Novel Stochastic and Deterministic Models for Polydisperse Flows Resulting from a Radiological Dispersal Device

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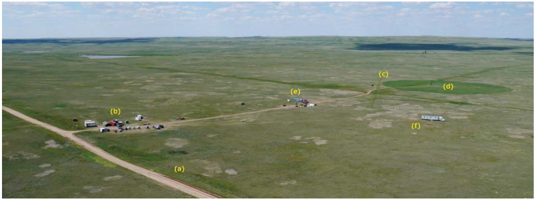
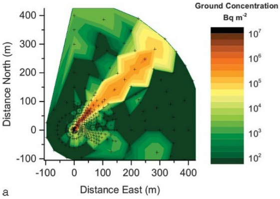
Radionuclide Dispersal Events

Full-Scale RDD Field Trials (DRDC Suffield Experiment Series)





Images source:

E. Korpach et al., "Real Time In Situ Gamma Radiation measurements of the Plume Evolution from the Full-Scale Radiological Dispersal Device Field Trials," *Health Physics*, 2016.

L. Erhardt et al., "Deposition Measurements from the Full-Scale Radiological Dispersal Device Field Trials," *Health Physics*, 2016.

Modelling RDDs

Necessity

- First response and decision making support
- A *priori* scenario analyses by response planners
- Physics-based dispersal engine in virtual training environments

Required Capabilities

- Predict dose from passing plume and contaminated surfaces
- Perform data assimilation with various sensors
- Deal with uncertainties/unknowns, e.g., the amount of explosive and radioactive material(s)

Modelling Stages

- Source term characterization
- Transport and dispersion
- Dose estimation (ground & cloud shine)

Flow Properties of Radionuclide Dispersal Events

Polydisperse

- Particle size is approximately log-normal

Multi-velocity

- Particles at a location will display a range of velocities

Multi-Regime

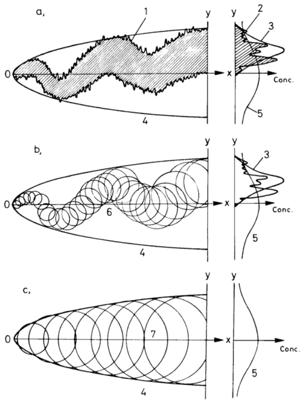
- Initially dense particle phase spreads over a large volume
- Initial strong deviations between particle and gas velocities decay to "simple convection"

Traditional Transport & Dispersion Models for RDDs

- Gaussian puffs (Lebel *et al.* (2016), others)
- Eulerian-Lagrangian (Fuka & Brechler (2011), others)

Unresolved Issues

- Characterization of the source term (e.g., treatment of blast and fireball dynamics)
- Predictions with traditional models could be quite inaccurate
- Trade-offs between accuracy and computational cost



Images source: S. Thykier-Nielsen et al., 1998

Outline

① Stochastic Approach: MCREXS Model

② A Kinetic Description of Polydisperse Flow

③ Deterministic Approach: A Moment Method for Polydisperse Flows

④ Conclusions & Ongoing Work

Improved Source Term Characterization for RDDs

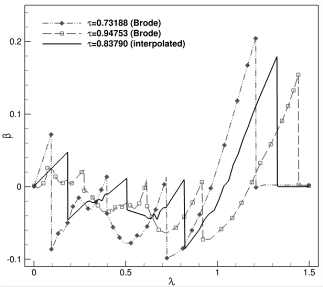
Hummel & Ivan, JER 172 (2017)

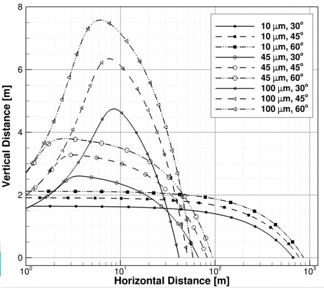
- Eulerian model for background flow
- $\vec{V}_{\mathrm{bf}}(t,x) = \vec{V}_{\mathrm{blast}}(t,x) + \vec{V}_{\mathrm{wind}}(t,x)$
- $\vec{V}_{\mathrm{blast}}$ provided by a surrogate model based on CFD data for a spherically-symmetric TNT explosion
- Lagrangian model for particles

$$\rho_p \frac{\pi d_p^3}{6} \frac{\mathrm{d}^2 x}{\mathrm{d}t^2} = F_{D_x} - F_{dP_x}$$

$$\rho_p \frac{\pi d_p^3}{6} \frac{\mathrm{d}^2 y}{\mathrm{d}t^2} = F_{D_y} - F_{dP_y}$$

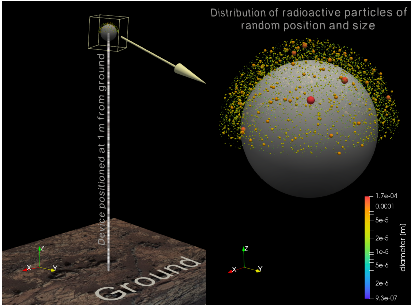
$$\rho_p \frac{\pi d_p^3}{6} \frac{\mathrm{d}^2 z}{\mathrm{d}t^2} = F_{D_z} - F_{dP_z} + F_B + F_G$$

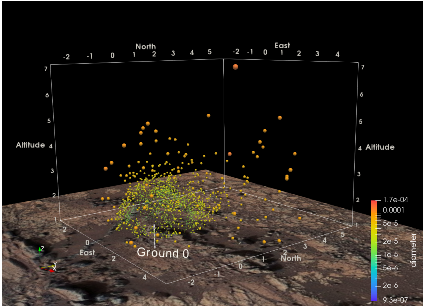




Stochastic Modelling Option: Direct Particle Tracking

L. Ivan *et al.*, JER 192 (2018)





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Phases of the MCREXS Procedure for RDD Simulation

MCREXS: Multi-Cloud Radiological EXplosive Source (L. Ivan *et al.*, JER 192 (2018))

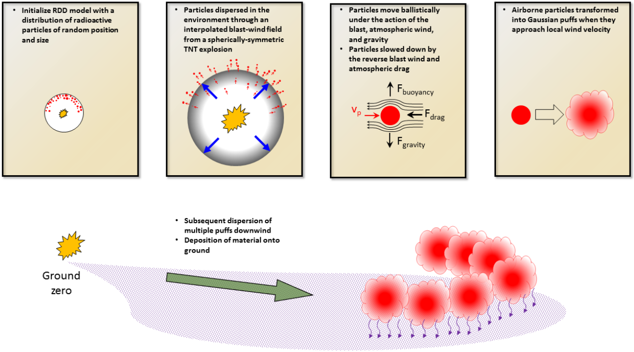
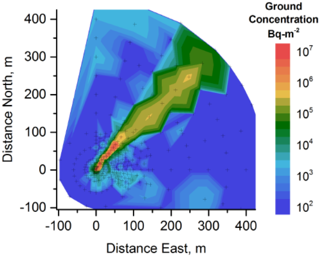


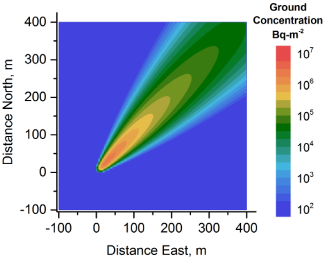
Figure: 1) Initialization of particles in the explosive device, 2) outward acceleration in the blast field, 3) deceleration in the atmosphere, 4) conversion to a Gaussian puff, and the subsequent dispersion and deposition onto the ground.

Shot 1 of the Suffield Full-Scale RDD Experiments

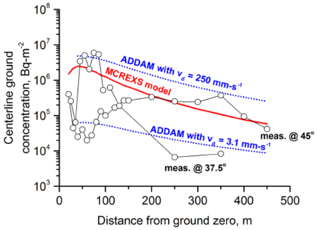
Ensemble Averaging Over 100 Puff Simulations with 12,800 Particles



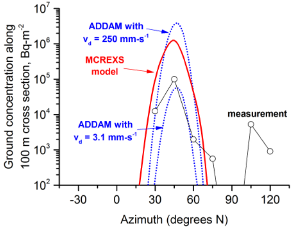
(a) Measured ground concentration



(b) Predicted ground concentration



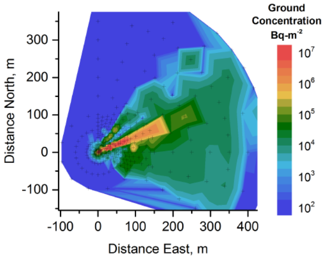
(c) Plume centreline deposition profile



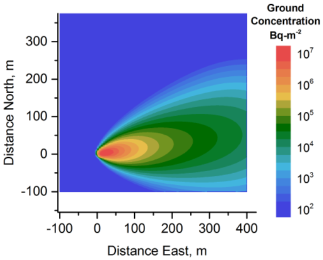
(d) Azimuthal cross-section of deposition profile at 100 m

Shot 2 of the Suffield Full-Scale RDD Experiments

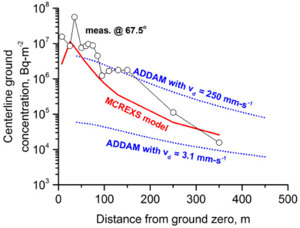
Ensemble Averaging Over 100 Puff Simulations with 12,800 Particles



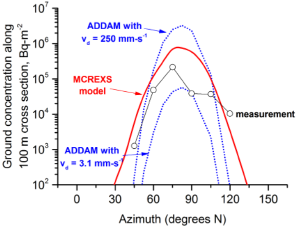
(a) Measured ground concentration



(b) Predicted ground concentration



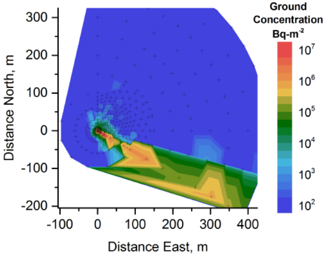
(c) Plume centreline deposition profile



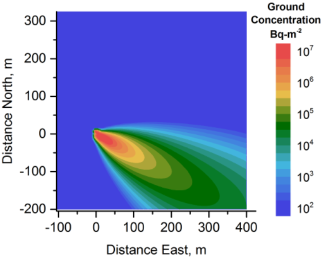
(d) Azimuthal cross-section of deposition profile at 100 m

Shot 3 of the Suffield Full-Scale RDD Experiments

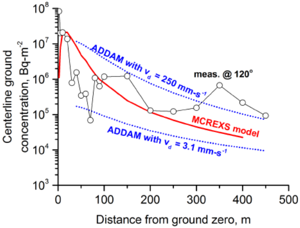
Ensemble Averaging Over 100 Puff Simulations with 12,800 Particles



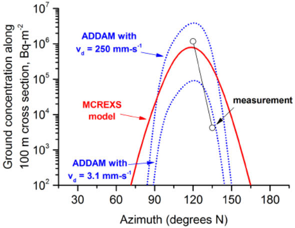
(a) Measured ground concentration



(b) Predicted ground concentration



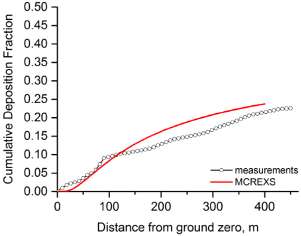
(c) Ground deposition profile along plume centreline



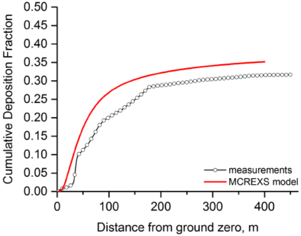
(d) Azimuthal cross-section of deposition profile at 100 m

Summary for the Suffield Full-Scale RDD Experiments

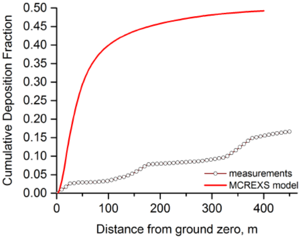
Ensemble Averaging Over 100 Puff Simulations with 12,800 Particles



(a) Shot 1



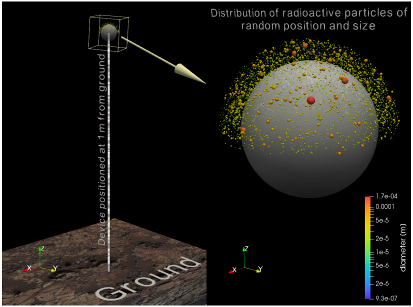
(b) Shot 2

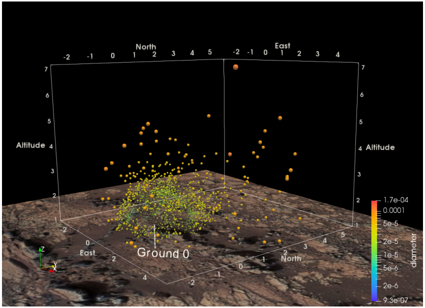


(c) Shot 3

Direct Particle Tracking

Drawbacks





- Expensive
- Stochastic
- Sensitivities are difficult to calculate (inverse problems are hard)

A Kinetic Description of Polydisperse Flows

F. Forgues *et al.*, under review in JCP (2019)

Multiphase flow can be considered similar to an ideal gas (many particles in seemingly “random” motion). Traditional Eulerian models can suffer from modelling artifacts in non-continuous regimes.

Kinetic theory defines a distribution function for the density of identical particles

$$\mathcal{F}(x_i, v_i, t)$$

To allow the particle to be differentiated by a collection of N properties (e.g., size, colour, temperature) the distribution function is extended as

$$\mathcal{F}(x_i, v_i, \zeta_0, \zeta_1, \ldots, \zeta_N, t)$$

The distribution function for particles with a range of sizes is extended to include a diameter space

$$\mathcal{F}(x_i, v_i, d, t)$$

Traditional Moments

Traditional "macroscopic" properties are related to $\mathcal{F}$ by moments

$$\int_0^\infty \iiint_\infty W(v_i, d)\mathcal{F}\, \mathrm{d}v_i\, \mathrm{d}d = \langle W(v_i, d)\mathcal{F}\rangle$$

$$nu_i = \langle v_i \mathcal{F}\rangle$$

$$n\Theta_{ij} = \langle c_i c_j \mathcal{F}\rangle$$

$$n\Psi_{id} = \langle c_i(\ln d - \mu)\mathcal{F}\rangle$$

$$n\Psi_{dd} = \left\langle (\ln d - \mu)^2 \mathcal{F}\right\rangle$$

where $c_i = v_i - u_i$ is the difference between a particle's velocity and the local average and μ is the local average of the logarithm of particle diameter.

Evolution of the Distribution Function

Extended Boltzmann equation:

$$\frac{\partial \mathcal{F}}{\partial t} + v_\alpha \frac{\partial \mathcal{F}}{\partial x_\alpha} + \frac{\partial}{\partial v_\alpha}\left(a_\alpha \mathcal{F}\right) + \sum_{\breve{i}=0}^{N} \frac{\partial}{\partial \zeta_{\breve{i}}}\left(\Upsilon_{\breve{i}} \mathcal{F}\right) = \left(\frac{\delta \mathcal{F}}{\delta t}\right)_{\text{collision}}$$

$$\frac{\partial \mathcal{F}}{\partial t} + v_i \frac{\partial \mathcal{F}}{\partial x_i} + \frac{\partial a_i \mathcal{F}}{\partial v_i} + \frac{\partial \phi \mathcal{F}}{\partial d} = \left(\frac{\delta \mathcal{F}}{\delta t}\right)_{\text{collision}}$$

Unfortunately,

- High-dimensional
- Expensive to compute
- Not all the information carried by the distribution is necessary
- It is better to take the velocity moments of the Boltzmann equation

Moment closure

Velocity moment of the kinetic equation (ignoring collisions and diameter changes):

$$\frac{\partial}{\partial t}\langle \boldsymbol{W}\mathcal{F}\rangle + \frac{\partial}{\partial x_i}\langle v_i \boldsymbol{W}\mathcal{F}\rangle + \left\langle \boldsymbol{W}\frac{\partial}{\partial v_i}(a_i\mathcal{F})\right\rangle + \left\langle \cancel{\boldsymbol{W}\frac{\partial \phi\mathcal{F}}{\partial d}}\right\rangle = \left\langle \cancel{\boldsymbol{W}\frac{\delta\mathcal{F}}{\delta t}}\right\rangle$$

- System is never closed
- Possible to close the system by choosing $\mathcal{F}$ as a function of free parameters
- Choose $\mathcal{F}$ in order to maximize entropy

$$\mathcal{F} = e^{\boldsymbol{\alpha}^{\mathrm{T}}\boldsymbol{W}}$$

Polydisperse Gaussian Distribution Function

Assumed form of the distribution function:

$$\mathcal{F} = \frac{n}{(2\pi)^2(\det \Psi_{ij})^{1/2}} e^{\left(-\frac{1}{2}\Psi_{ij}^{-1}\tilde{c}_i\tilde{c}_j\right)} .$$

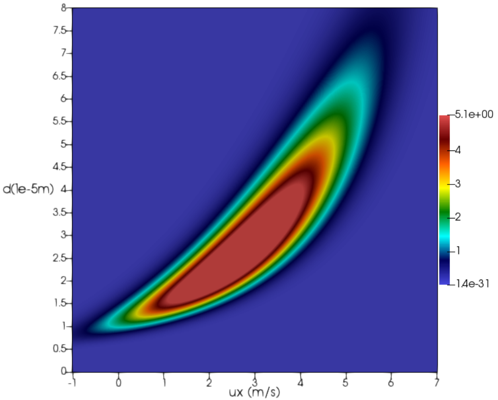
Data show the diameter to be log-normal where

$$\tilde{c}_i = \begin{bmatrix} v_x - u_x \\ v_y - u_y \\ v_z - u_z \\ \ln(d) - \mu \end{bmatrix} \qquad \Psi = \begin{bmatrix} \Theta_{xx} & \Theta_{xy} & \Theta_{xz} & \Psi_{xd} \\ \Theta_{xy} & \Theta_{yy} & \Theta_{yz} & \Psi_{yd} \\ \Theta_{xz} & \Theta_{yz} & \Theta_{zz} & \Psi_{zd} \\ \Psi_{xd} & \Psi_{yd} & \Psi_{zd} & \Psi_{dd} \end{bmatrix}$$

A generalized Gaussian distribution function can be written for a set of N properties

Polydisperse Gaussian Distribution Function

An example distribution in v_x-d space:



- Particles display a range of velocities and diameters.
- Particles with large diameters are more likely to have higher speeds.
- $\Psi_{xd} > 0$

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Polydisperse Gaussian Model (PGM)

Polydisperse Flows Subject to Aerodynamic Drag, Gravity and Buoyancy Forces

Application of Gaussian moment closure leads to a 15 first-order hyperbolics PDEs of the form

$$\frac{\partial \boldsymbol{U}}{\partial t} + \frac{\partial \boldsymbol{F}_x}{\partial x} + \frac{\partial \boldsymbol{F}_y}{\partial y} + \frac{\partial \boldsymbol{F}_z}{\partial z} = \boldsymbol{S}$$

Polydisperse Gaussian Model (PGM)

$$\boldsymbol{U} = n \begin{bmatrix} 1 \\ u_x \\ u_y \\ u_z \\ (u_x^2 + \Theta_{xx}) \\ (u_x u_y + \Theta_{xy}) \\ (u_x u_z + \Theta_{xz}) \\ (u_y^2 + \Theta_{yy}) \\ (u_y u_z + \Theta_{yz}) \\ (u_z^2 + \Theta_{zz}) \\ \mu \\ (\mu u_x + \Psi_{xd}) \\ (\mu u_y + \Psi_{yd}) \\ (\mu u_z + \Psi_{zd}) \\ (\mu^2 + \Psi_{dd}) \end{bmatrix} \qquad \boldsymbol{F}_x = n \begin{bmatrix} u_x \\ (u_x^2 + \Theta_{xx}) \\ (u_x u_y + \Theta_{xy}) \\ (u_x u_z + \Theta_{xz}) \\ (u_x^3 + 3u_x\Theta_{xx}) \\ (u_x^2 u_y + 2u_x\Theta_{xy} + u_y\Theta_{xx}) \\ (u_x^2 u_z + 2u_x\Theta_{xz} + u_z\Theta_{xx}) \\ (u_x u_y^2 + u_x\Theta_{yy} + 2u_y\Theta_{xy}) \\ (u_x u_y u_z + u_x\Theta_{yz} + u_y\Theta_{xz} + u_z\Theta_{xy}) \\ (u_x u_z^2 + u_x\Theta_{zz} + 2u_z\Theta_{xz}) \\ (\mu u_x + \Psi_{xd}) \\ (\mu u_x^2 + 2u_x\Psi_{xd} + \mu\Theta_{xx}) \\ (\mu u_x u_y + u_x\Psi_{yd} + u_y\Psi_{xd} + \mu\Theta_{xy}) \\ (\mu u_x u_z + u_x\Psi_{zd} + u_z\Psi_{xd} + \mu\Theta_{xz}) \\ (\mu^2 u_x + 2\mu\Psi_{xd} + u_x\Psi_{dd}) \end{bmatrix}$$

Polydisperse Gaussian Model (PGM)

The original ten wavespeed from the ten-moment model for gases remain and are supplemented by five new waves.

$$\lambda_{1-10} = \begin{pmatrix} u_x + \sqrt{3\Theta_{xx}} \\ u_x - \sqrt{3\Theta_{xx}} \\ u_x + \sqrt{\Theta_{xx}} \\ u_x - \sqrt{\Theta_{xx}} \\ u_x + \sqrt{\Theta_{xx}} \\ u_x - \sqrt{\Theta_{xx}} \\ u_x \\ u_x \\ u_x \\ u_x \end{pmatrix} \qquad \lambda_{11-15} = \begin{pmatrix} u_x + \sqrt{\Theta_{xx}} \\ u_x - \sqrt{\Theta_{xx}} \\ u_x \\ u_x \\ u_x \end{pmatrix}$$

Stokes Drag

Finally, a drag law is needed to completely close the system.

$$F_{D_i} = \begin{cases} C_d \rho_a \dfrac{\pi d_p^2}{8} ||\vec{v}|| v_i & : \text{Re} \geq 1 \\ 3\pi d_p \mu_a v_i & : \text{Re} < 1 \,, \end{cases}$$

$$C_d = \frac{24}{\text{Re}} + \frac{4.4}{\sqrt{\text{Re}}} + 0.42$$

For now, we assume Stokes drag, i.e., $C_d = \dfrac{24}{\text{Re}}$.

Acceleration of particle:

$$\vec{a}_d(t,x) = \frac{\vec{V}(t,\vec{x}) - \vec{v}_p}{\tau}, \quad \tau = \frac{\rho_p d_p^2}{18\mu_f}$$

Polydisperse Gaussian Model (PGM)

Source Term Accounting for the Effect of the Aerodynamic Drag

$$
\boldsymbol{S}_1 = \frac{n}{\tau_{\mathcal{G}}}
\begin{bmatrix}
0 \\
V_x - (u_x - 2\Psi_{xd}) \\
V_y - (u_y - 2\Psi_{yd}) \\
V_z - (u_z - 2\Psi_{zd}) \\
2\left(V_x(u_x - 2\Psi_{xd}) - (u_x^2 - 4u_x\Psi_{xd} + 4\Psi_{xd}^2 + \Theta_{xx})\right) \\
V_x(u_y - 2\Psi_{yd}) + V_y(u_x - 2\Psi_{xd}) - 2(u_x u_y - 2u_x\Psi_{yd} - 2u_y\Psi_{xd} + 4\Psi_{xd}\Psi_{yd} + \Theta_{xy}) \\
V_x(u_z - 2\Psi_{zd}) + V_z(u_x - 2\Psi_{xd}) - 2(u_x u_z - 2u_x\Psi_{zd} - 2u_z\Psi_{xd} + 4\Psi_{xd}\Psi_{zd} + \Theta_{xz}) \\
2\left(V_y(u_y - 2\Psi_{yd}) - (u_y^2 - 4u_y\Psi_{yd} + 4\Psi_{yd}^2 + \Theta_{yy})\right) \\
V_y(u_z - 2\Psi_{zd}) + V_z(u_y - 2\Psi_{yd}) - 2(u_y u_z - 2u_y\Psi_{zd} - 2u_z\Psi_{yd} + 4\Psi_{yd}\Psi_{zd} + \Theta_{yz}) \\
2\left(V_z(u_z - 2\Psi_{zd}) - (u_z^2 - 4u_z\Psi_{zd} + 4\Psi_{zd}^2 + \Theta_{zz})\right) \\
0 \\
V_x(\mu - 2\Psi_{dd}) - (\mu u_x - 2\mu\Psi_{xd} - 2u_x\Psi_{dd} + 4\Psi_{dd}\Psi_{xd} + \Psi_{xd}) \\
V_y(\mu - 2\Psi_{dd}) - (\mu u_y - 2\mu\Psi_{yd} - 2u_y\Psi_{dd} + 4\Psi_{dd}\Psi_{yd} + \Psi_{yd}) \\
V_z(\mu - 2\Psi_{dd}) - (\mu u_z - 2\mu\Psi_{zd} - 2u_x\Psi_{dd} + 4\Psi_{dd}\Psi_{zd} + \Psi_{zd}) \\
0
\end{bmatrix},
$$

$$
\tau_{\mathcal{G}} = \frac{\rho_p}{18\mu_f} e^{2\mu - 2\Psi_{dd}}, \quad \vec{V}_{\mathrm{bf}}(t, x) = (V_x, V_y, V_z)
$$

Polydisperse Gaussian Model (PGM)

Source Term Accounting for the Effect of Gravity and Buoyance Forces

$$
\boldsymbol{S}_2 = n \begin{bmatrix} 0 \\ \phi_x \\ \phi_y \\ \phi_z \\ 2u_x\phi_x \\ u_x\phi_y + u_y\phi_x \\ u_x\phi_z + u_z\phi_x \\ 2u_y\phi_y \\ u_y\phi_z + u_y\phi_x \\ 2u_z\phi_z \\ 0 \\ \mu\phi_x \\ \mu\phi_y \\ \mu\phi_z \\ 0 \end{bmatrix},
$$

$$
\phi_i = \frac{\rho_p - \rho_f}{\rho_p} g_i
$$

A Polydisperse Sedimentation Problem

Challenge: capture accurately the different relaxation rates of the particle phase to the terminal velocities for the complete range of particle diameters

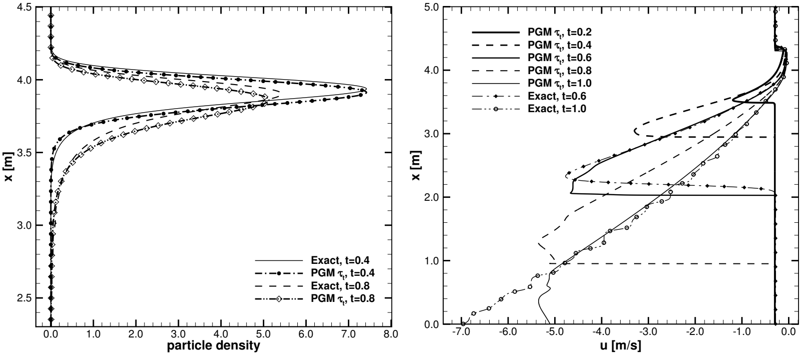

Figure: Comparison between the PGM predictions and exact solution for the particle density and velocity as a function of the vertical spatial coordinate

Conclusions

MCREXS Model :

- A hybrid stochastic model for RDD has been developed
- The model is an improvement relative to previously proposed models
- Comparisons to RDD experimental data show good agreement

Gaussian Polydisperse Model :

- A new deterministic polydisperse model for a wide range of multiphase flow regimes
- The model is globally hyperbolic and well-posed
- One-dimensional solutions demonstrate the potential for improved Eulerian predictions

Ongoing Work

- Account for the presence complex obstacles in the MCREXS model
- Implement the Gaussian model in an higher-order accurate multi-dimensional numerical framework
- Investigate problems with background flow that models the detonation of a radiological dispersal device
- Investigate high-performance algorithms for computational speed-up

Supplementary Material

- Proof of Wellposedness
- Exact Solution to the Kinetic Equation
- Numerical Method
- Assess the Drag Law for a Space-Homogeneous Case
- A Riemann Problem with Different Drag Strengths

Proof of Wellposedness

- The resulting PDEs are hyperbolic and well-posed whenever n and Ψ is positive definite.
- If one premultiplies the PDE for Ψ by Ψ^{-1} and uses the identity

$$\partial_s \log(\det(\Psi)) = \text{trace}(\Psi^{-1}\partial_s\Psi)$$

along with the continuity equation, one finds

$$\frac{\partial \log\left(\frac{\det\Psi}{n^2}\right)}{\partial t} + u_i \frac{\partial \log\left(\frac{\det\Psi}{n^2}\right)}{\partial x_i} = -108\left(\frac{\mu_f}{\rho_p} e^{-2\mu+2\Psi_{dd}}\right)$$

- The determinant of Ψ decays exponentially, but never reaches zero.

Back

Exact Solution to the Kinetic Equation

The kinetic equation for Stokes drag with zero background flow:

$$\frac{\partial \mathcal{F}}{\partial t} + v_i \frac{\partial \mathcal{F}}{\partial x_i} - \frac{\partial}{\partial v_i}\left(\frac{v_i}{\tau}\mathcal{F}\right) = 0$$

With initial conditions, $\mathcal{F}_0(x_i, v_i, d)$, this has an exact solution:

$$\mathcal{F}(x_i, v_i, d, t) = A\ \mathcal{F}_0(B_i, C_i, d)\ ,$$

with

$$A = e^{\frac{3t}{\tau}}\ ,$$

$$B_i = x_i + v_i\tau(1 - e^{\frac{t}{\tau}})\ ,$$

$$C_i = v_i e^{\frac{t}{\tau}}\ .$$

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Assess the Drag Law for a Space-Homogeneous Case

Normal distribution function relaxing to a zero velocity; Solution at time $t = 0$

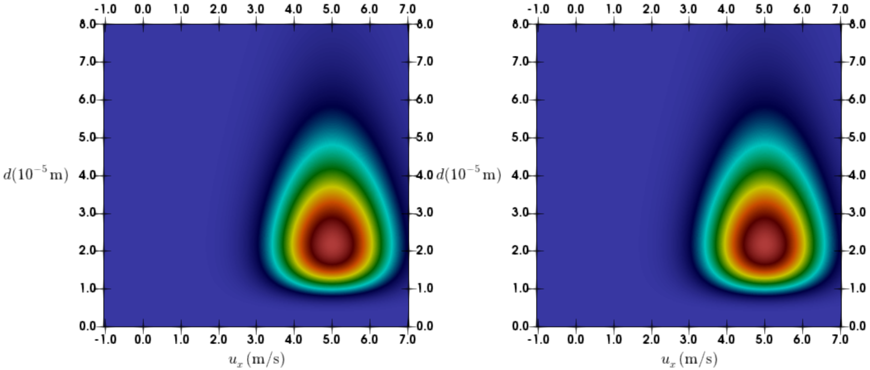

Figure: Kinetic solution (left) and moment solution (right)

Assess the Drag Law for a Space-Homogeneous Case

Normal distribution function relaxing to a zero velocity; Solution at time $t \approx 0.61$ s

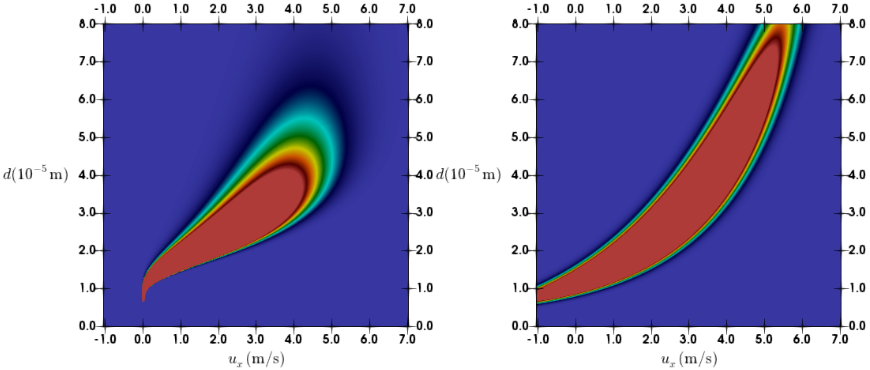

Figure: Kinetic solution (left) and moment solution (right)

Assess the Drag Law for a Space-Homogeneous Case

Normal distribution function relaxing to a zero velocity; Solution at time $t \approx 1.82\,\mathrm{s}$

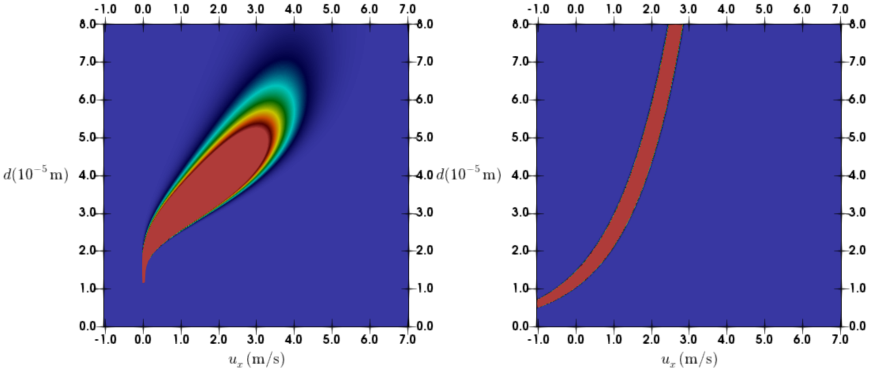

Figure: Kinetic solution (left) and moment solution (right)

Assess the Drag Law for a Space-Homogeneous Case

Normal distribution function relaxing to a zero velocity; Solution at time $t \approx 3.03$ s

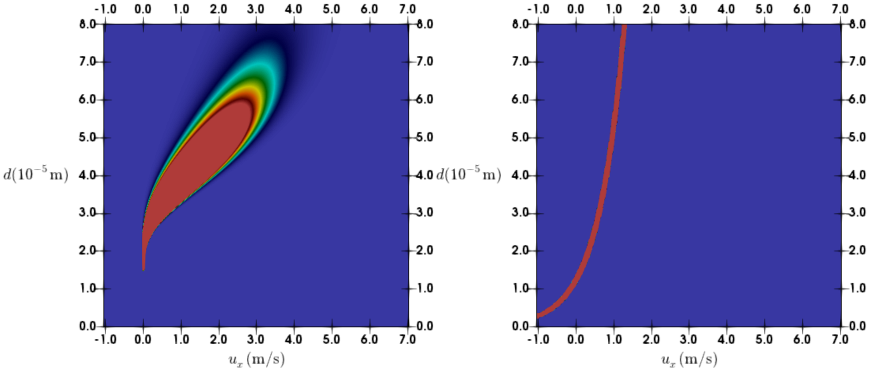

Figure: Kinetic solution (left) and moment solution (right)

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Numerical Method (operator splitting)

Discretization of the Moment Model

- Simple first-order Godunov-type finite-volume scheme for the hyperbolic part:

$$\widetilde{U}_i^{n+1} = \bar{U}_i^n - \frac{\Delta t}{\Delta x}\left(\hat{F}_{i+\frac{1}{2}} - \hat{F}_{i-\frac{1}{2}}\right)$$

- The possibly stiff source term is then evaluated analytically to account for drag.

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Comparisons are made to a common “single-velocity” multiphase treatment:

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x_j}(n u_j) = 0\,,$$

$$\frac{\partial}{\partial t}(n u_i) + \frac{\partial}{\partial x_j}(n u_i u_j) = S_i\,,$$

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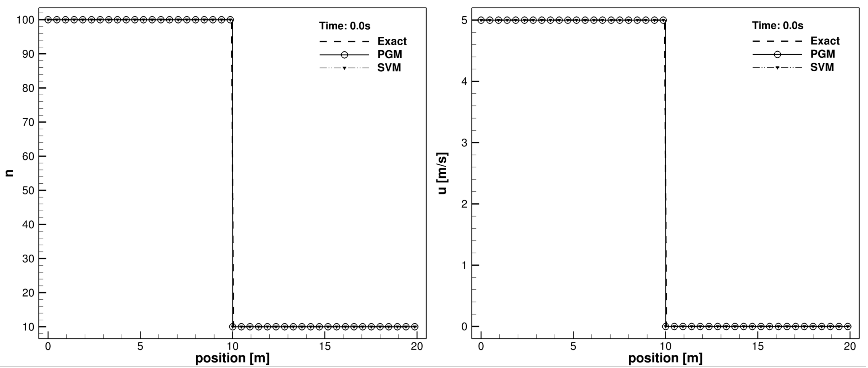
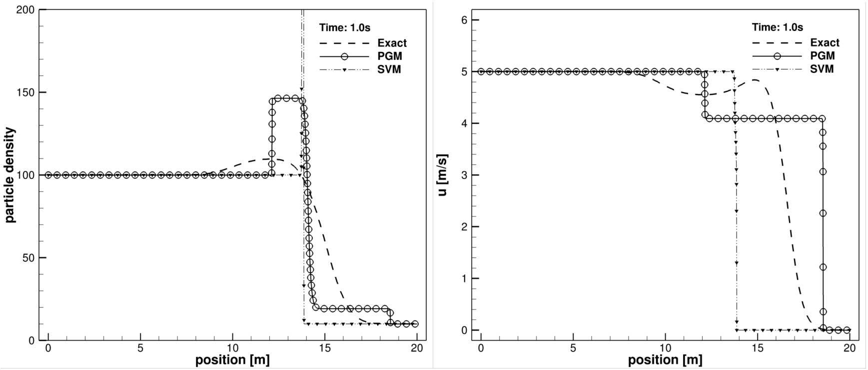
Numerical Result - ICs for a Riemann problem



For the whole domain Θ_{xx} is equal to $1.0\,m^2/s^2$, Ψ_{xd} is equal to $0\,m/s$, μ is equal to $\ln(28 \times 10^{-6})$ and Ψ_{dd} is equal to 0.25. A grid of 4000 cells with a CFL number of 0.5 is used for all cases.

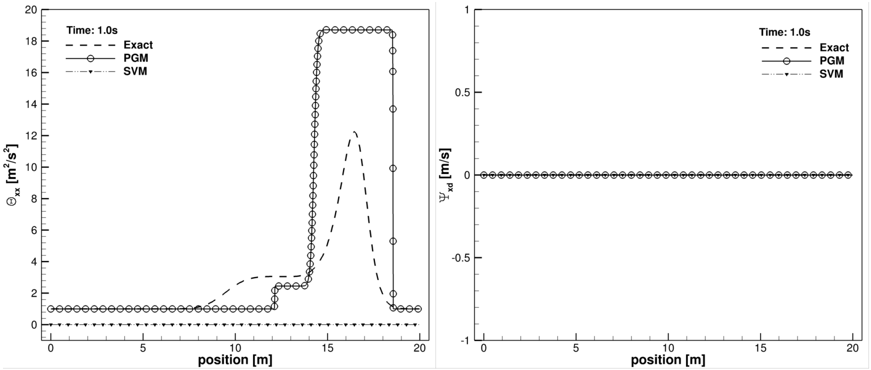
No drag $\tau = \infty$

Particle number (left) and velocity (right) at time $t = 1$ s



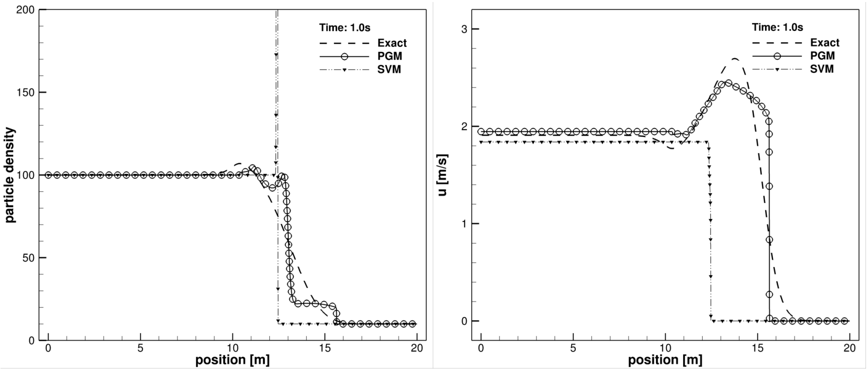
No drag $\tau = \infty$

Θ_{xx} (left) and Ψ_{xd} (right) at time $t = 1$ s



Medium drag $\tau = 1$ s

Particle number (left) and velocity (right) at time $t = 1$ s



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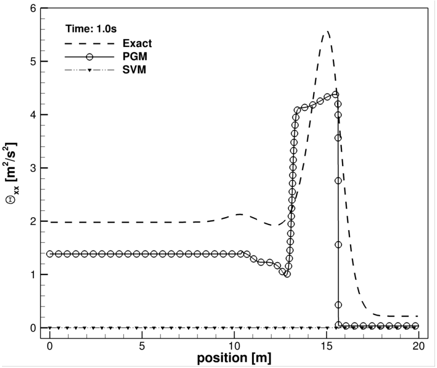
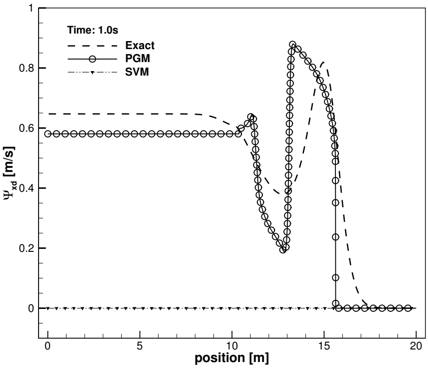
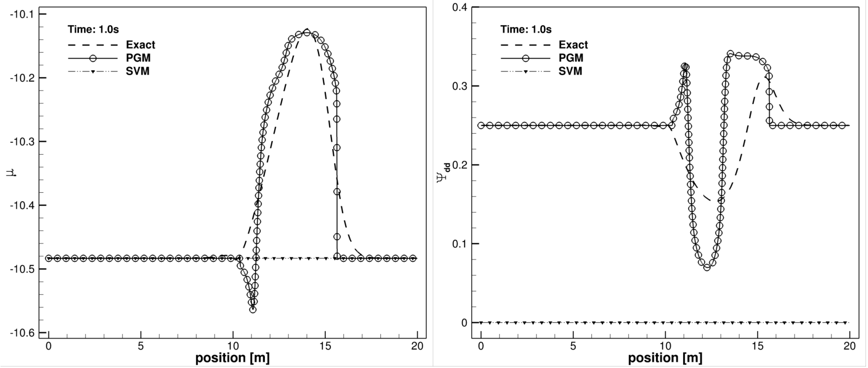




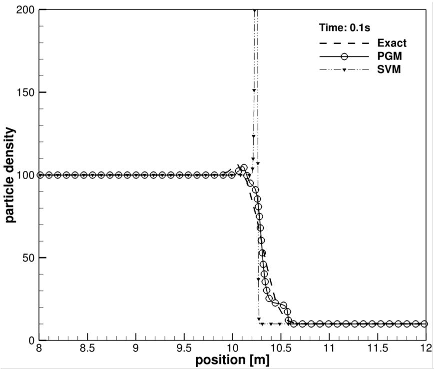
Medium drag $\tau = 1$ s

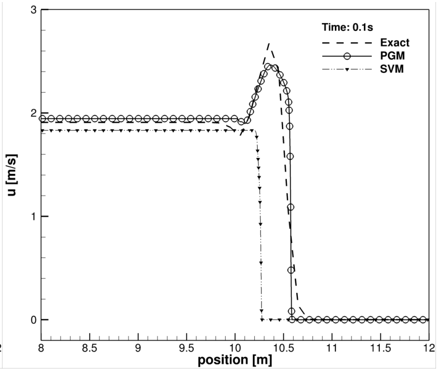
Mean diameter (left) and Ψ_{dd} (right) at time $t = 1$ s



Strong drag $\tau = 0.1$ s

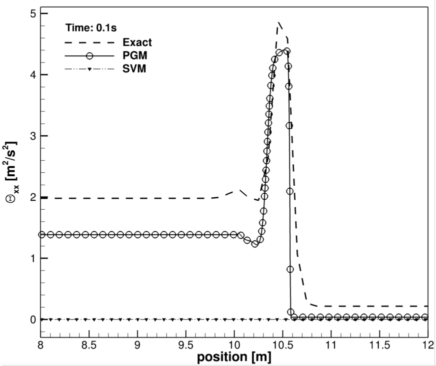
Particle number (left) and velocity (right) at time $t = 0.1$ s

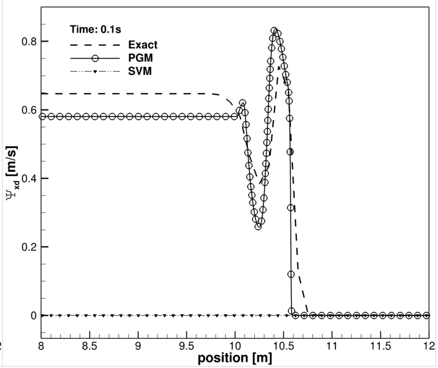




Strong drag $\tau = 0.1$ s

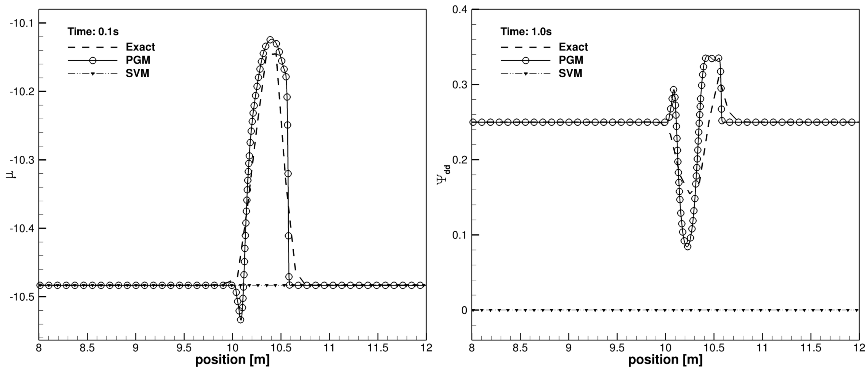
Θ_{xx} (left) and Ψ_{xd} (right) at time $t = 0.1$ s





Strong drag $\tau = 0.1$ s

Mean diameter (left) and Ψ_{dd} (right) at time $t = 0.1$ s



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