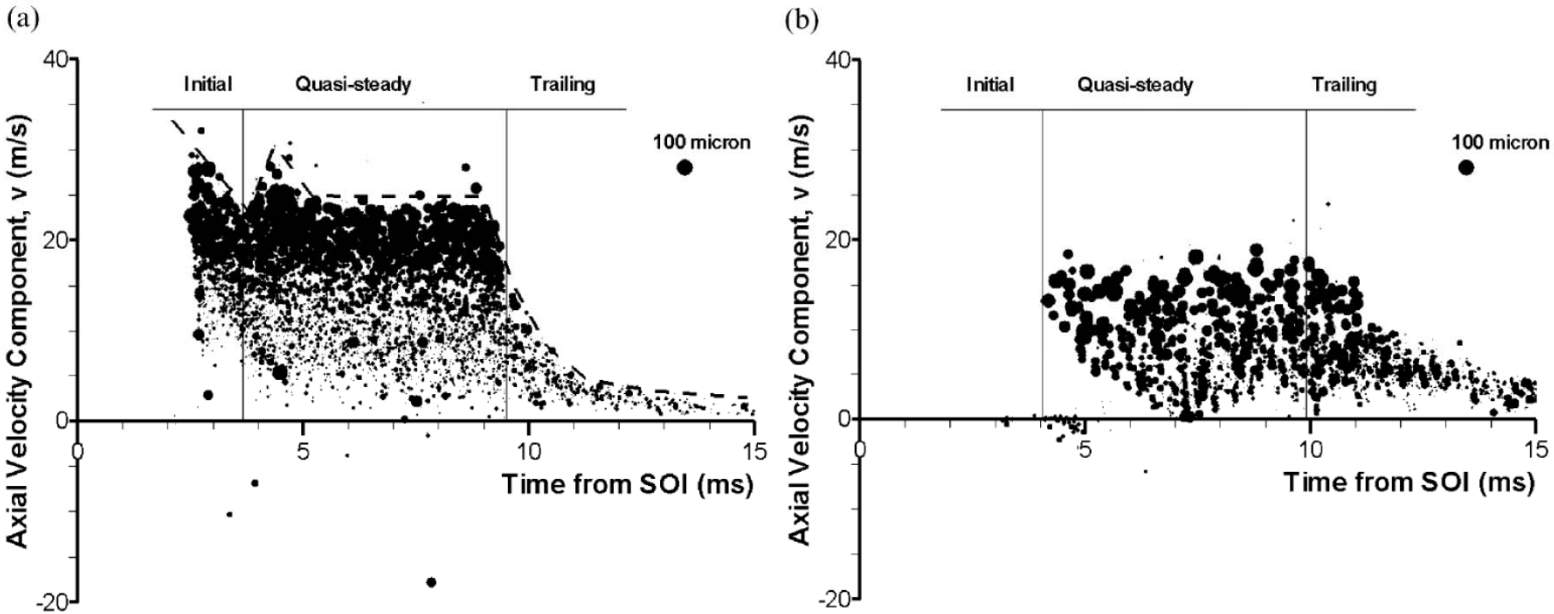


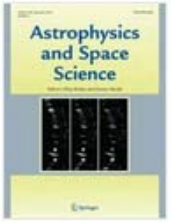
Fig. 3 Distribution of droplet diameters and velocities in the PFI injector spray plotted against time from SOI when (a) $r = 0$ mm and $x = 15$ mm and (b) when $r = 6$ mm and $x = 55$ mm

S. Begg, F. Kaplanski, S. Sazhin, M. Hindle, M. Heikal. *Int J. Engine Res*. 2009

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

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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Lagrangian Modelling of Dust Admixture in Gas Flows

Authors | Authors and affiliations

A.N. Osiptsov 1

1. Institute of Mechanics, Lomonosov Moscow State University, Moscow, Russia

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Standard FLA

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

Continuity equation

$$n_d\,|J| = n_{d0},$$

Energy balance

$$c_{dl}\frac{\partial T_d}{\partial t} = q_d,$$

Momentum balance

$$\frac{\partial \mathbf{r}_d}{\partial t} = \mathbf{v}_d, \qquad \frac{\partial \mathbf{v}_d}{\partial t} = \mathbf{f}_d,$$

Equations for Jacobian components

$$\frac{\partial J_{ij}}{\partial t} = q_{ij}, \qquad \frac{\partial q_{ij}}{\partial t} = \frac{\partial f_{id}}{\partial x_{j0}}$$

$$|J| \equiv |\det(J)|$$

$$J_{ij} = \partial x_i / \partial x_{j0}$$

Jacobian of the transformation form Eulerian to Lagrangian coordinates

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

$$\tilde{n}_d\left(t, \mathbf{x}, r_d\right)\left|J\right| = \tilde{n}_{d0},$$

Jacobian of the transformation form Eulerian to Lagrangian coordinates

$$\left|J\right| \equiv \left|\det(J)\right|$$

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

FLA for polydisperse admixture

For a chosen particle trajectory, we have the following system of ODE:

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

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

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

$$\frac{\partial J_{4j}}{\partial t} = \frac{\partial \dot{r}_d}{\partial x_{0j}} J_{4j}, \quad \frac{\partial J_{44}}{\partial t} = \frac{\partial \dot{r}_d}{\partial r_d} J_{44}, \quad i, j = 1, 2, 3.$$

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:

$$\mathbf{f}_d = 6\pi r_d^* \mu \left(\mathbf{v}^* - \mathbf{v}_d^*\right)$$

$$q_d = 4\pi r_d^* \lambda (T^* - T_d^*)$$

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

$$\dot{m} = \frac{q_d}{H}$$

Non-dimensional parameters:

$$x_{(d)} = \frac{x_{(d)}^*}{l_\tau}, \; u_{(d)} = \frac{u_{(d)}^*}{U}, \; t = \frac{Ut^*}{l_{\tau 0}}, \; r_d = \frac{r_d^*}{r_0}, \; \tilde{n}_d = \frac{\tilde{n}_d^*}{n_{dt}},$$

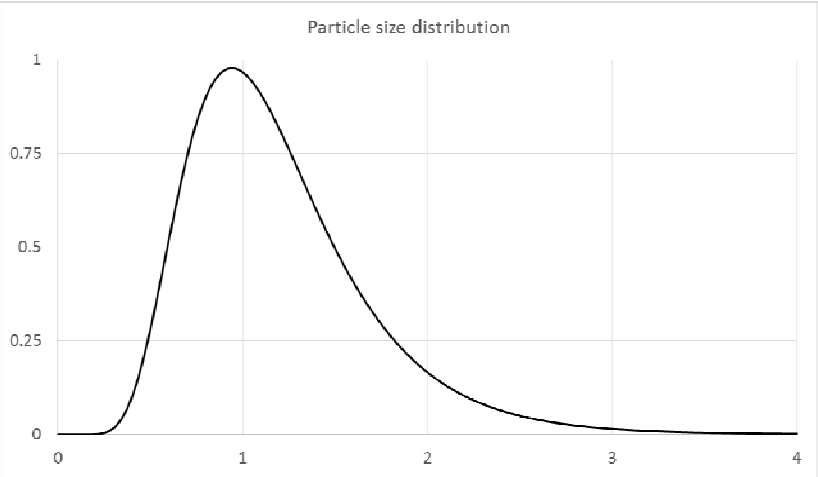
$$T(T_s) = \frac{T^*(T_s^*) - T_0}{T_a - T_0}. \quad l_{\tau 0} = \frac{m_0 U}{6\pi r_0 \mu}, \; m_0 = \frac{4}{3}\pi r_0^3 \rho_{dl}$$

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

$$\tilde{n}_d\left(t, \mathbf{x}, r_d\right)|J| = \tilde{n}_{d0},$$

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

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:

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

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

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

$$J11 = 1,$$

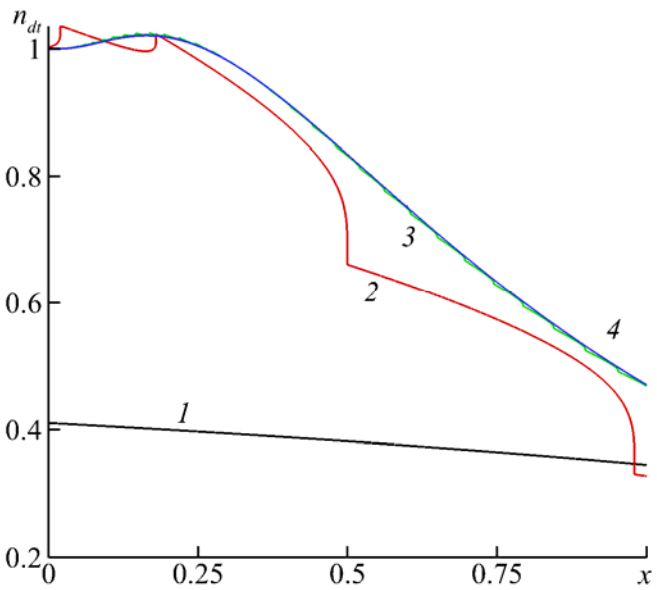
$$J22 = \frac{r_{d0}}{r_d},$$

$$q11 = 0.$$

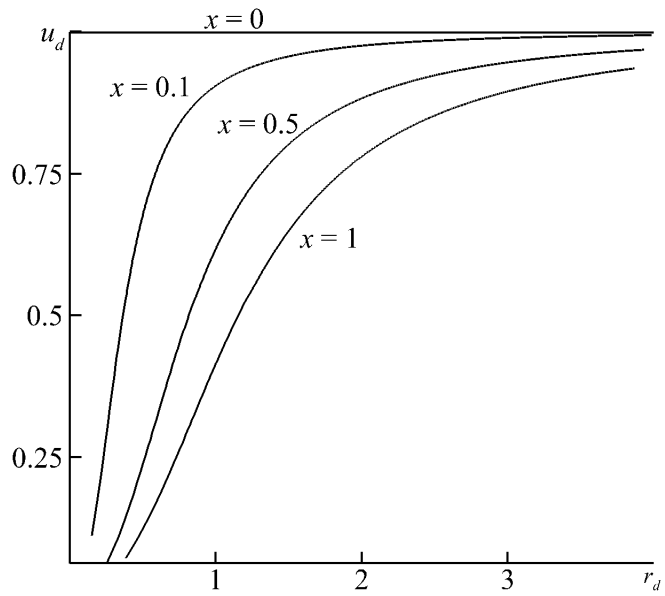
The system was solved numerically using 4th order Runge-Kutta method. Numerical solution was verified against the analytical solution

1D flow of droplets in still hot air

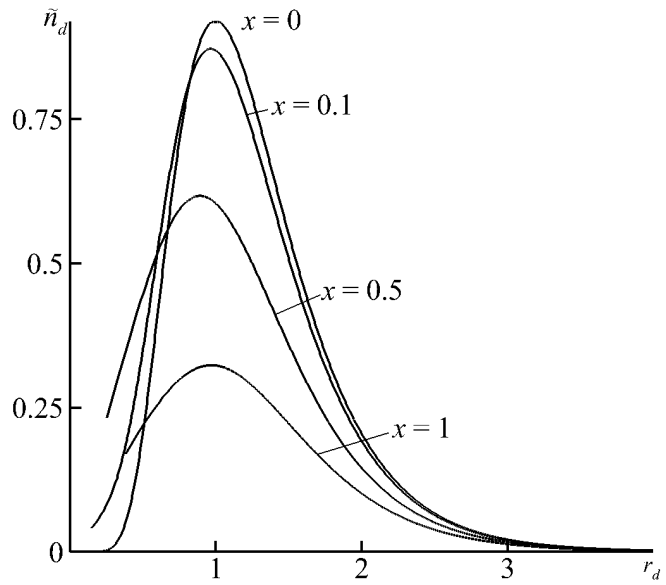
$\delta = 1$



Total number density



Velocity distribution vs size



Number density vs size

Discretisation: *1* - 1, *2* - 10, *3* - 100, *4* - 1000

2D flow Poiseuille flow hot gas and droplets

Force and heat flux on the droplet:

$$\mathbf{f}_d = 6\pi r_d^* \mu \left(\mathbf{v}^* - \mathbf{v}_d^*\right)$$

$$q_d = 4\pi r_d^* \lambda (T^* - T_d^*)$$

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

$$\dot{m} = \frac{q_d}{H}$$

Non-dimensional parameters:

$$x_{(d)} = \frac{x_{(d)}^*}{a},\ u_{(d)} = \frac{u_{(d)}^*}{U_m},\ t = \frac{Ut^*}{a},\ r_d = \frac{r_d^*}{r_0},\ \tilde{n}_d = \frac{\tilde{n}_d^*}{n_{dt0}},$$

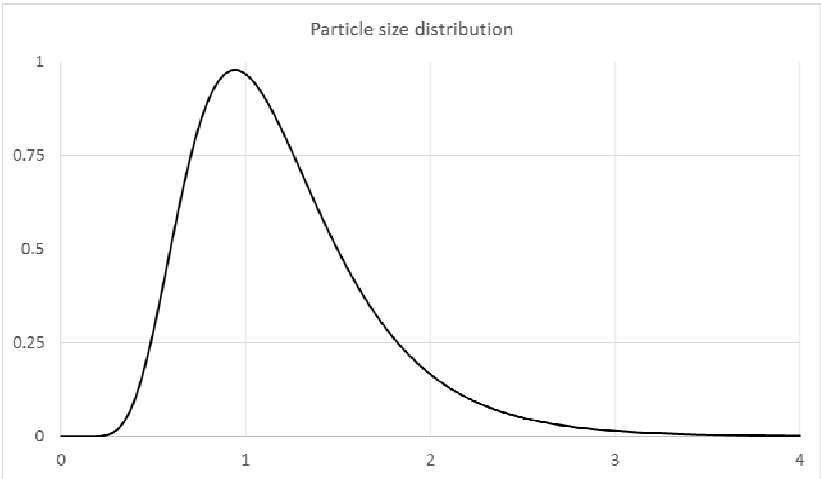
$$l_{\tau 0} = \frac{m_0 U_m}{6\pi r_0 \mu},\ m_0 = \frac{4}{3}\pi r_0^3 \rho_{dl},\ T(T_s) = \frac{T^*(T_s^*) - T_0}{T_a - T_0}.\ \delta = \frac{4}{9}\frac{\lambda\left(T_a - T_0\right)}{\mu H}\quad \beta = \frac{a}{l_\tau}$$

Characteristic droplet radius, r_0, maximum air velocity U_m and temperature T_0, n_{dt0} total initial droplet number density at x_0

2D flow Poiseuille flow hot gas and droplets

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

$$\tilde{n}_{d0} = \frac{1}{r_d}\frac{1}{S\sqrt{2\pi}}\exp\left(-\frac{(\ln r_d - M)^2}{2S^2}\right)$$



2D flow Poiseuille flow hot gas and droplets

$$\frac{dx_d}{dt} = u_d, \quad \frac{dy_d}{dt} = v_d, \quad \frac{du_d}{dt} = \frac{\beta}{r_d^2}\left(u - u_d\right), \quad \frac{dv_d}{dt} = \frac{\beta}{r_d^2}\left(v - v_d\right),$$

$$T_d = 0, \quad \frac{dr_d^2}{dt} = -\delta,$$

$$\frac{dJ_{11}}{dt} = q_{11}, \quad \frac{dJ_{12}}{dt} = q_{12}, \quad \frac{dJ_{13}}{dt} = q_{13},$$

$$\frac{dJ_{21}}{dt} = q_{21}, \quad \frac{dJ_{22}}{dt} = q_{22}, \quad \frac{dJ_{23}}{dt} = q_{23},$$

$$\frac{dJ_{31}}{dt} = 0, \quad \frac{dJ_{32}}{dt} = 0, \quad \frac{dJ_{33}}{dt} = \frac{\delta}{2r_d^2} J_{33},$$

$$\frac{dq_{11}}{dt} = \frac{\beta}{r_d^2}\left(\frac{\partial u}{\partial x} J_{11} + \frac{\partial u}{\partial y} J_{21} - q_{11}\right) - \frac{2\beta}{r_d^3}\left(u - u_d\right) J_{31},$$

$$\frac{dq_{12}}{dt} = \frac{\beta}{r_d^2}\left(\frac{\partial u}{\partial x} J_{12} + \frac{\partial u}{\partial y} J_{22} - q_{12}\right) - \frac{2\beta}{r_d^3}\left(u - u_d\right) J_{32},$$

$$\frac{dq_{13}}{dt} = \frac{\beta}{r_d^2}\left(\frac{\partial u}{\partial x} J_{13} + \frac{\partial u}{\partial y} J_{23} - q_{13}\right) - \frac{2\beta}{r_d^3}\left(u - u_d\right) J_{33},$$

$$\frac{dq_{21}}{dt} = \frac{\beta}{r_d^2}\left(\frac{\partial v}{\partial x} J_{11} + \frac{\partial v}{\partial y} J_{21} - q_{21}\right) - \frac{2\beta}{r_d^3}\left(v - v_d\right) J_{31},$$

$$\frac{dq_{22}}{dt} = \frac{\beta}{r_d^2}\left(\frac{\partial v}{\partial x} J_{12} + \frac{\partial v}{\partial y} J_{22} - q_{22}\right) - \frac{2\beta}{r_d^3}\left(v - v_d\right) J_{32},$$

$$\frac{dq_{23}}{dt} = \frac{\beta}{r_d^2}\left(\frac{\partial v}{\partial x} J_{13} + \frac{\partial v}{\partial y} J_{23} - q_{23}\right) - \frac{2\beta}{r_d^3}\left(v - v_d\right) J_{33},$$

2D flow Poiseuille flow hot gas and droplets

$$\tilde{n}_d\left(t, \mathbf{x}, r_d\right)|J| = \tilde{n}_{d0},$$

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

Initial conditions:

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

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

$$q_{ij} = 0.$$

2D flow Poiseuille flow hot gas and droplets

The system can be solved analytically:

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

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

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

$$y_d = y_0, \; v_d = 0,$$

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

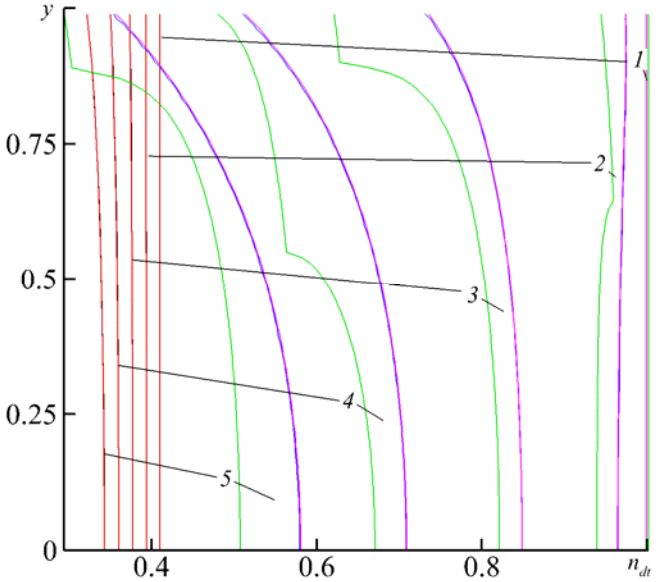
$$q_{11} = 0, \quad q_{21} = 0, \quad q_{22} = 0, \quad q_{23} = 0,$$

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

The system was solved numerically using 4th order Runge-Kutta method.

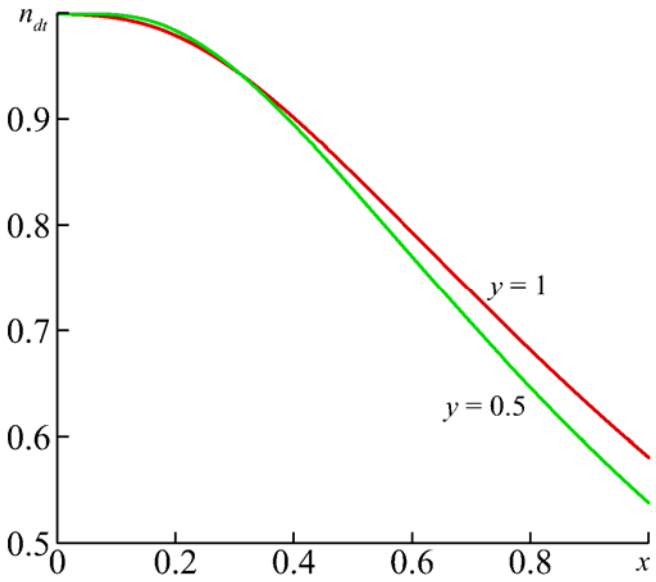
2D flow Poiseuille flow hot gas and droplets

$\delta = 1$, $\beta = 1$



1 x = 0,
2 x = 0.25,
3 x = 0.5,
4 x = 0.75
5 x = 1

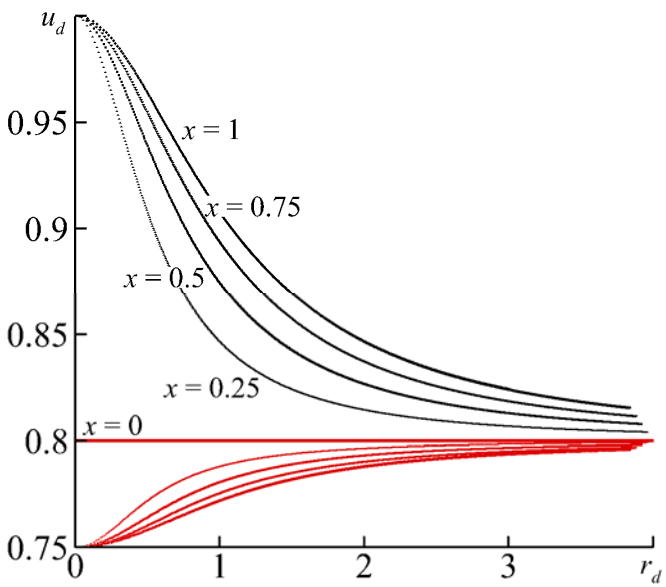
Total number density at different *x* cross-sections for different discretisations



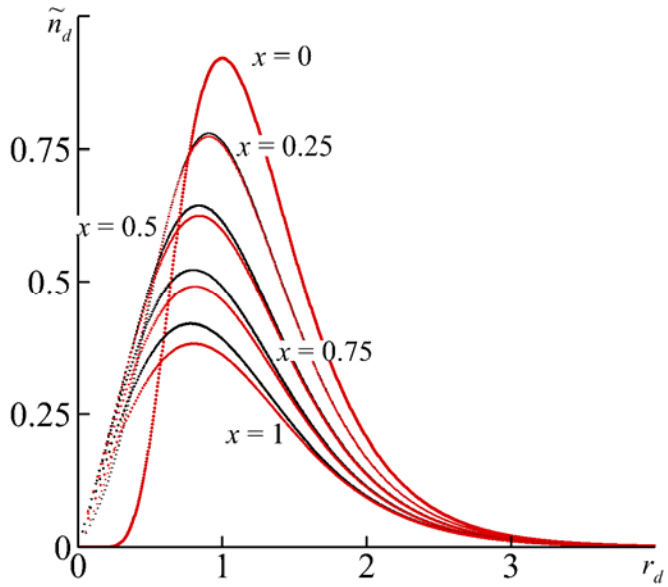
Total number density at different *y* cross-sections

2D flow Poiseuille flow hot gas and droplets

δ = 1, β = 1



Velocity distribution vs size



Number density vs size

red y = 0.5,
black y = 0

Acknowledgements

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Thank you for your attention

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