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Spray and Combustion SIGs meeting
8 April 2019

Recent developments in gas-droplet flow simulations based on the Fully Lagrangian Approach

Oyuna Rybdylova

EPSRC Engineering and Physical Sciences Research Council

Outline

- Background
- Basic equations (droplets): original and generalised FLA
- Application of generalised FLA to 1D and 2D flow and preliminary results
- Outlook

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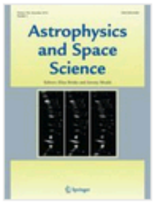
How to model droplet concentration evolution?



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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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Dr Oyuna Rybdylova, Dr Timur Zaripov, Dr Yuan Li)

Motivation

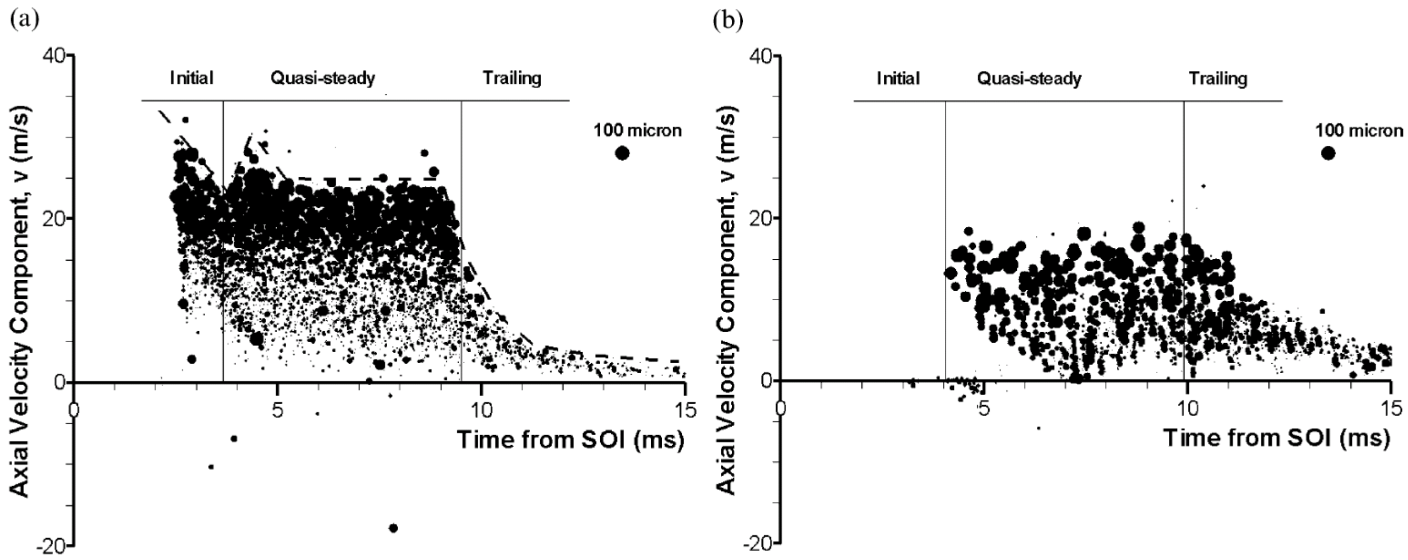


Fig. 3 Distribution of droplet diameters and velocities in the PFI injector spray plotted against time from SOI when (a) $r = 0$ mm and $x = 15$ mm and (b) when $r = 6$ mm and $x = 55$ mm

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

Standard FLA

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

Continuity equation

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

Momentum balance

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

Energy balance

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

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

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

Jacobian of the transformation form Eulerian to Lagrangian coordinates

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

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

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:
$$\mathbf{f}_d = 6\pi r_d^* \mu \left(\mathbf{v}^* - \mathbf{v}_d^*\right)$$
$$q_d = 4\pi r_d^* \lambda (T^* - T_d^*)$$

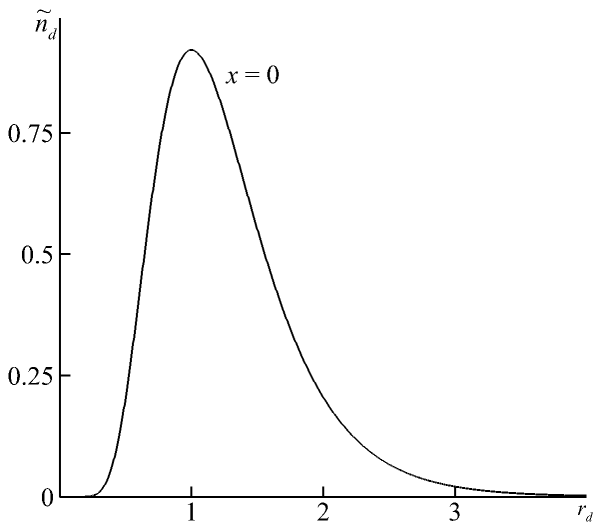
Assume all the heat that reaches the droplet is spent on evaporation:
$$\dot{m} = \frac{q_d}{H}$$

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

$$\frac{dx_d}{dt} = u_d, \quad \frac{du_d}{dt} = -\frac{1}{r_d^2} u_d,$$

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

$$\frac{dJ_{12}}{dt} = q_{12}, \quad \frac{dq_{12}}{dt} = -\frac{1}{r_d^2} q_{12} + \frac{2}{r_d^3} u_d J_{22}$$

$$\frac{dJ_{22}}{dt} = \frac{\delta}{2r_d^2} J_{22}$$

$$\delta = \frac{4}{9} \frac{\lambda \left(T_a - T_0\right)}{\mu H}.$$

1D flow of droplets in still hot air

$$\tilde{n}_d\left(t, x, r_d\right)\begin{vmatrix} u_d & \partial x/\partial r_{d0} \\ \dot{r} & \partial r_d/\partial r_{d0} \end{vmatrix} = \tilde{n}_{d0}u_{d0}$$

Initial conditions:

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

$$J_{12} = 0, \quad J_{22} = 1, \quad q_{12} = 0.$$

1D flow of droplets in still hot air

The system can be solved analytically:

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

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

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

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

$$J12 = -\frac{2}{r_{d0}}\left(1-\frac{\delta t}{r_{d0}^2}\right)^{1/\delta} t,$$

$$\tilde{n}_d = \tilde{n}_{d0}\left(1-\frac{\delta t}{r_{d0}^2}\right)^{-1/2} = \tilde{n}_{d0}\frac{r_{d0}}{r_d}$$

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

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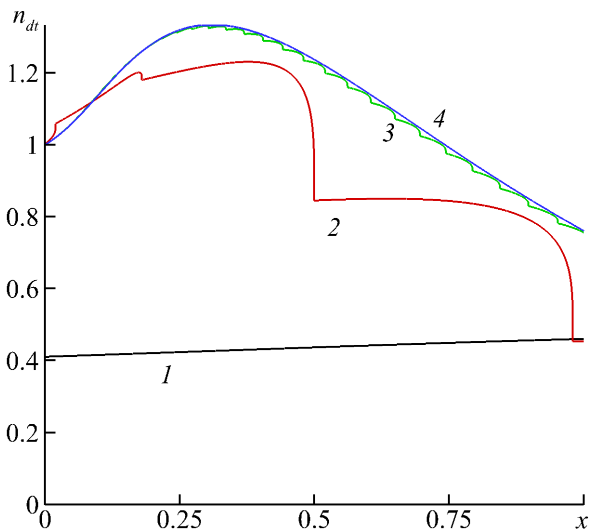
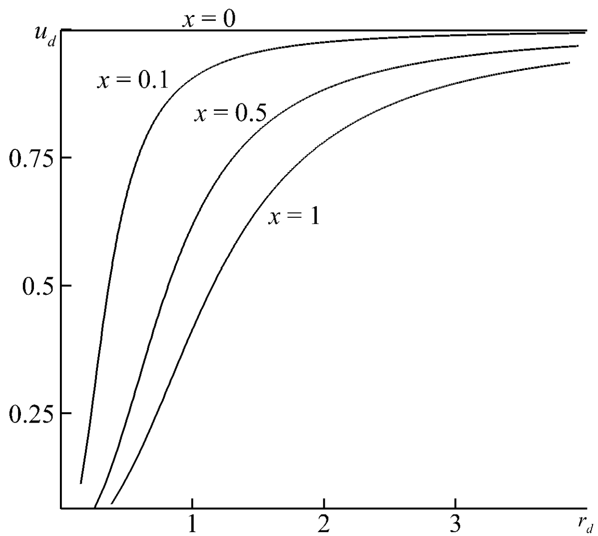
1D flow of droplets in still hot air

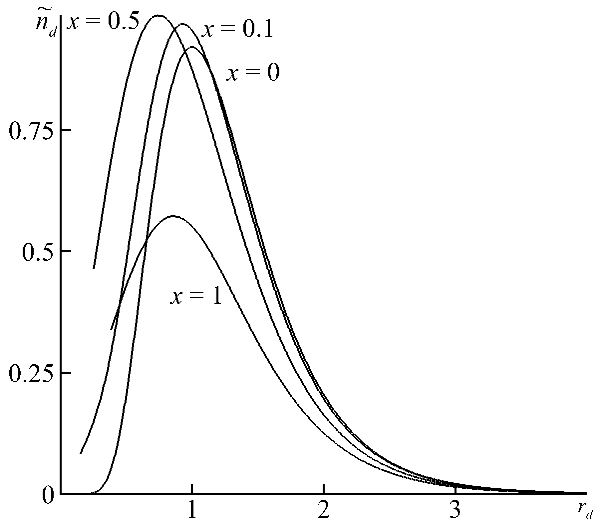
δ = 1



Total number density



Velocity distribution vs size



Number density vs size

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

2D spray in cross flow

$$\tilde{n}_d\left(t,x,r_d\right)\left|\det\begin{pmatrix} J_{11} & u_d & J_{13} \\ J_{21} & v_d & J_{23} \\ J_{31} & \dot{r} & J_{33}\end{pmatrix}\right| = \tilde{n}_{d0}v_{d0}$$

$$\delta = \frac{4}{9}\frac{\lambda\left(T_a - T_0\right)}{\mu H}$$

Initial conditions:

$$x = x_0 \in [-\epsilon,\epsilon],\ y=0,\ u_d = U_j\cos\left(-\frac{\pi}{4}\cdot\frac{x_0}{\epsilon}+\frac{\pi}{2}\right),\ v_d = U_j\sin\left(-\frac{\pi}{4}\cdot\frac{x_0}{\epsilon}+\frac{\pi}{2}\right),$$

$$T_d = 0, \tilde{n}_d = \tilde{n}_{d0}, r_d = r_{d0}$$

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

$$q_{11} = \frac{1}{\epsilon}\frac{\pi}{4}U_j\cos\left(\frac{\pi}{4}\frac{x_0}{\epsilon}\right),\ q_{13}=0,\ q_{21} = -\frac{1}{\epsilon}\frac{\pi}{4}U_j\sin\left(\frac{\pi}{4}\frac{x_0}{\epsilon}\right),\ q_{23}=0.$$

2D spray in cross flow

$$\frac{dx_d}{dt} = u_d, \quad \frac{dy_d}{dt} = v_d, \quad \frac{du_d}{dt} = \frac{1}{r_d^2}\left(1 - u_d\right), \quad \frac{dv_d}{dt} = -\frac{1}{r_d^2} v_d$$

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

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

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

$$\frac{dq_{11}}{dt} = -\frac{1}{r_d^2} q_{11} - \frac{2}{r_d^3}\left(1 - u_d\right) J_{31},$$

$$\frac{dq_{13}}{dt} = -\frac{1}{r_d^2} q_{13} - \frac{2}{r_d^3}\left(1 - u_d\right) J_{33},$$

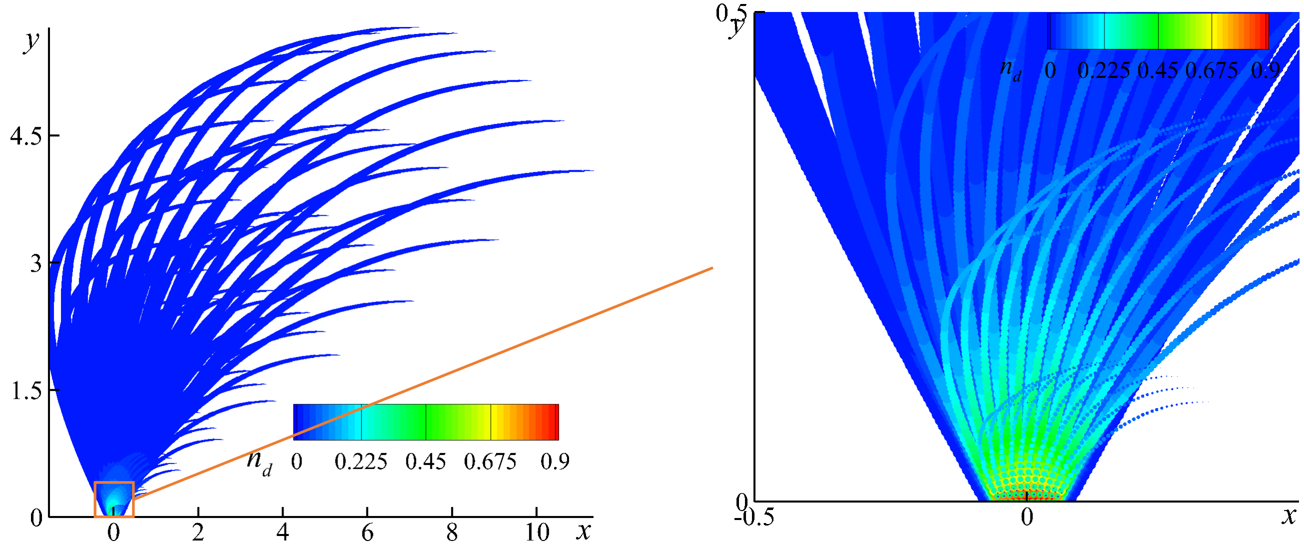
$$\frac{dq_{21}}{dt} = -\frac{1}{r_d^2} q_{21} + \frac{2}{r_d^3} v_d J_{31},$$

$$\frac{dq_{23}}{dt} = -\frac{1}{r_d^2} q_{23} + \frac{2}{r_d^3} v_d J_{33},$$

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

2D spray in cross flow

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

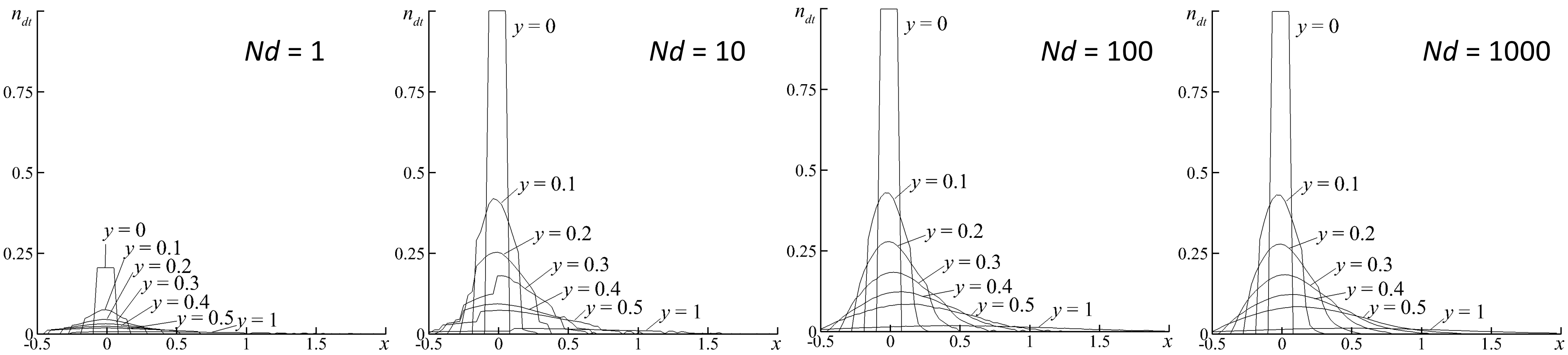


Number density along trajectories

2D spray in cross flow

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

Discretisation:



Total number density in horizontal cross-sections

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