Gravity-based percolation of small particles through an assembly of large particles

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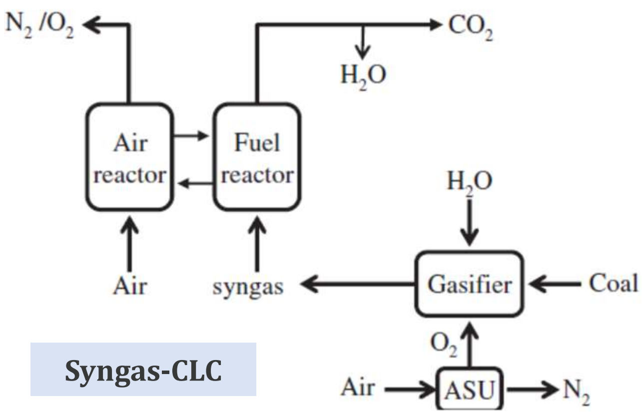
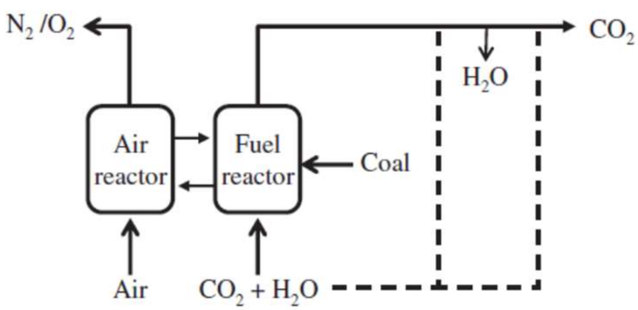
Context: Chemical-Looping Combustion

Coal-fueled Options

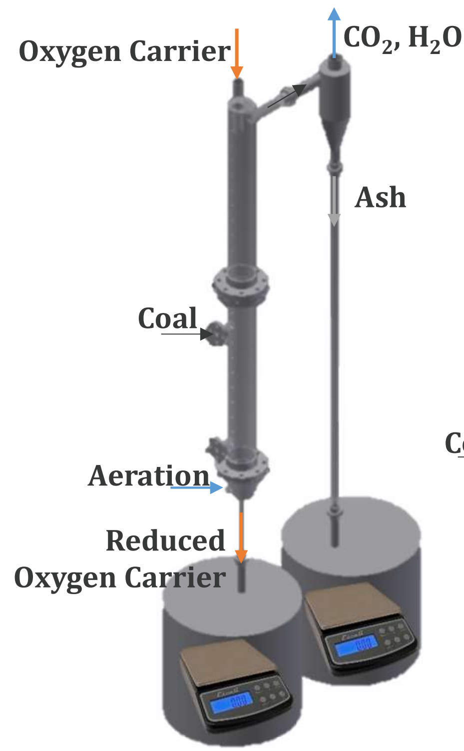


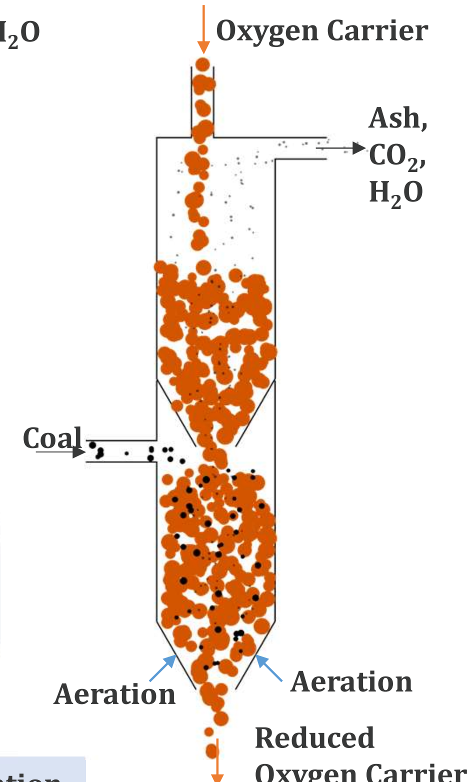
Syngas-CLC



In-Situ Gasification-CLC

In-Situ Coal Gasification and Waste (Ash) Removal





NETL Cold Moving Bed: Fluidization-Based Percolation

Solid-Fueled Moving Bed Operation

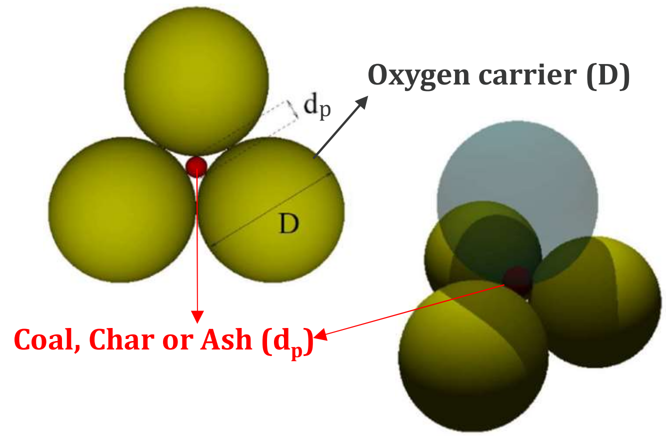
Hydrodynamics

- Transport/Separation (by Elutriation): carrier-fuel/waste
  - Flow regimes, Dispersion, Transit time, …etc.
- Packed bed pressure drop

Heat and Mass transfers

- Temperature distribution
- Reaction rates

Percolation (Fluidization-based)



Percolation constraint (spherical particles):

$$\frac{D}{d_p} > 6.46$$

➔ **Get insight first with "simple" flows: Gravity-based percolation**

Outline

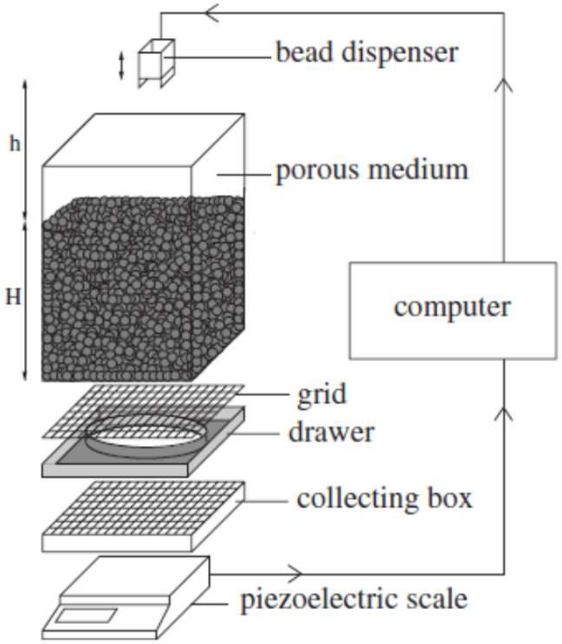
1. **Percolation Experiments of Lomine & Oger (2006)**
   - “Simple” mono-disperse intruder flow

2. **Discrete Element Method Simulations of Lomine & Oger’s Exp.**
   - Goal: Gain Understanding to be fed into KTGF Models

3. **Preliminary assessments of Poly-disperse KTGF models**
   - e.g. Syamlal’s Friction-based Poly-disperse Particle-Particle Drag (1987)

4. **Conclusion – Future plans**

Percolation Experiments of Lomine & Oger



Material	Diameter	Density
Porous medium bed (Large, Glass beads)	16mm	2500kg/m^3
Intruder (Fine, Steel)	1mm	7800kg/m^3

Dimensions	
Porous medium	26cm x 26cm x H
Dispenser (fine)	5.2cm x 5.2cm x h

$$N_p\left(N,\frac{d_p}{D}\right)=\frac{N\frac{\pi}{6}d_p^3}{\frac{\sqrt{2}-2\Omega}{12}\Phi_{RCP}D^3}\approx 31.5N\left(\frac{d_p}{D}\right)^3$$

Lominé F., Oger L., Journal of Statistical Mechanics: Theory and Exp. (2006)

- **What measurements were performed?**
  1. Collect intruder with respect to time (scale) ➔ Mean transit time (➔ mean velocity)
  2. Intruder total mass in each cell of collecting box ➔ Position variance (➔ dispersion coefficients)

- **Objective: Describe flow behavior using Advection-Dispersion model**

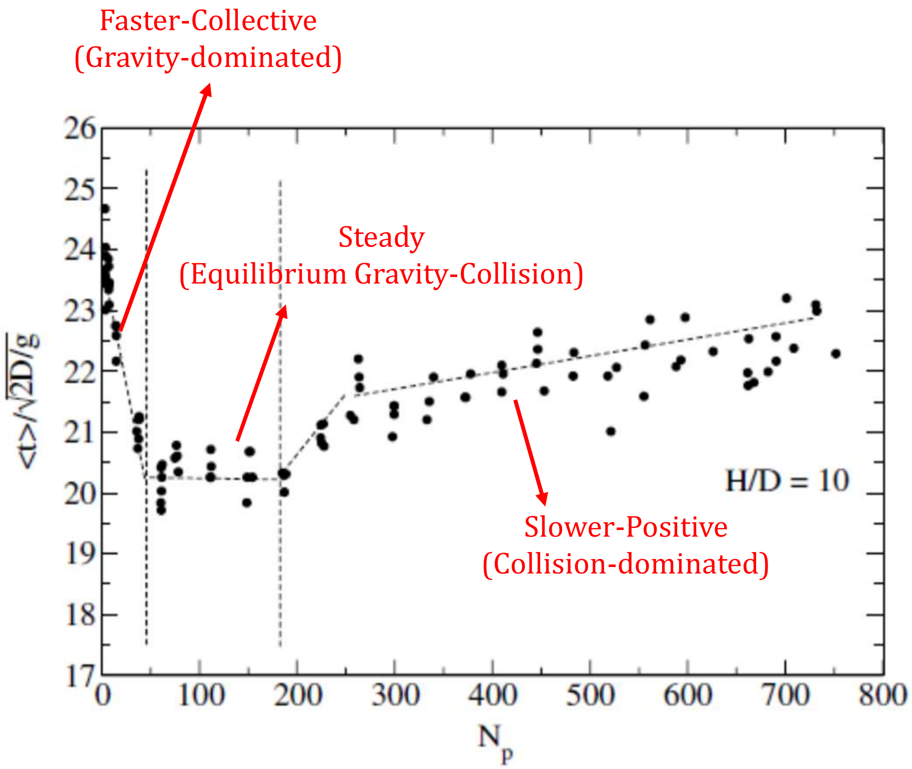
$$\frac{\partial C(r,t)}{\partial t}+U\cdot\nabla C(r,t)=D_{\parallel}\frac{\partial^2 C(r,t)}{\partial r_{\parallel}^2}+D_{\perp}\frac{\partial^2 C(r,t)}{\partial r_{\perp}^2}$$

Mean velocity

Longitudinal & Transverse dispersion coefficients

Cooperative Percolation Flow Regimes

Flow Regimes (from Mean Transit Time)



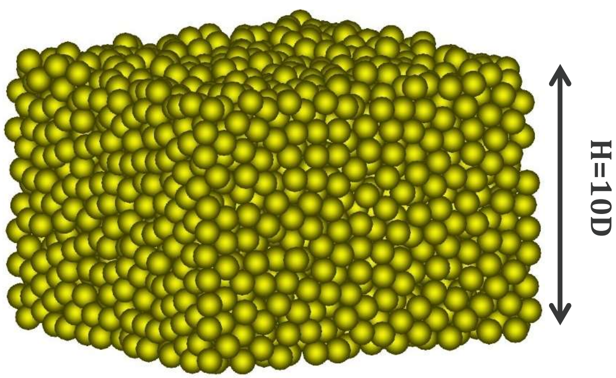
- (May be) useful to guide, design and operation of the moving bed solid-fueled reactors
- How well can the flow regimes be captured with DEM models?
- What mechanisms control these flow regimes? (useful for the KTGF models)
  - Intruder-Intruder interactions (➔dispersion)
  - Intruder-Fixed bed interactions (➔dispersion)
  - Pore jamming
  - Bed dispersivity (local structure arrangement)

Lominé F., Oger L., Journal of Statistical Mechanics: Theory and Exp. (2006)

Packed Bed Generation

Lagrangian DEM-based Gravitational Settling

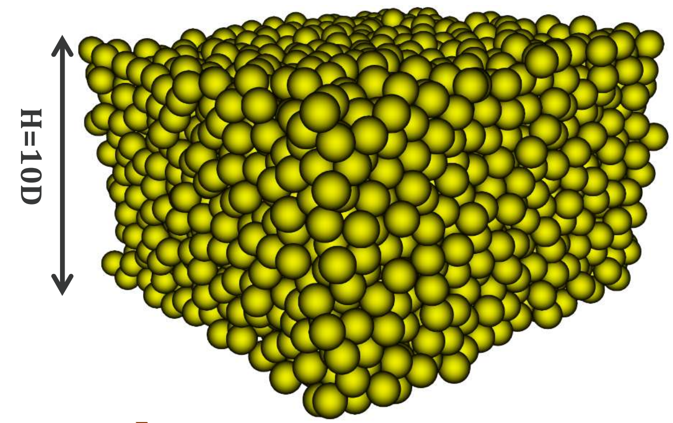
(release and settling of large amount of particles in larger container ➔ cut to match domain of interest)



➔ Average porosity = 0.435

Modified Lubachevsky-Stillinger[1] algorithm

(Random Sequential Addition init., Particle grow, Hard Sphere Coll, Solid Pressure ➔ cut to match domain of interest)



Donev NYU Packing Code

➔ Average porosity = 0.376

(Lominé & Oger reported bed porosity around 0.4)

➔ (*The effects*) Pore distribution, Tortuosity, Spatial randomness etc. … have not been investigated yet

[1]M. Skoge, A. Donev, F. H. Stillinger, and S. Torquato, Phys. Rev. E, Vol. 74: 041127 (2006)

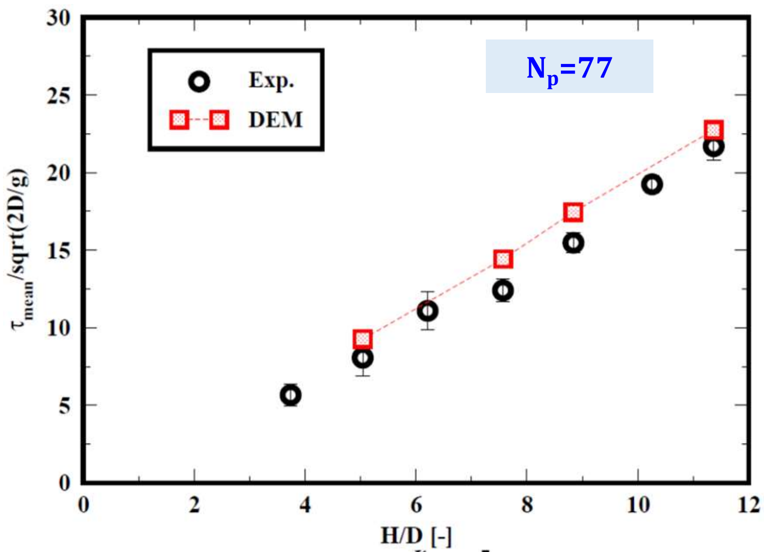
Steady Percolation Dynamics

(4 beds constructed from the same parent)

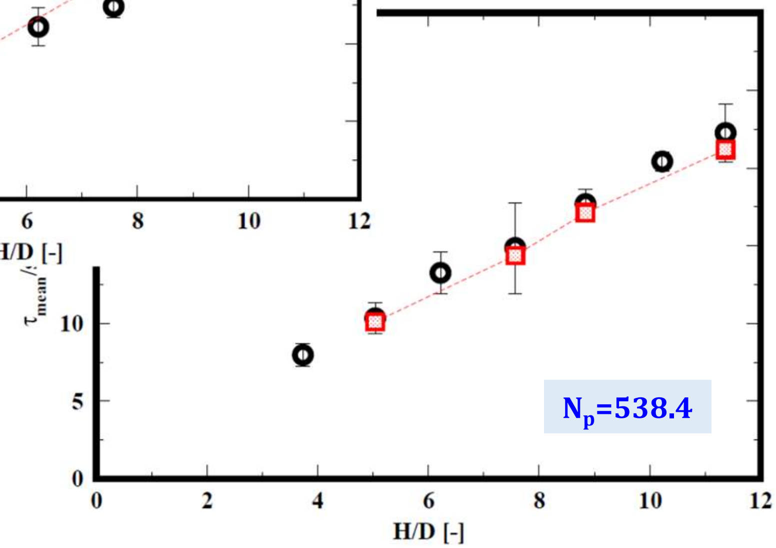
H/D	5.04	7.57	8.84	10.0	11.37
Number large particle	1428	2152	2523	2851	3257
Porosity	0.438	0.436	0.434	0.435	0.432

(3 amounts of intruder particles)

Number of intruder: N [-]	500	10,000	70,000
Dimensionless number: N_p[-]	3.8	77.0	538.4

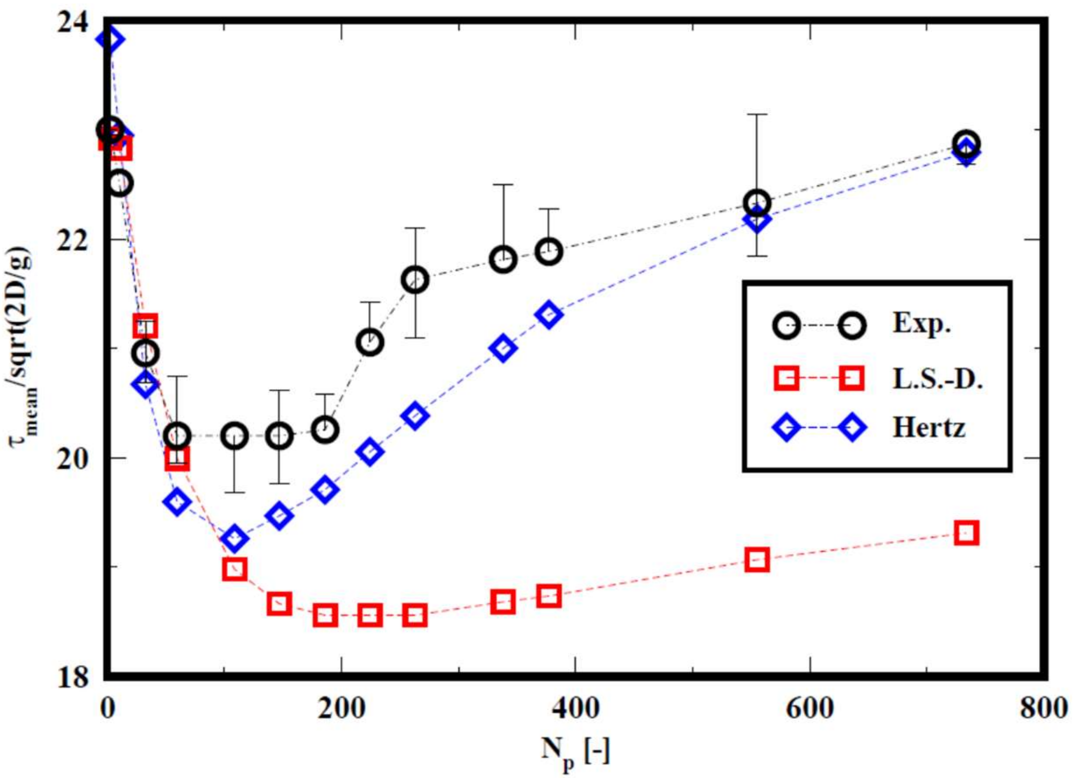


Mean transit time



- Predictions within exp. uncertainties ➔ porous medium geometrical structures seem adequately captured
- Mean transit velocity is constant regardless bed height

Flow Regime Predictions



- Percolation dynamics appears quite dependent on the inter-particle interaction models (especially for the collision-dominated regime)
- The dependence of the restitution coefficient to impact velocity with Hertz model force calculations (contrary to the Linear Spring-Dashpot) may have been critical in the predictions for that regime

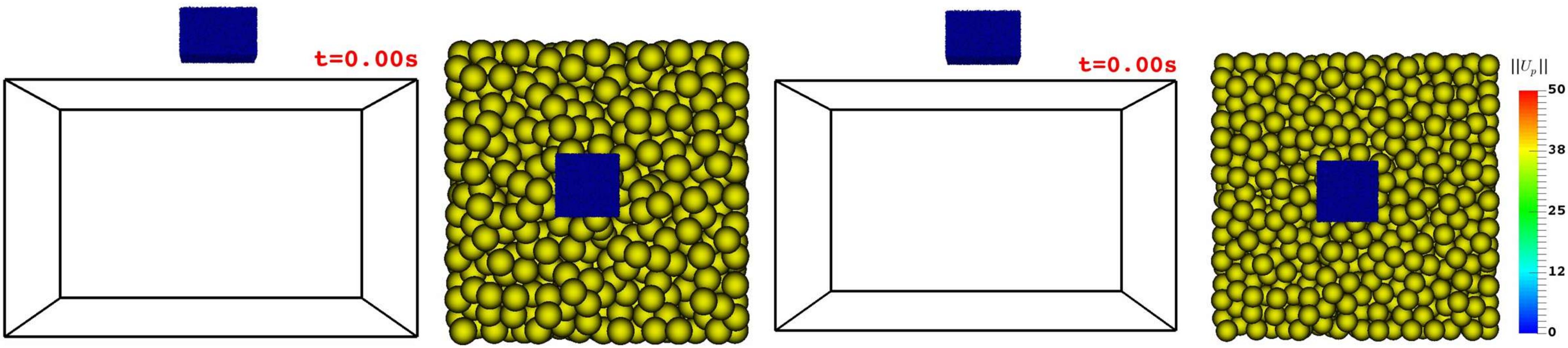
Exp. data from Lominé F., Oger L., Journal of Statistical Mechanics: Theory and Exp. (2006)

Animation (Intruder: N=95,404 or N_p=734)

Linear Spring-Dashpot | **Hertz**

(colored by the magnitude of the intruder velocities)

Side View | Top View | Side View | Top View

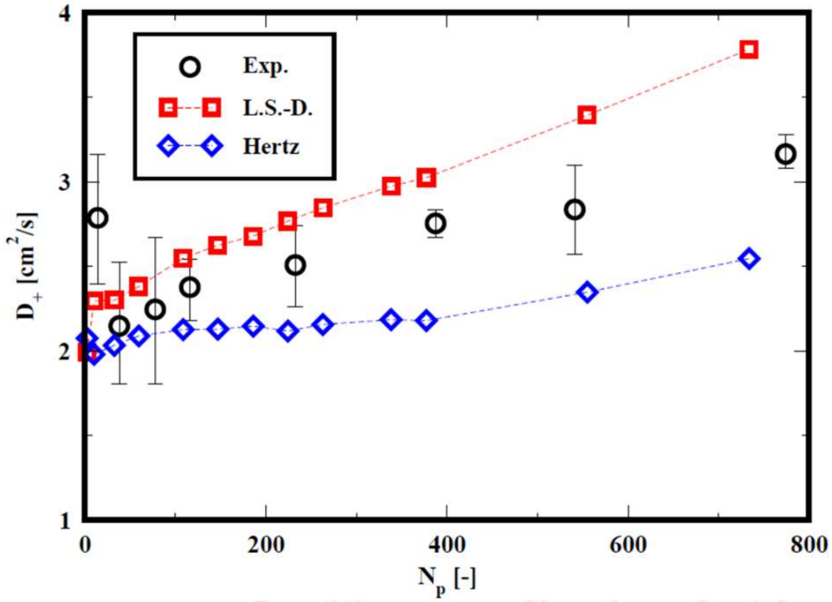


➔ **The intruder particles percolate through the porous medium by remaining a bulb**

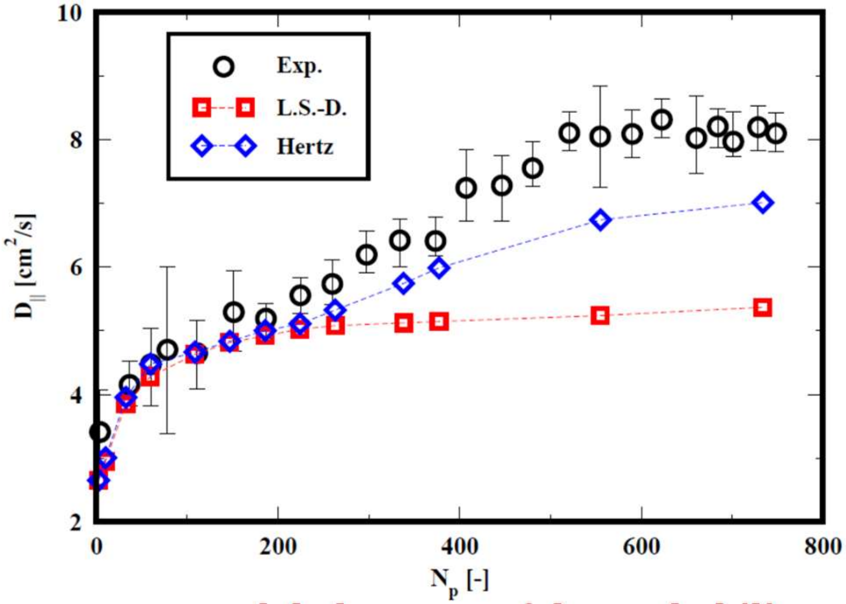
➔ **Intruder scattering is wider at the bed with L.S.-D. compared to Hertz**

Dispersion Coefficients

Transverse Dispersion



Longitudinal Dispersion



➔ **Wider spreading found with L.S-D. versus Hertz model: decrease of the probability of Intruder-Intruder interactions with L.S-D. model**

➔ **Intruder bed expands more vertically with Hertz model as in the experiments**

Exp. data from Nominé F., Oger L., Physical Review E 79 (2009)

Uncertainty due to Bed Porosity

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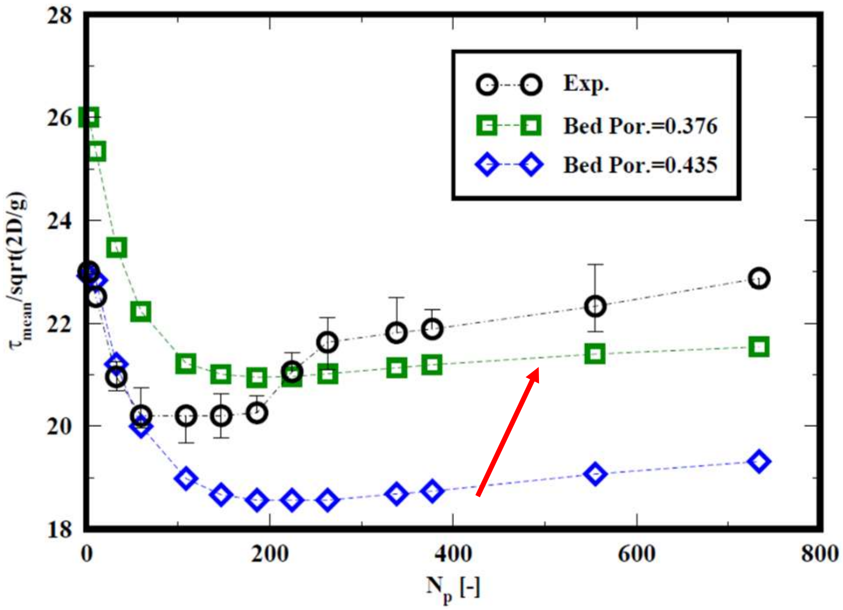
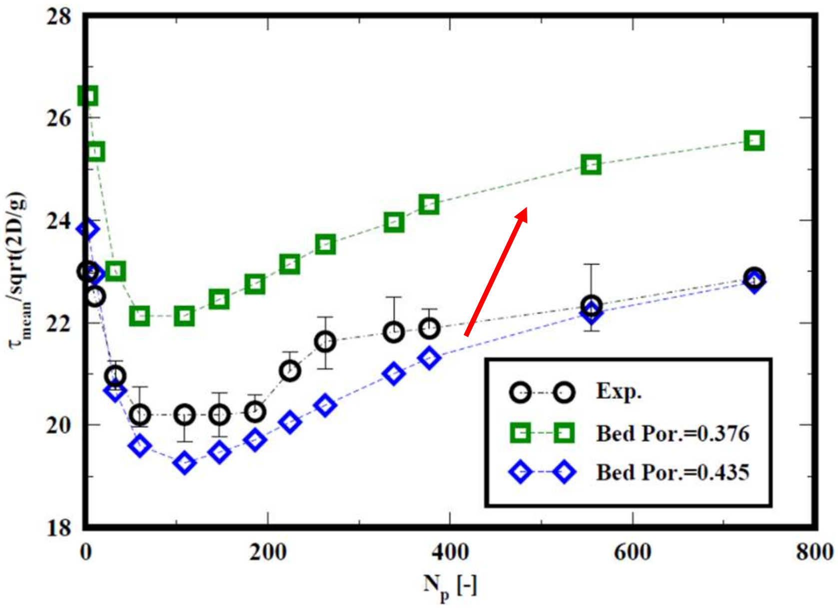
Linear Spring-Dashpot



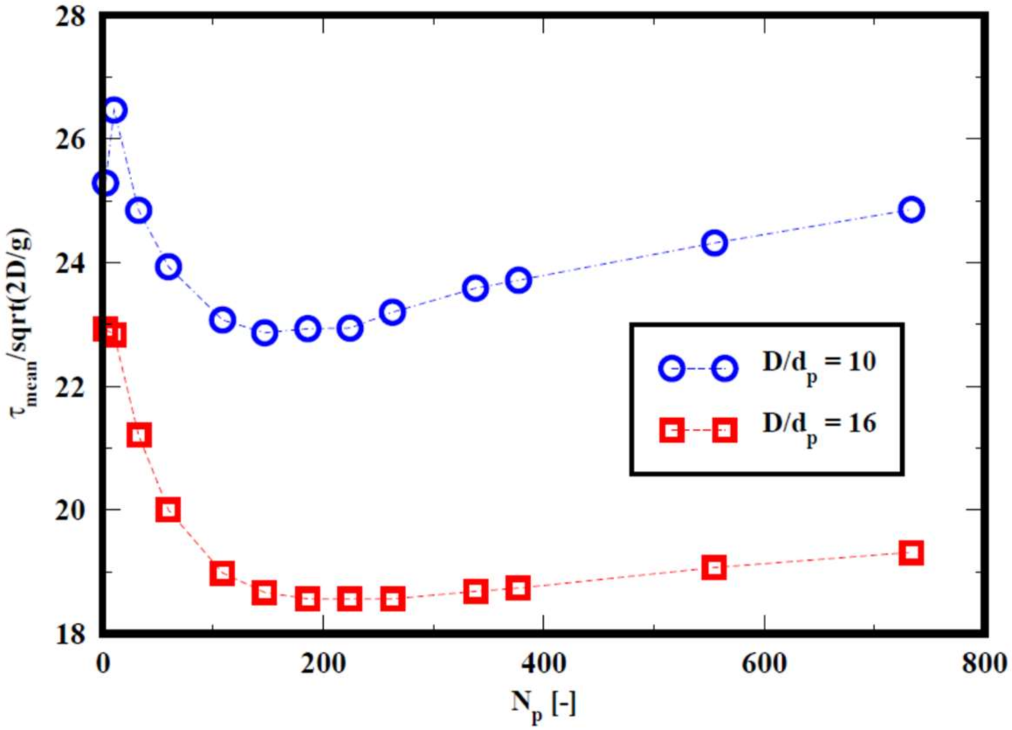
Hertz



➔ **Flow regime predictions appear independent of the uncertainty in the bed porosity, even though the denser bed unsurprisingly slowed down the intruder particles**

Flow Regime Dependence on Intruder Size

Linear Spring-Dashpot



$$N_p\left(N, \frac{d_p}{D}\right) \approx 31.5N\left(\frac{d_p}{D}\right)^3$$

➔ **Larger size intruders transited slowly but percolation dynamics (in terms of flow regime) appears independent of the diameter ratio (at least using the Linear Spring-Dashpot force calculation).**

Preliminary assessments of KTGF models

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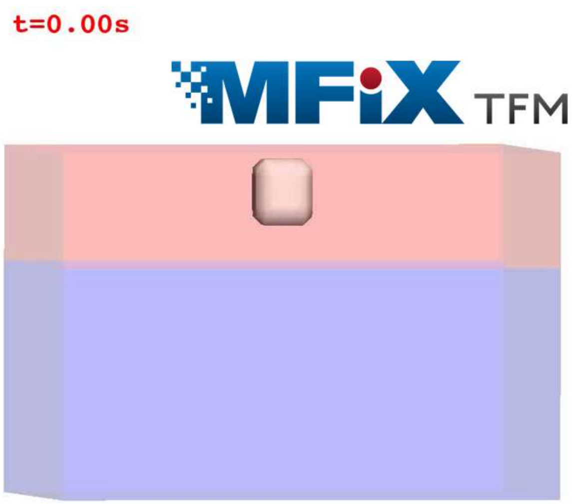
Kinetic Theory-based Poly-Disperse Model

- Syamlal (1987): translational-based motion, friction between particles
- Maximum packing: Yu & Standish (1987)
- Constant restitution and friction coefficients (interaction between particles by collisions)



Influence of the Fixed Bed Height: 10,000 small particles

H/D	5.04		7.57		8.84		11.37	
	Exp.	Sim.	Exp.	Sim.	Exp.	Sim.	Exp.	Sim.
Transit time [s]	0.471	0.599	0.724	0.806	0.900	0.909	1.259	1.124
$\langle(\Delta r)^2\rangle$ [cm^2]	-	2.915	-	4.023	10.07	4.020	-	2.951
$D_\perp$ [cm^2/s]	-	1.217	-	1.248	2.797	1.106	-	0.656
$\langle(\Delta z)^2\rangle$ [cm^2]	-	1.687	-	2.826	-	3.511	-	5.371
$D_\parallel$ [cm^2/s]	5.312	1.409	-	1.753	-	1.931	-	2.388

→ Relatively small errors in the prediction of mean transit time (27%, 11%, 1% and -11%)

→ Low scattering and expansion of intruder particles

Despite:

- Constant restitution, friction coefficients
- Translational-based motion Kinetic theory-based model (Syamlal, 1987) assuming:
  - Dirac velocity distribution function → momentum transfer doesn't account for agitation of the particles
  - Energy redistribution due to inter-particle collisions between different particle phases
- Additional dispersion induced by the porous medium assembly → dispersivity not accounted in the kinetic theory model (local structure of the arrangement)

- **Gray potato** → iso-surface volume fraction small particles
- **Blue color**: fixed bed

Conclusion – Future works

- **Conclusions:**
  - Hertz model (in contrast) to LS-D predicts the experimentally measured variation in the mean transit time (intruder velocity) with respect to the intruder concentration.
  - Hertz under-predicts the transverse and axial dispersion
  - LS-D over-predicts the transfer and under-predicts the axial dispersion
  - Predicted sensitivity of the transit time with respective to material properties is consistent with experimental observations
- **Future**
  - Trajectory/collision analysis
  - Hertz model parameters sensitivity
  - Continuum/large scale modeling

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NETL 2018 Workshop on Multiphase Flow Science
August 7-9, 2018
University of Houston, Houston, TX
Abstract submission: workshop@mfix.netl.doe.gov by June 1, 2018
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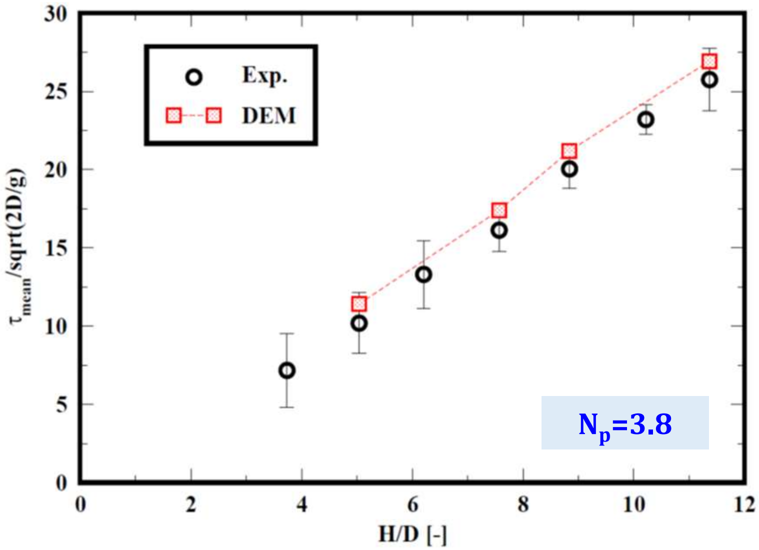
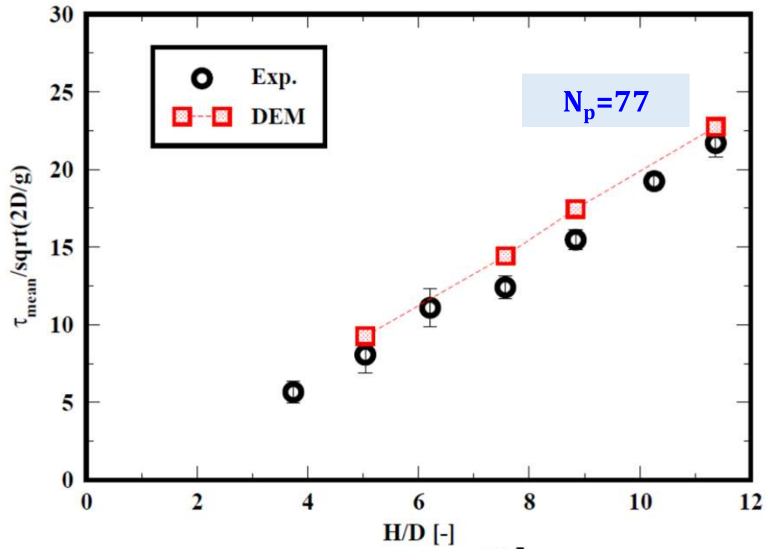
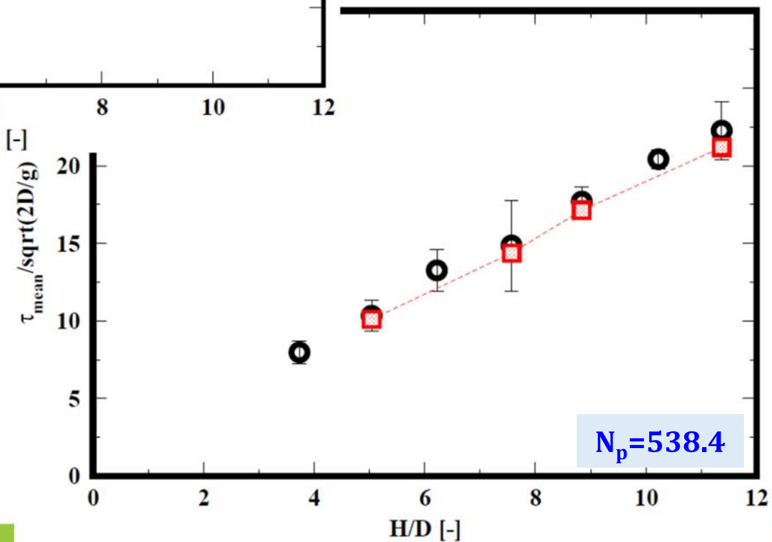
LSU

Back-up: Steady Percolation Dynamics





Mean transit time



(Linear Spring-Dashpot collision parameters)

Particle	Small-Small	Small-Large
Normal stiffness	10^5 g/s^2	
Normal restitution	0.99	0.84
Tangential stiffness	$2/7 \times 10^5$ g/s^2	
Friction coefficient	0.10	

Back-up: Sensitivity Study (L.S-D.)

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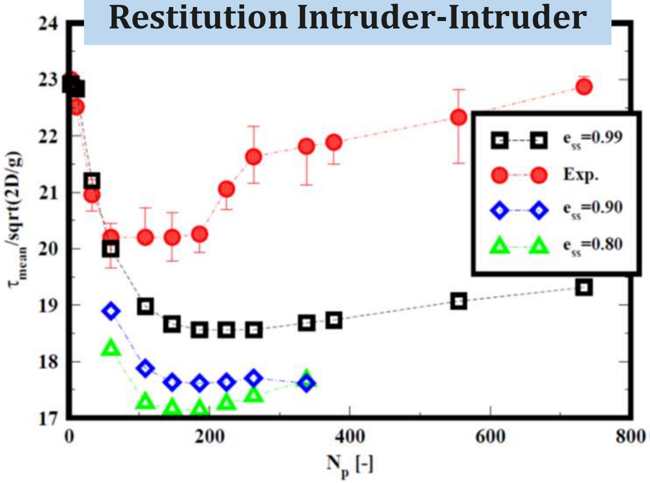
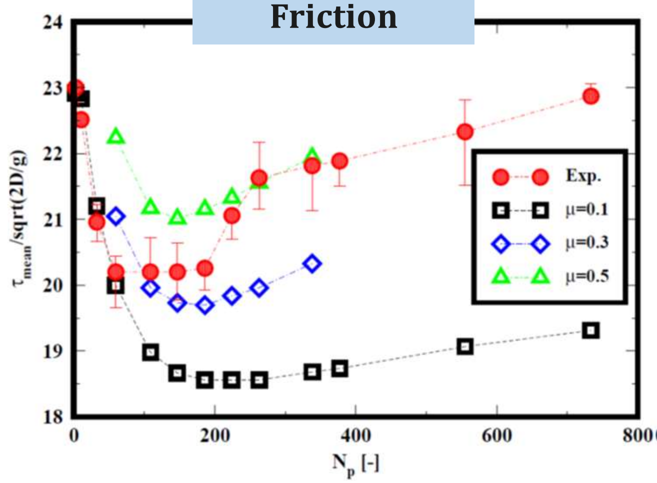
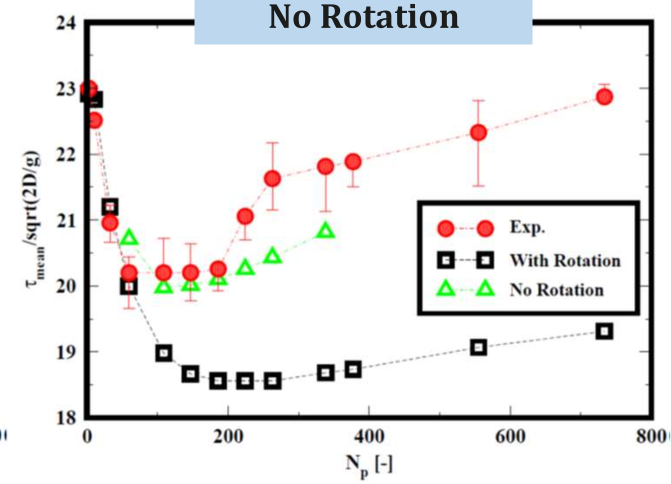
	Restitution Intruder-Intruder	Friction	No Rotation

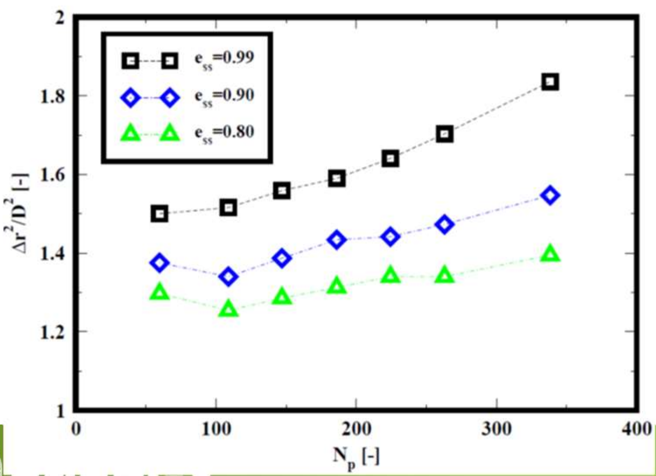
Mean Transit Time

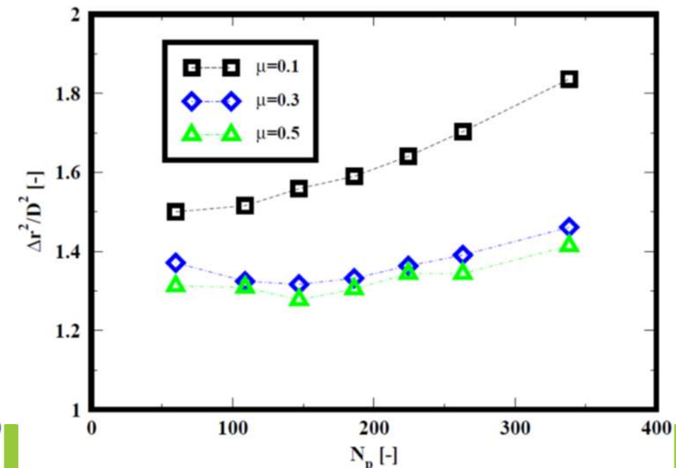


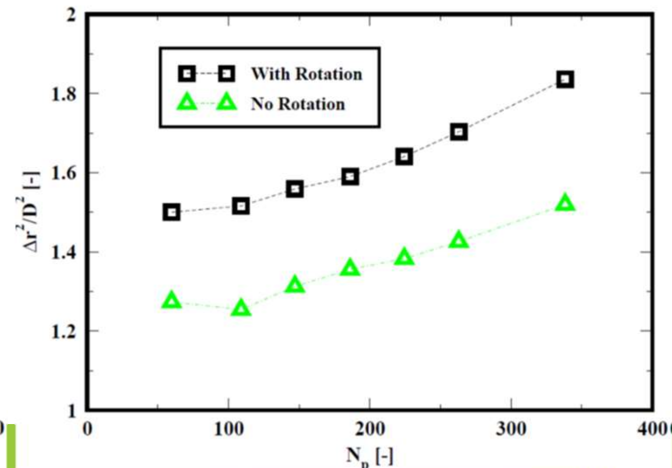




Radial Position Variance







Back-up: Post-process (as in experiments)

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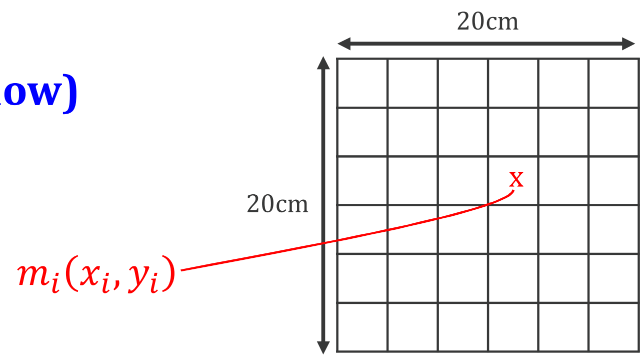
- **Mean transit time**

$$\tau_{mean} = \int_0^\infty t\varphi(t)dt \quad \text{with} \quad \varphi(t) = \frac{d}{dt}\left(\frac{m(t)}{\int_0^\infty m(t)dt}\right)$$

- **Transverse variance & dispersion (i.e. orthogonal to mean flow)**

$$\langle(\Delta r)^2\rangle = \sum_i p_i(r_i - \langle r\rangle)^2 = 4D_\perp\, \tau_{mean}$$

$$p_i = \frac{m_i(x_i, y_i)}{\sum_i m_i(x_i, y_i)}$$



- **Longitudinal variance & dispersion (i.e. mean flow direction)**

Assumption: Intruder transport through medium described by advection-dispersion model

$$m(z = H, t) = \frac{m_0}{2}\left[exp\left(\frac{zV}{D_\parallel}\right) erfc\left(\frac{z + Vt}{\sqrt{4D_\parallel t}}\right) + erf\left(\frac{z - Vt}{\sqrt{4D_\parallel t}}\right)\right]$$

$$\langle(\Delta z)^2\rangle = 2D_\parallel \tau_{mean}$$

← Find $D_\parallel$ which best fits normalized collected mass (Nonlinear Least Squares minimization algorithm: augmented Gauss-Newton and Levenberg-Marquardt)