Modeling Material/Species Transport

Reacting Flows - Lecture 8

Instructor: André Bakker

http://www.bakker.org

© André Bakker (2006)

Outline

- In addition to flow fields, we often need to model additional physics.
- The fluid velocities transport a number of properties:
  - Mass of one or more materials.
  - Momentum.
  - Energy.
- Proper modeling of material transport is necessary if we want to model mixing or reaction.
- Methods to model material transport:
  - Discrete phase modeling (DPM), aka particle tracking.
  - Species transport, aka scalar transport.
  - Multiphase flow modeling, e.g. Eulerian flow models.

Multiphase flow → multiple momentum eqns.

- Multiphase flow is simultaneous flow of:
  - Materials with different states or phases (i.e. gas, liquid or solid).
  - Materials in the same state or phase, but that are immiscible (i.e. liquid-liquid systems such as oil droplets in water).
- Each phase has its own velocity field and its own momentum.
- It is therefore often necessary to solve multiple sets of momentum equations, one set for each phase.
- Interaction between the phases requires the introduction of momentum exchange terms.
- Models are often complex, and time consuming to solve.
- Will not discuss here.

Systems with single set of momentum eqns.

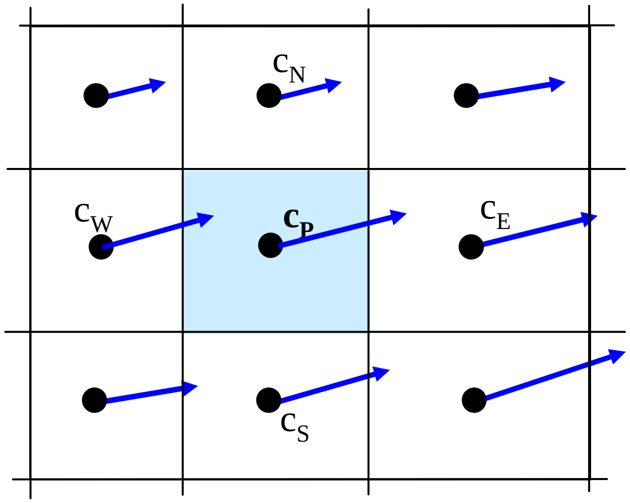
- We will discuss material transport in systems that are adequately described by a single set of momentum eqns:
  - Species or scalar transport.
  - Particle tracking (DPM).
- One fluid flow field is solved.
- The rate of transport of the species or particles is derived from that single fluid flow field.
- The local concentration of species or particles may affect the flow field itself.

Species transport

- The species transport equation (constant density, incompressible flow) is given by:

$$\frac{\partial c}{\partial t}+\frac{\partial}{\partial x_i}(u_i c)=\frac{\partial}{\partial x_i}\left(\mathbf{D}\frac{\partial c}{\partial x_i}\right)+S$$

- The concentration of the chemical species is c.
- The velocity is u_i.
- $\mathbf{D}$ is the diffusion coefficient.
- S is a source term.
- This equation is solved in discretized form to calculate the transport and local species concentrations.

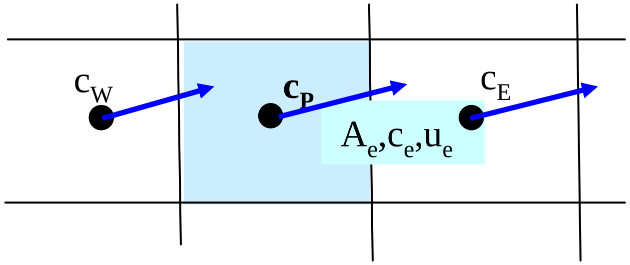


Species transport – the convective term

- Convection is transport of material due to the velocity of the fluid.

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial x_i}(u_i c) = \frac{\partial}{\partial x_i}\left(\mathbf{D}\frac{\partial c}{\partial x_i}\right) + S$$

- Flux from one grid cell to the next is area times normal-velocity times concentration.
- From cell “p” to “E”: $A_e.u_e.c_e$.



- Values at cell faces required!
- Implication: for best accuracy, use higher order discretization.

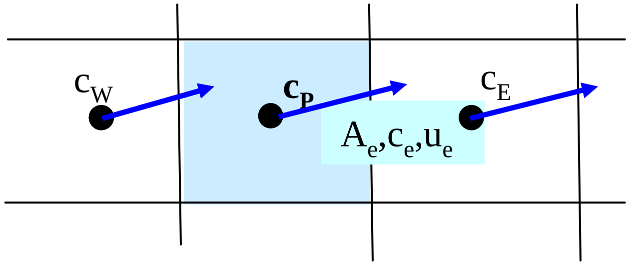
Species transport – the diffusive term

- Diffusion is transport resulting from concentration gradients.

$$\frac{\partial c}{\partial t}+\frac{\partial}{\partial x_i}(u_i c)=\frac{\partial}{\partial x_i}\left(\mathbf{D}\frac{\partial c}{\partial x_i}\right)+S$$

- Diffusion flux from one grid cell to the next is area times the concentration gradient times the diffusion coefficient.
- From cell “p” to “E”:

$$\mathbf{D}A_e \left.\frac{dc}{dx}\right|_e$$



- Gradient at interface between cells is easily calculated.
- The main difficulty is the calculation of the diffusion coefficient.

The diffusion term - molecular

- Molecular diffusion:
  - As a result of concentration gradients: mass diffusion.
  - As a result of temperature gradients: thermodiffusion.
- Mass diffusion coefficient:
  - Constant dilute approximation: same constant for all species.
  - Dilute approximation: different constant for each species.
  - Multi-component: a separate binary diffusion coefficient $\mathbf{D}_{ij}$ for each combination of species "i" into species "j".
- Thermodiffusion: flux is proportional to thermal diffusion coefficient $\mathbf{D}_T$ and temperature gradients:

$$\mathbf{D}_T \frac{\nabla T}{T}$$

  - Not usually important in industrial chemical reactors.

The diffusion term - turbulence

- Turbulent diffusion: transport due to the mixing action of the chaotic turbulent velocity fluctuations.
- The turbulent diffusion coefficient is calculated from the turbulent viscosity μ_t:

$$\mathbf{D}_{\mathrm{t}} = \frac{\mu_t}{\rho Sc_t}$$

- The turbulent Schmidt number Sc_t is a model constant. Recommended values are:
  - 0.7 if an eddy viscosity turbulence model is used, e.g. k-ε.
  - 1.0 if the Reynolds stress model (RSM) is used.

Species transport – source terms

- The source term:

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial x_i}(u_i c) = \frac{\partial}{\partial x_i}\left(\mathbf{D}\frac{\partial c}{\partial x_i}\right) + S$$

- This describes all other effects:
  - Creation or destruction of species due to chemical reaction.
  - Any other physical phenomena the user wants to implement.

Model setup

- Model setup:
  - Specify which species are present in the mixture.
  - Specify properties of all species.
  - If N species are present, N-1 equations are solved. The concentration of the Nth species follows from the fact that all mass fractions Y_i should sum to unity.

$$\sum_i Y_i = 1$$

$$\text{mass fraction:} \quad Y_i = \frac{c_i (kg/m^3)}{\rho_{mixture} (kg/m^3)}$$

$$\text{mixture density:} \quad \rho_{mixture} = \sum_i c_i$$

Boundary conditions

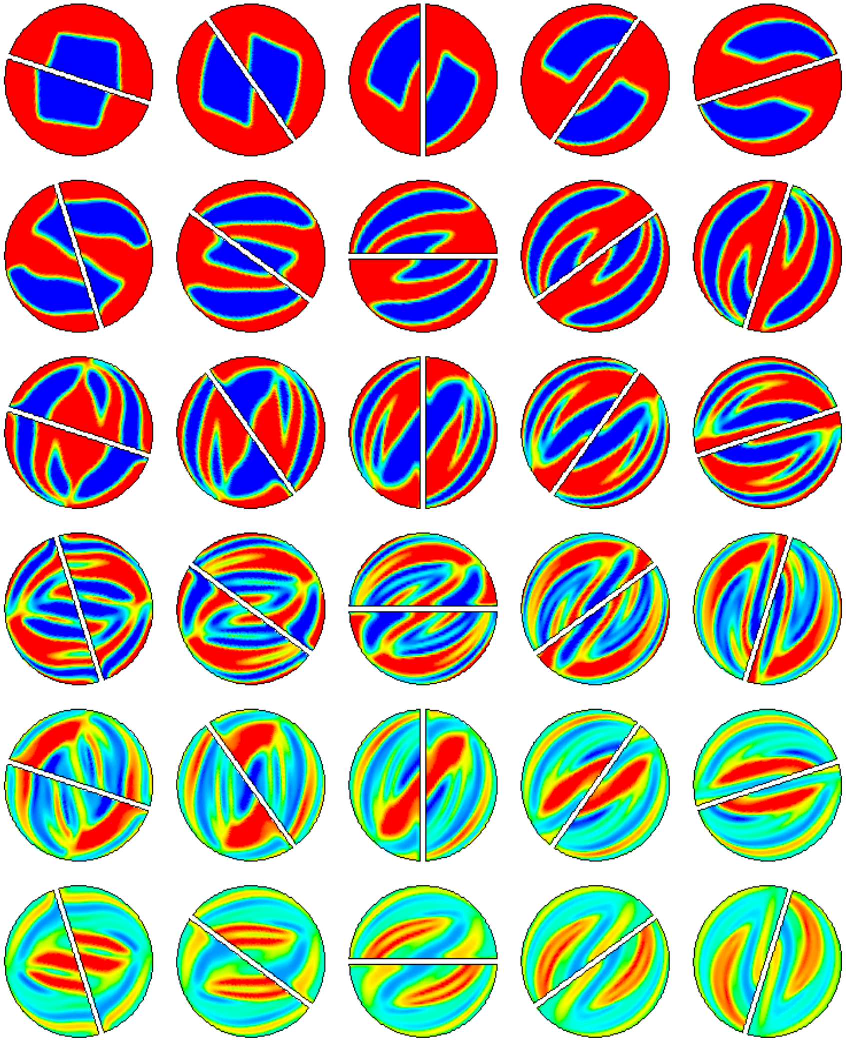
- Wall boundary conditions:
  - Either specified mass fraction, or zero flux.

- Inlet boundary conditions:
  - At inlets, the inlet flux is calculated as: $u_n c - \mathbf{D}\dfrac{\partial c}{\partial x_n}$
    - Need to specify inlet concentration/mass fraction.
    - The inlet diffusion flux depends on the concentration gradient. Value can not be predicted beforehand. If a fixed mass flow rate is desired, this term should be disabled.
- Outlet boundary conditions: specify species mass fraction in case backflow occurs at outlet.

Species equation is one-way!

- All species have the same convective velocity.
- Diffusion usually reduces concentration gradients → mixing.
- As a result, the diffusion equation can not usually be used to model separation!
- To model separation, multiphase models where the phases have different velocities are necessary.
- Exceptions:
  - Some laminar flow, thermal diffusion dominated cases.
  - Cases with complex transport models implemented through source terms.

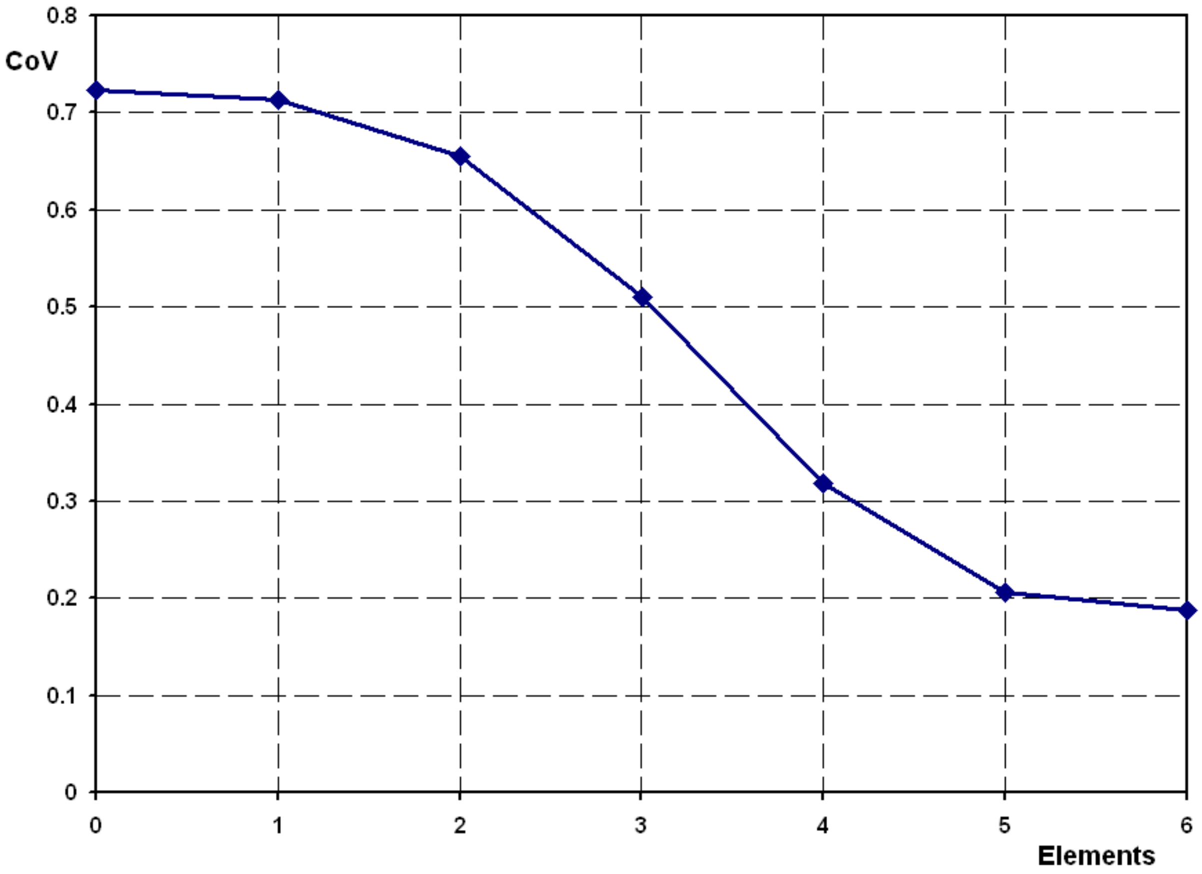
Mixing mechanism



- Laminar mixing.
- CFD simulation.
- Six elements.
- Each element splits, stretches and folds the fluid parcels.
- Every two elements the fluid is moved inside-out.

Mixing quantification

- Species concentration in sample points at different axial locations.
- Coefficient of variance: $CoV = \dfrac{stdev(c)}{average(c)}$



Kenics mixer

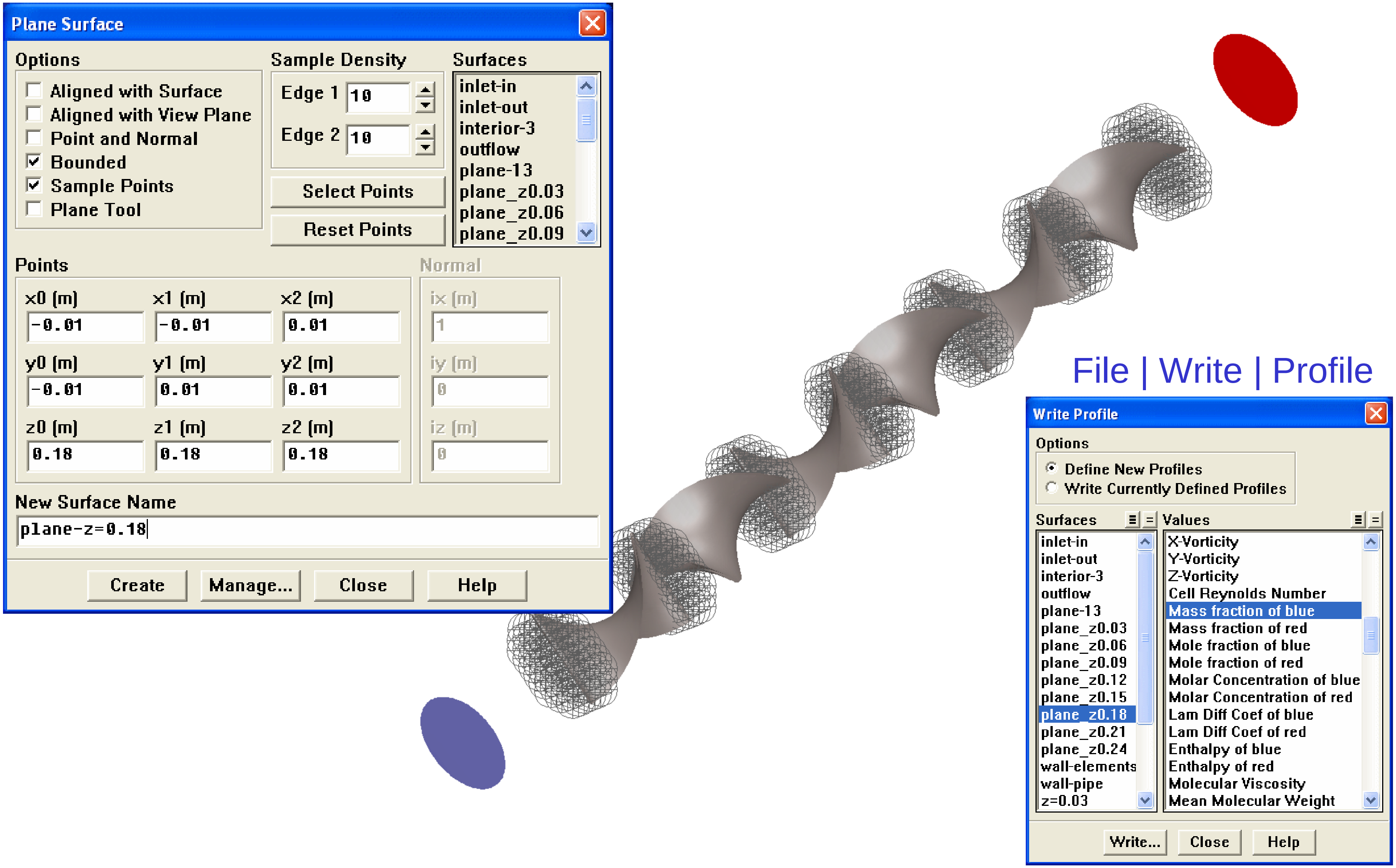
Six elements

Re=10

88 evenly spaced sample points in each axial plane.

Locations of sample plane points

Surfaces | Plane



Plane Surface

Options
- ☐ Aligned with Surface
- ☐ Aligned with View Plane
- ☐ Point and Normal
- ☑ Bounded
- ☑ Sample Points
- ☐ Plane Tool

Sample Density
- Edge 1: 10
- Edge 2: 10

Surfaces
- inlet-in
- inlet-out
- interior-3
- outflow
- plane-13
- plane_z0.03
- plane_z0.06
- plane_z0.09

Points

x0 (m)	x1 (m)	x2 (m)
-0.01	-0.01	0.01

y0 (m)	y1 (m)	y2 (m)
-0.01	0.01	0.01

z0 (m)	z1 (m)	z2 (m)
0.18	0.18	0.18

Normal
- ix (m): 1
- iy (m): 0
- iz (m): 0

New Surface Name: plane-z=0.18

File | Write | Profile

Write Profile

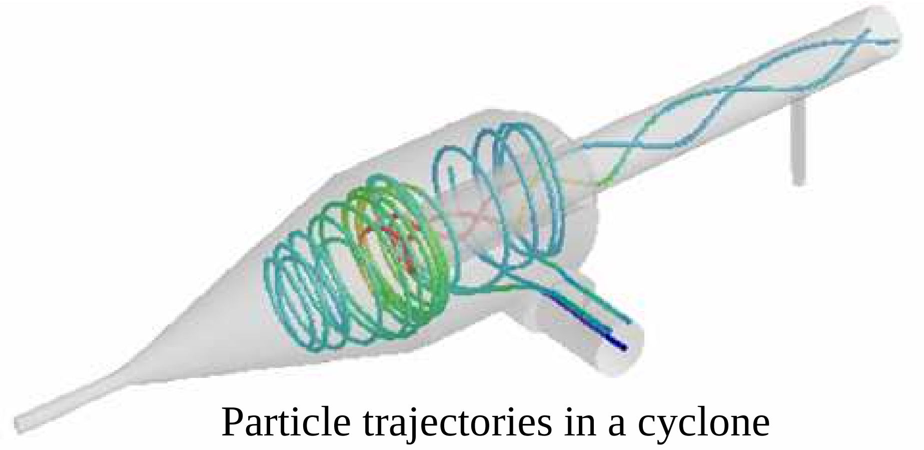
Options
- ● Define New Profiles
- ○ Write Currently Defined Profiles

Surfaces
- inlet-in
- inlet-out
- interior-3
- outflow
- plane-13
- plane_z0.03
- plane_z0.06
- plane_z0.09
- plane_z0.12
- plane_z0.15
- plane_z0.18
- plane_z0.21
- plane_z0.24
- wall-elements
- wall-pipe
- z=0.03

Values
- X-Vorticity
- Y-Vorticity
- Z-Vorticity
- Cell Reynolds Number
- Mass fraction of blue
- Mass fraction of red
- Mole fraction of blue
- Mole fraction of red
- Molar Concentration of blue
- Molar Concentration of red
- Lam Diff Coef of blue
- Lam Diff Coef of red
- Enthalpy of blue
- Enthalpy of red
- Molecular Viscosity
- Mean Molecular Weight

Particle tracking

- Solve one set of momentum equations for the fluid flow.
  - In an Eulerian reference frame, i.e. on the grid locations.
- Simulate a second, discrete phase consisting of individual particles.
  - Known as discrete phase modeling (DPM).
  - In a Lagrangian frame of reference, i.e. following the particles.
  - Trajectories are calculated, as well as particle heat and mass transfer.
  - Particles may affect fluid flow field. This is done by introducing source terms in the fluid flow equations.



Particle trajectories in a cyclone

DPM theory

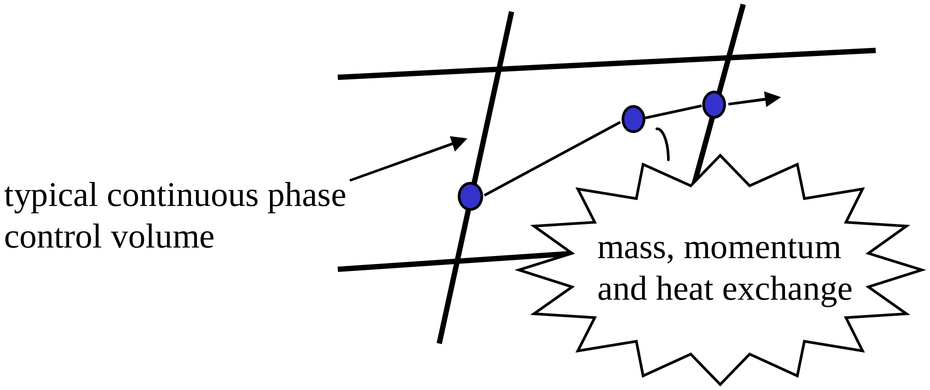
Trajectory is calculated by integrating the particle force balance equation:

$$\frac{du_i^p}{dt} = F_D\left(u_i - u_i^p\right) + g_i(\rho_p - \rho)/\rho_p + F_i/\rho_p$$

drag force is a function of the relative velocity

Gravity force

Additional forces:
- Pressure gradient
- Thermophoretic
- Rotating reference frame
- Brownian motion
- Saffman lift
- Other (user defined)

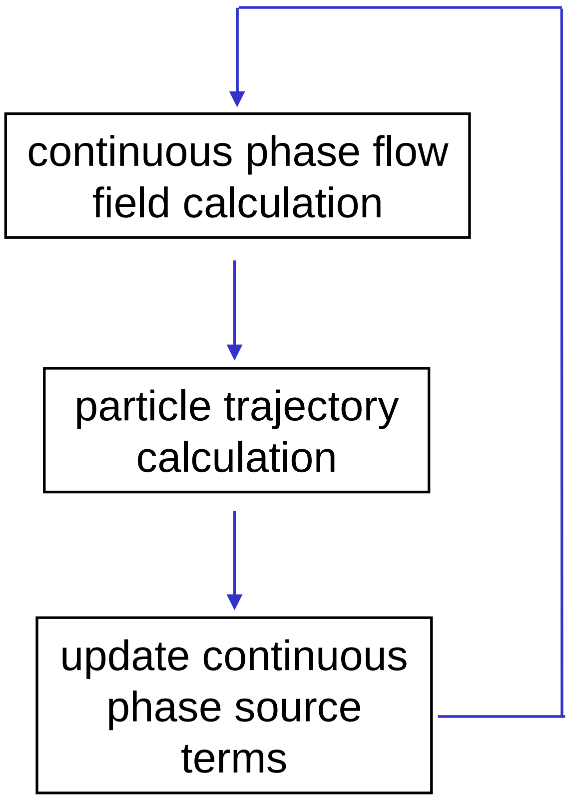


Coupling between phases

- One-way coupling:
  - Fluid phase influences particulate phase via drag and turbulence.
  - Particulate phase has no influence on the gas phase.
- Two-way coupling:
  - Fluid phase influences particulate phase via drag and turbulence.
  - Particulate phase influences fluid phase via source terms of mass, momentum, and energy.
  - Examples include:
    - Inert particle heating and cooling.
    - Droplet evaporation.
    - Droplet boiling.
    - Devolatilization.
    - Surface combustion.

Discrete phase model

- Trajectories of particles/droplets are computed in a Lagrangian frame.
  - Exchange (couple) heat, mass, and momentum with Eulerian frame gas phase.
- Discrete phase *volume* fraction should preferably be less than 10%.
  - *Mass* loading can be large (+100%).
  - No particle-particle interaction or break up.
- Turbulent dispersion modeled by:
  - Stochastic tracking.
  - Particle cloud model.
- Model particle separation, spray drying, liquid fuel or coal combustion, etc.


continuous phase flow field calculation

particle trajectory calculation

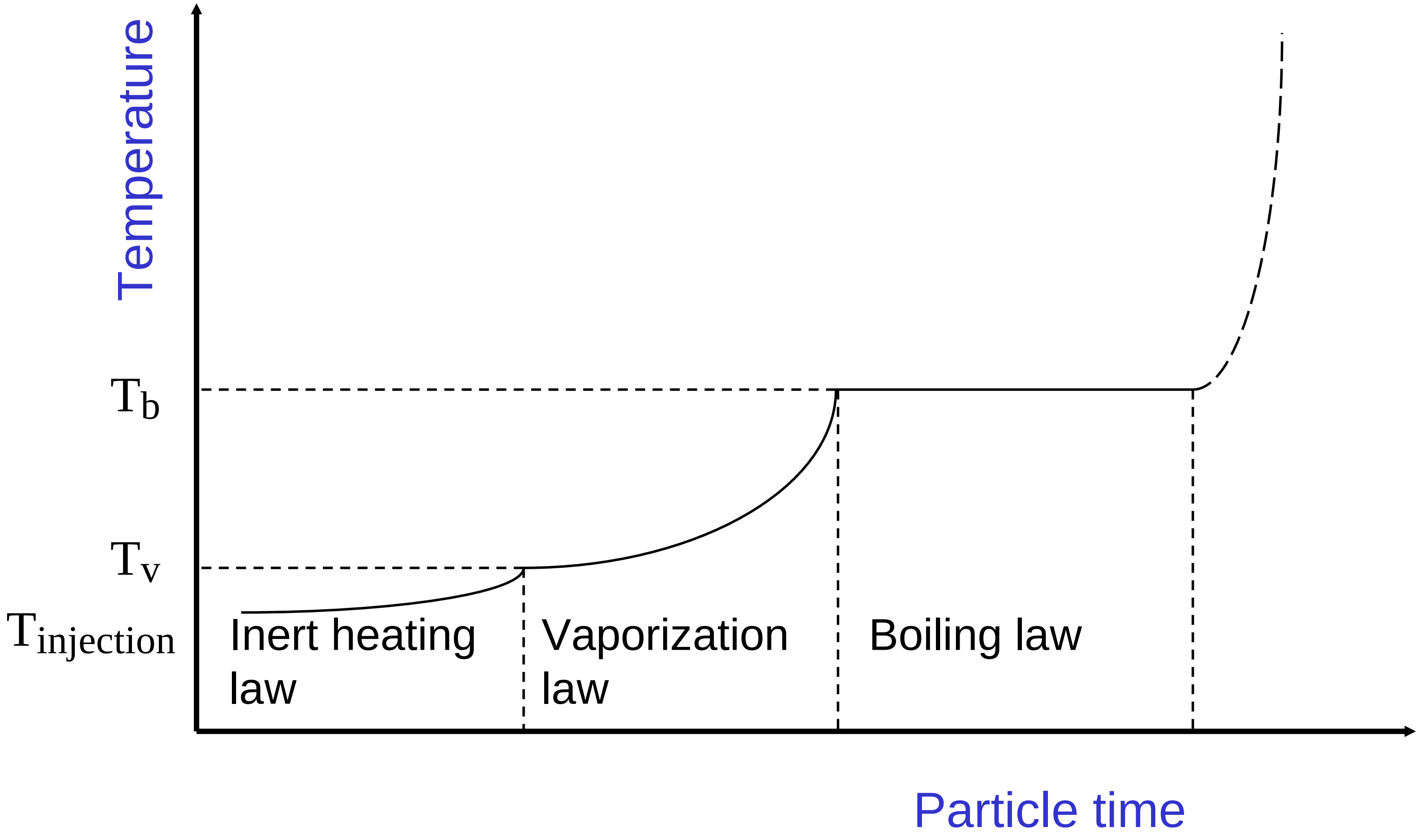
update continuous phase source terms

Particle types

- Particle types are inert, droplet and combusting particle.

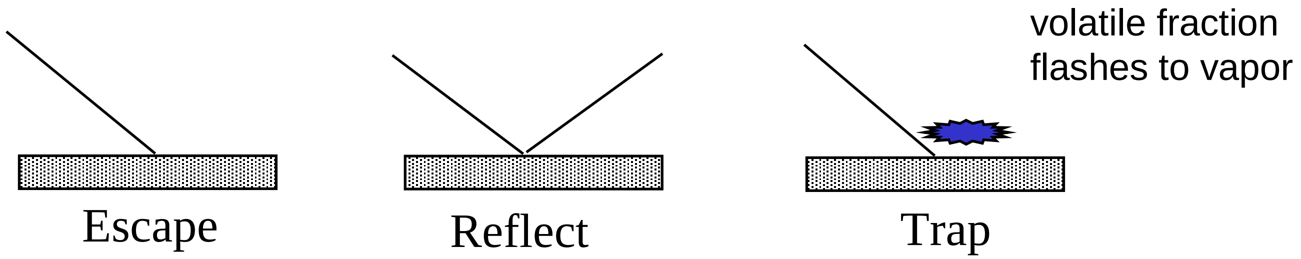
Particle Type	**Description**
Inert.	Inert/heating or cooling
Droplet (e.g. oil).	Heating/evaporation/boiling. Requires modeling of heat transfer and species.
Combusting (e.g. coal).	Heating. Evolution of volatiles/swelling. Heterogeneous surface reaction. Requires modeling of heat transfer and species.

Heat and mass transfer to a droplet



Particle-wall interaction

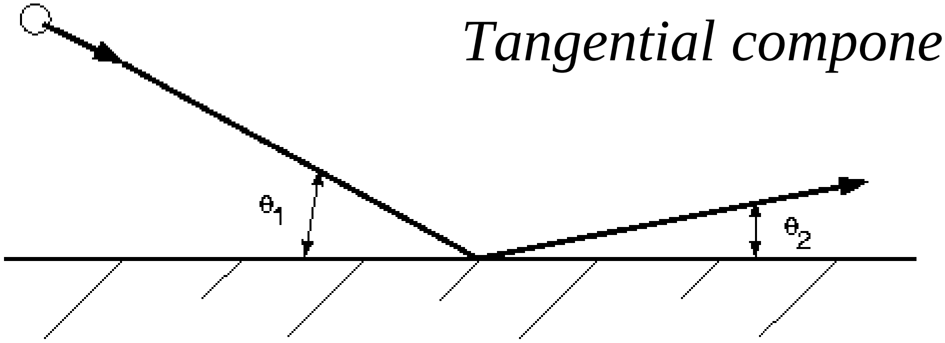
- Particle boundary conditions at walls, inlets, and outlets:



- For particle reflection, a restitution coefficient *e* is specified:

$$\textit{Normal component:}\ \ e_n = \frac{v_{2,n}}{v_{1,n}}$$

$$\textit{Tangential component:}\ \ e_t = \frac{v_{2,t}}{v_{1,t}}$$



Particle fates

- “Escaped” trajectories are those that terminate at a flow boundary for which the “escape” condition is set.
- “Incomplete” trajectories are those that were terminated when the maximum allowed number of time steps was exceeded.
- “Trapped” trajectories are those that terminate at a flow boundary where the “trap” condition has been set.
- “Evaporated” trajectories include those trajectories along which the particles were evaporated within the domain.
- “Aborted” trajectories are those that fail to complete due to numerical/round-off reasons. If there are many aborted particles, try to redo the calculation with a modified length scale and/or different initial conditions.

Turbulent dispersion of particles

- Dispersion of particles due to turbulent fluctuations in the flow can be modeled using either:
  - Stochastic tracking (discrete random walk).
  - Particle cloud model.
- Turbulent dispersion is important because:
  - Physically more realistic (at an added computational expense).
  - Enhances stability by smoothing source terms and eliminating local spikes in coupling to the gas phase.

Turbulence: discrete random walk tracking

- Each injection is tracked repeatedly in order to generate a statistically meaningful sampling.
- Mass flow rates and exchange source terms for each injection are divided equally among the multiple stochastic tracks.
- Turbulent fluctuations in the flow field are represented by defining an instantaneous fluid velocity:

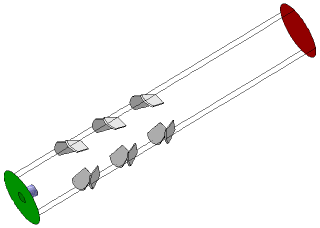
$$u_i = \overline{u_i} + u'_i$$

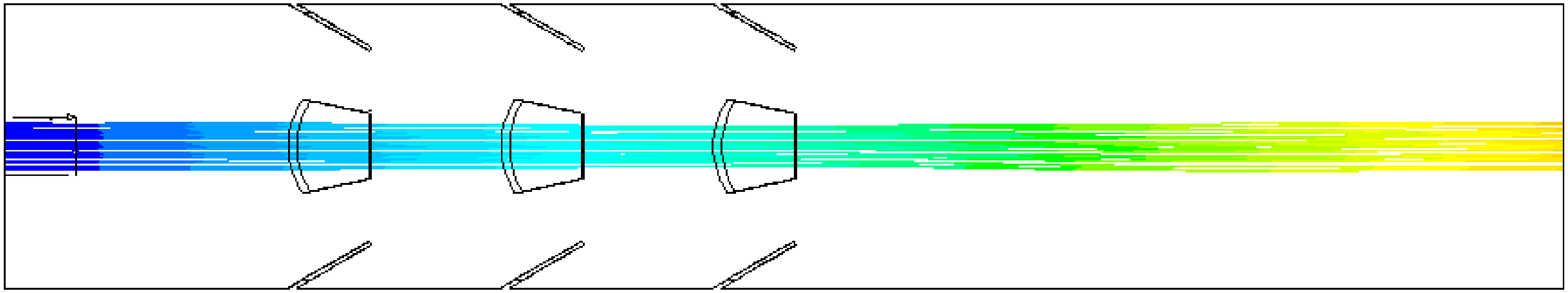
- where u'_i is derived from the local turbulence parameters:

$$u'_i = \varsigma \sqrt{\frac{2k}{3}}$$

- and ς is a normally distributed random number.

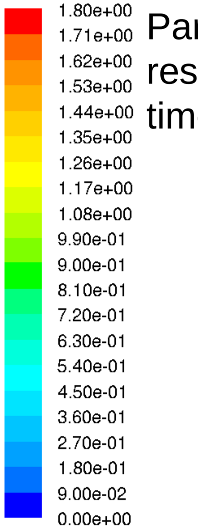
Stochastic tracking – static mixer

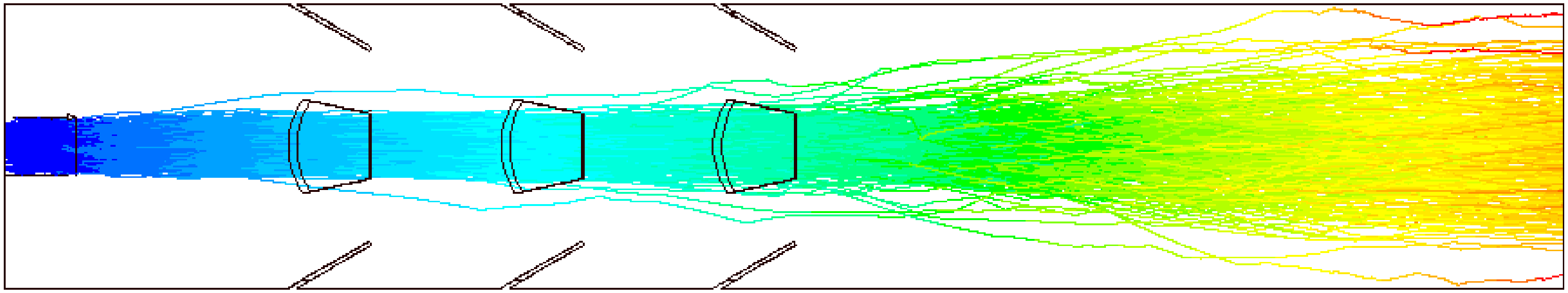




- Stochastic tracking turned off.
- One track per injection point.
- Uses steady state velocities only and ignores effect of turbulence.

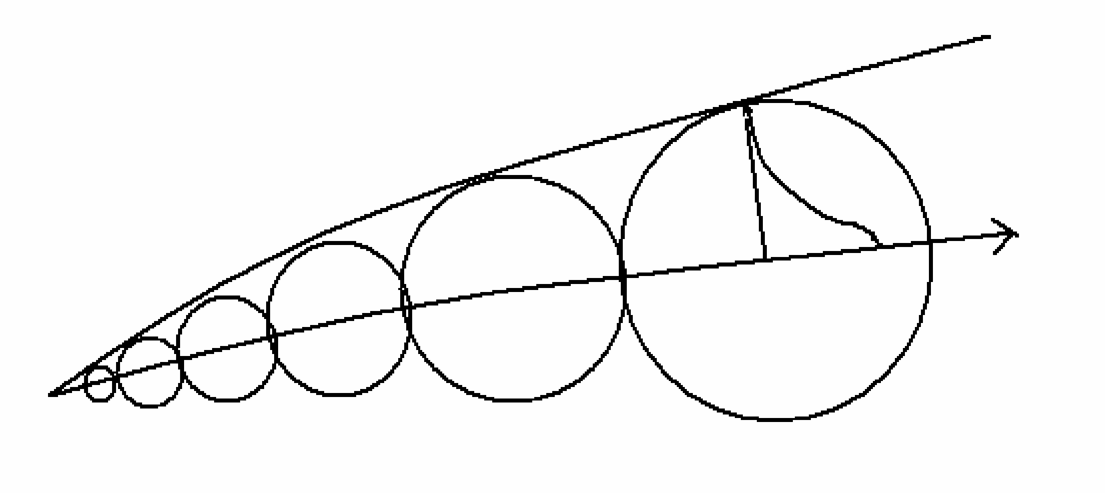
- Stochastic tracking turned on.
- Ten tracks per injection point.
- Adds random turbulent dispersion to each track.
- Tracks that start in the same point are all different.





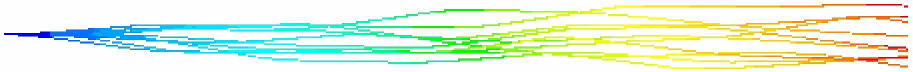
Turbulence: cloud tracking

- Uses statistical methods to trace the turbulent dispersion of particles about a mean trajectory.
- Calculate mean trajectory from the ensemble average of the equations of motion for the particles represented in the cloud.
- Distribution of particles inside the cloud is represented by a Gaussian probability density function.

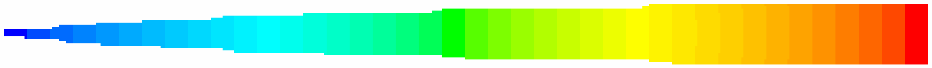


Stochastic vs. cloud tracking

- Stochastic tracking:



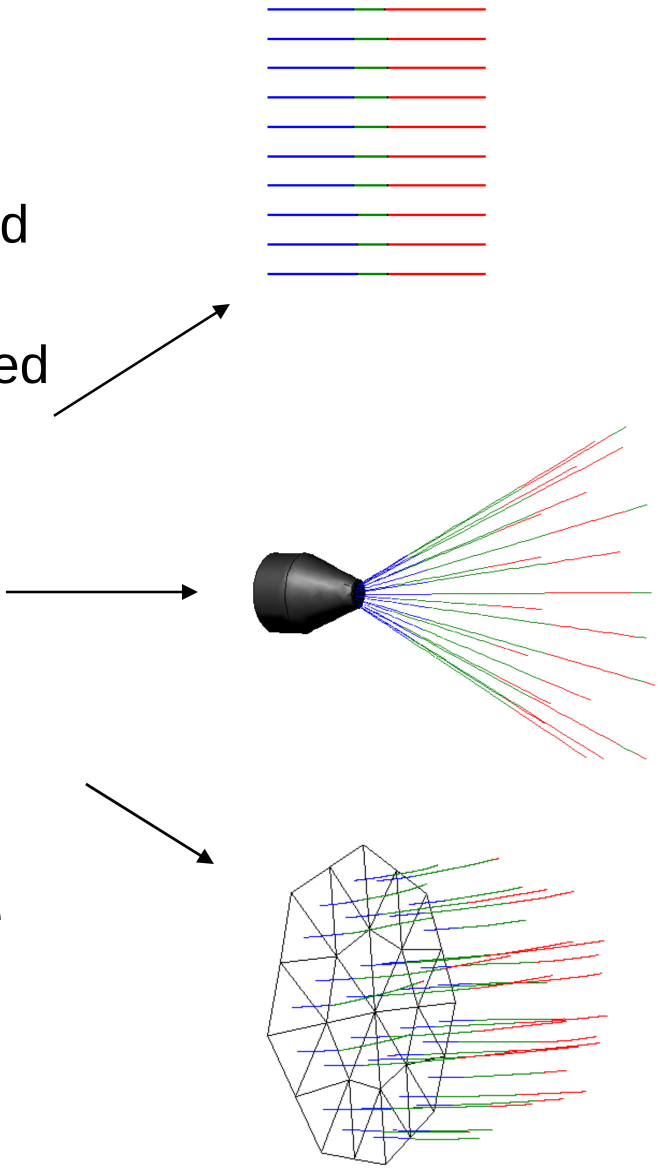
  - Accounts for local variations in flow properties.
  - Requires a large number of stochastic tries in order to achieve a statistically significant sampling (function of grid density).
  - Insufficient number of stochastic tries results in convergence problems due to non-smooth particle source term distributions.
  - Recommended for use in complex geometry.
- Cloud tracking:



  - Local variations in flow properties get averaged inside the particle cloud.
  - Smooth distributions of particle coupling source terms.
  - Each diameter size requires its own cloud trajectory calculation.

Injection set-up

- Injections may be defined as:
  - Single: a particle stream is injected from a single point.
  - Group: particle streams are injected along a line.
  - Cone: (3-D) particle streams are injected in a conical pattern.
  - Surface: particle streams are injected from a surface (one from each face).
  - File: particle streams injection locations and initial conditions are read in from an external file.



Injection definition

- Every injection definition includes:
  - Particle type (inert, droplet, or combusting particle).
  - Material (from data base).
  - Initial conditions (except when read from a file).
- Combusting particles and droplets require definition of destination species.
- Combusting particles may include an evaporating material.
- Turbulent dispersion may be modeled by stochastic tracking.

Solution strategy: particle tracking

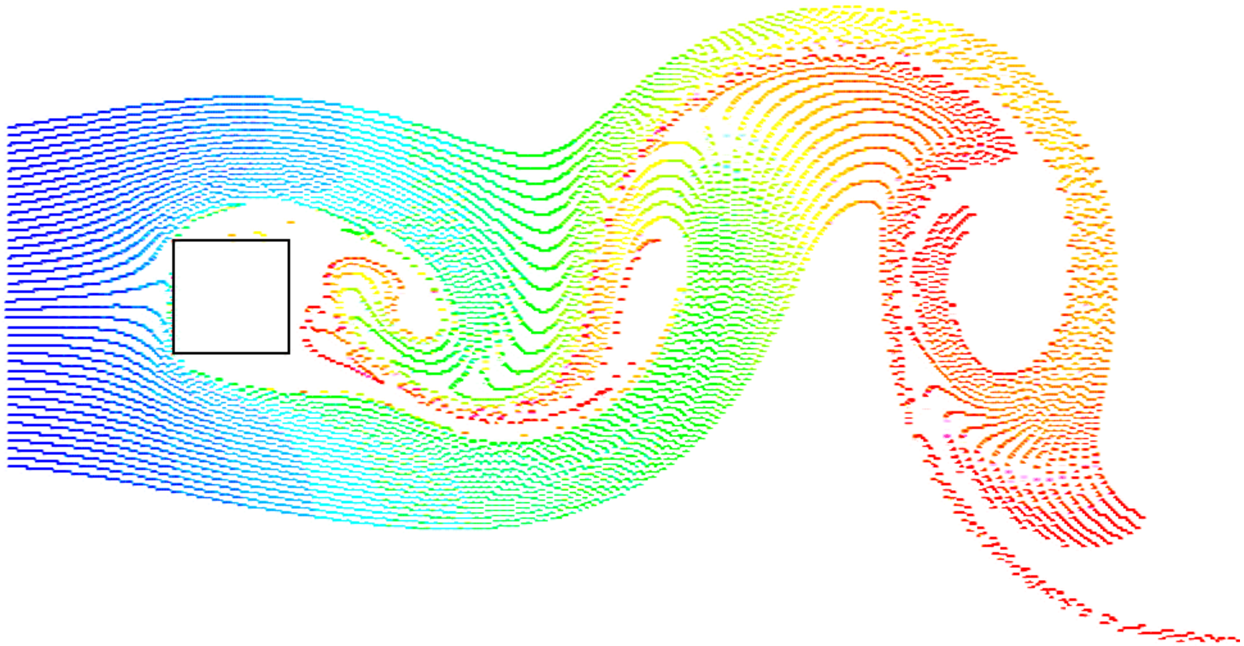
- Cell should be crossed in a minimum of two or three particle steps. More is better.
- Adjust step length to either a small size, or 20 or more steps per cell.
- Adjust “Maximum Number of Steps.”
- Take care for recirculation zones.
- Heat and mass transfer: reduce the step length if particle temperature wildly fluctuates at high vaporization heats.

Solution strategy: coupled calculation

- Two strategies possible:
  - Closer coupling between dispersed and continuous flow:
    - Increase underrelaxation for discrete phase.
    - Decrease number of continuous phase calculations between trajectory calculations to less than three.
    - Reduce underrelaxation factors for continuous phase.
  - Decoupling of dispersed and continuous flow:
    - Reduce underrelaxation factor for discrete phase.
    - Increase number of continuous phase calculations between trajectory calculations to more than fifteen.
- Smooth out particle source terms.
  - Increase number of particle trajectories.

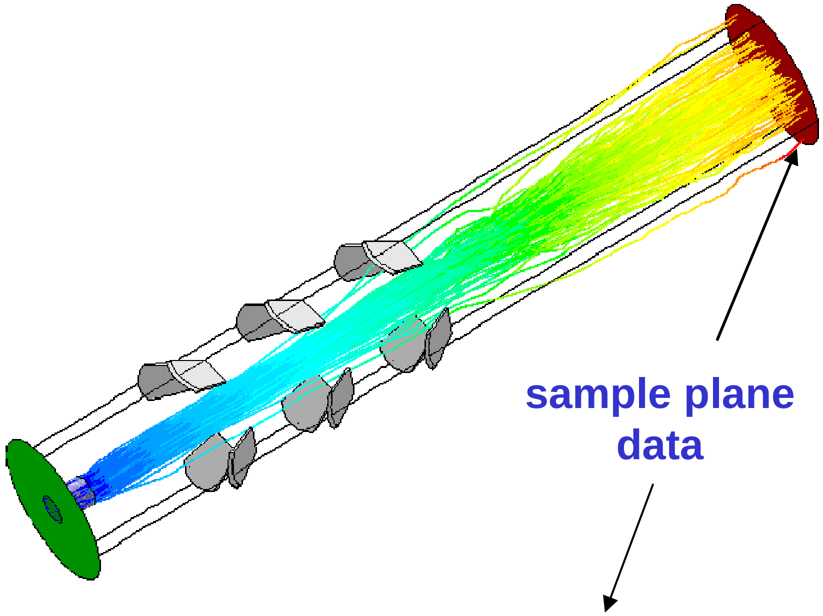
Particle tracking in unsteady flows

- Each particle advanced in time along with the flow.
- For coupled flows using implicit time stepping, sub-iterations for the particle tracking are performed within each time step.
- For non-coupled flows or coupled flows with explicit time stepping, particles are advanced at the end of each time step.

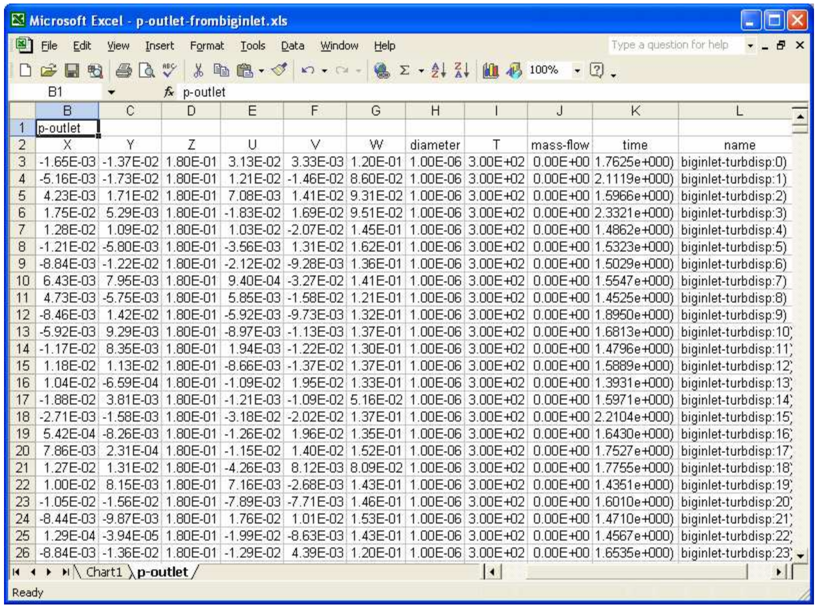


Sample planes and particle histograms

- Track mean particle trajectory as particles pass through sample planes (lines in 2D), properties (position, velocity, etc.) are written to files.
- These files can then be read into the histogram plotting tool to plot histograms of residence time and distributions of particle properties.
- The particle property mean and standard deviation are also reported.



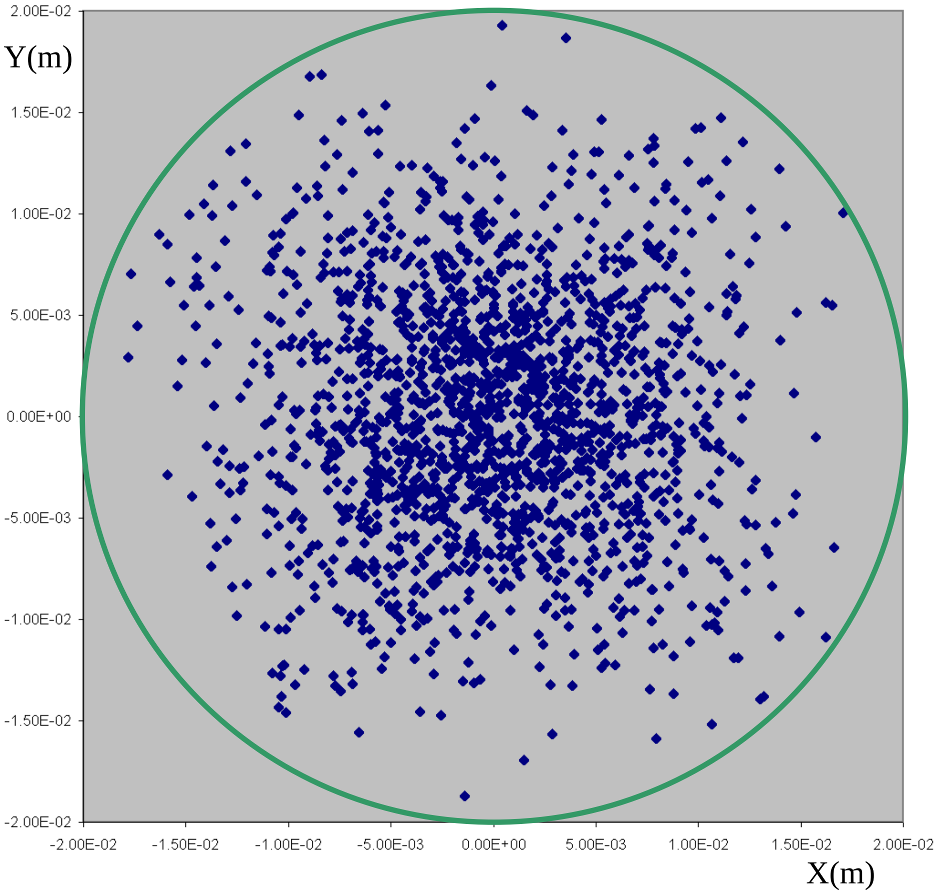
sample plane data



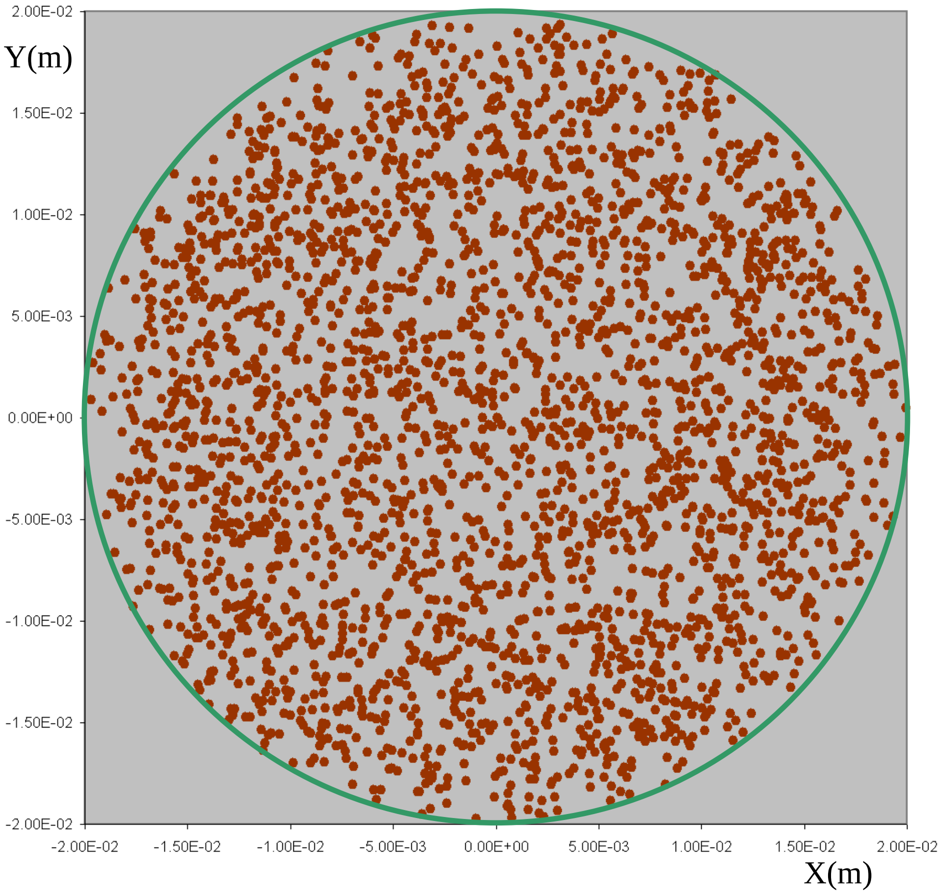
	B	C	D	E	F	G	H	I	J	K	L
1	p-outlet										
2	X	Y	Z	U	V	W	diameter	T	mass-flow	time	name
3	-1.65E-03	-1.37E-02	1.80E-01	3.13E-02	3.33E-03	1.20E-01	1.00E-06	3.00E+02	0.00E+00	1.7625e+000)	biginlet-turbdisp:0)
4	-5.16E-03	-1.73E-02	1.80E-01	1.21E-02	-1.46E-02	8.60E-02	1.00E-06	3.00E+02	0.00E+00	2.1119e+000)	biginlet-turbdisp:1)
5	4.23E-03	1.71E-02	1.80E-01	7.08E-03	1.41E-02	9.31E-02	1.00E-06	3.00E+02	0.00E+00	1.5966e+000)	biginlet-turbdisp:2)
6	1.75E-02	5.29E-03	1.80E-01	-1.83E-02	1.69E-02	9.51E-02	1.00E-06	3.00E+02	0.00E+00	2.3321e+000)	biginlet-turbdisp:3)
7	1.28E-02	1.09E-02	1.80E-01	1.03E-02	-2.07E-02	1.45E-01	1.00E-06	3.00E+02	0.00E+00	1.4862e+000)	biginlet-turbdisp:4)
8	-1.21E-02	-5.80E-03	1.80E-01	-3.56E-03	1.31E-02	1.62E-01	1.00E-06	3.00E+02	0.00E+00	1.5323e+000)	biginlet-turbdisp:5)
9	-8.84E-03	-1.22E-02	1.80E-01	-2.12E-02	-9.28E-03	1.36E-01	1.00E-06	3.00E+02	0.00E+00	1.5029e+000)	biginlet-turbdisp:6)
10	6.43E-03	7.95E-03	1.80E-01	9.40E-04	-3.27E-02	1.41E-01	1.00E-06	3.00E+02	0.00E+00	1.5547e+000)	biginlet-turbdisp:7)
11	4.73E-03	-5.75E-03	1.80E-01	5.85E-03	-1.58E-02	1.21E-01	1.00E-06	3.00E+02	0.00E+00	1.4525e+000)	biginlet-turbdisp:8)
12	-8.46E-03	1.42E-02	1.80E-01	-5.92E-03	-9.73E-03	1.32E-01	1.00E-06	3.00E+02	0.00E+00	1.8950e+000)	biginlet-turbdisp:9)
13	-5.92E-03	9.29E-03	1.80E-01	-8.97E-03	-1.13E-03	1.37E-01	1.00E-06	3.00E+02	0.00E+00	1.6813e+000)	biginlet-turbdisp:10
14	-1.17E-02	8.35E-03	1.80E-01	1.94E-03	-1.22E-02	1.30E-01	1.00E-06	3.00E+02	0.00E+00	1.4796e+000)	biginlet-turbdisp:11
15	1.18E-02	1.13E-02	1.80E-01	-8.66E-03	-1.37E-02	1.37E-01	1.00E-06	3.00E+02	0.00E+00	1.5889e+000)	biginlet-turbdisp:12
16	1.04E-02	-6.59E-04	1.80E-01	-1.09E-02	1.95E-02	1.33E-01	1.00E-06	3.00E+02	0.00E+00	1.3931e+000)	biginlet-turbdisp:13
17	-1.88E-02	3.81E-03	1.80E-01	-1.21E-03	-1.09E-02	5.16E-02	1.00E-06	3.00E+02	0.00E+00	1.5971e+000)	biginlet-turbdisp:14
18	-2.71E-03	-1.58E-03	1.80E-01	-3.18E-02	-2.02E-02	1.37E-01	1.00E-06	3.00E+02	0.00E+00	2.2104e+000)	biginlet-turbdisp:15
19	5.42E-04	-8.26E-03	1.80E-01	-1.26E-02	1.96E-02	1.35E-01	1.00E-06	3.00E+02	0.00E+00	1.6430e+000)	biginlet-turbdisp:16
20	7.86E-03	2.31E-04	1.80E-01	-1.15E-02	1.40E-02	1.52E-01	1.00E-06	3.00E+02	0.00E+00	1.7527e+000)	biginlet-turbdisp:17
21	1.27E-02	1.31E-02	1.80E-01	-4.26E-03	8.12E-03	8.09E-02	1.00E-06	3.00E+02	0.00E+00	1.7755e+000)	biginlet-turbdisp:18
22	1.00E-02	8.15E-03	1.80E-01	7.16E-03	-2.68E-03	1.43E-01	1.00E-06	3.00E+02	0.00E+00	1.4351e+000)	biginlet-turbdisp:19
23	-1.05E-02	-1.56E-02	1.80E-01	-7.89E-03	-7.71E-03	1.46E-01	1.00E-06	3.00E+02	0.00E+00	1.6010e+000)	biginlet-turbdisp:20
24	-8.44E-03	-9.87E-03	1.80E-01	1.76E-02	1.01E-02	1.53E-01	1.00E-06	3.00E+02	0.00E+00	1.4710e+000)	biginlet-turbdisp:21
25	1.29E-04	-3.94E-05	1.80E-01	-1.99E-02	-8.63E-03	1.43E-01	1.00E-06	3.00E+02	0.00E+00	1.4567e+000)	biginlet-turbdisp:22
26	-8.84E-03	-1.36E-02	1.80E-01	-1.29E-02	4.39E-03	1.20E-01	1.00E-06	3.00E+02	0.00E+00	1.6535e+000)	biginlet-turbdisp:23

Particle locations at outlet (HEV)

- Flow following particles.



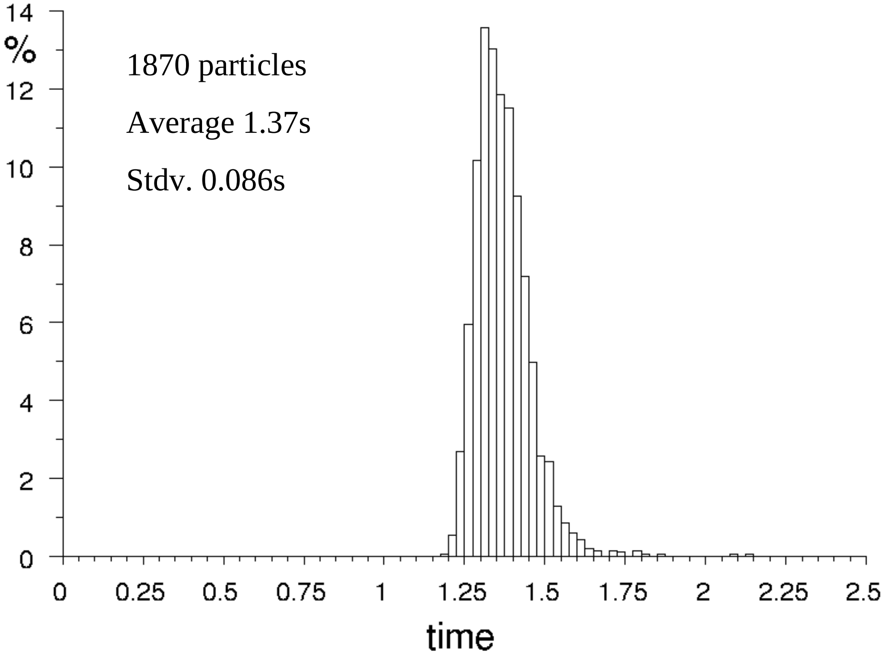
Particles from small center inlet



Particles from large outer inlet

Residence time distribution

- Residence time histograms can be made from particle times at outlet for flow following particles.
- For this mixer, volume is 0.275 l, total volumetric flow rate is 0.152 l/s, and an average residence time of 1.8 s is expected.

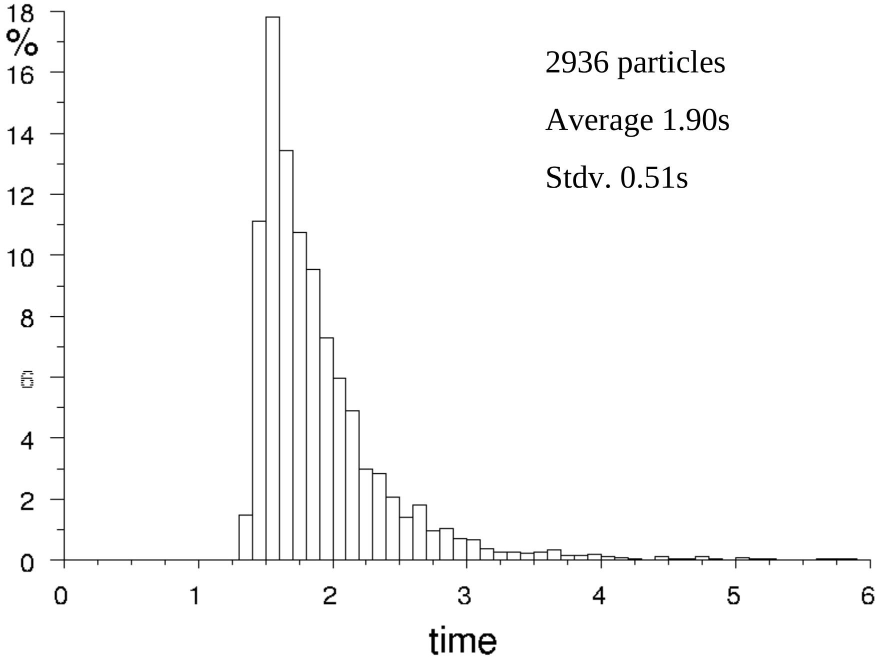


1870 particles

Average 1.37s

Stdv. 0.086s

Particles from small center inlet



2936 particles

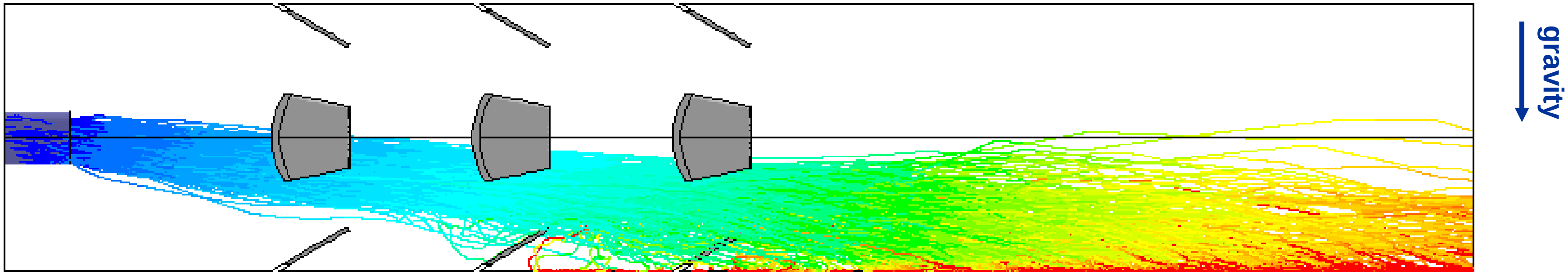
Average 1.90s

Stdv. 0.51s

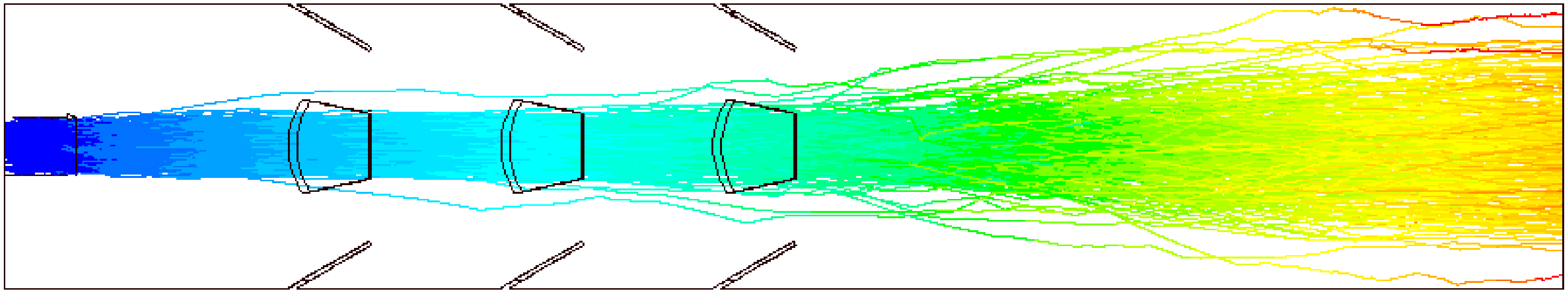
Particles from large outer inlet

Effect of particle properties

- Sand particles (0.2mm, 2000 kg/m^3).

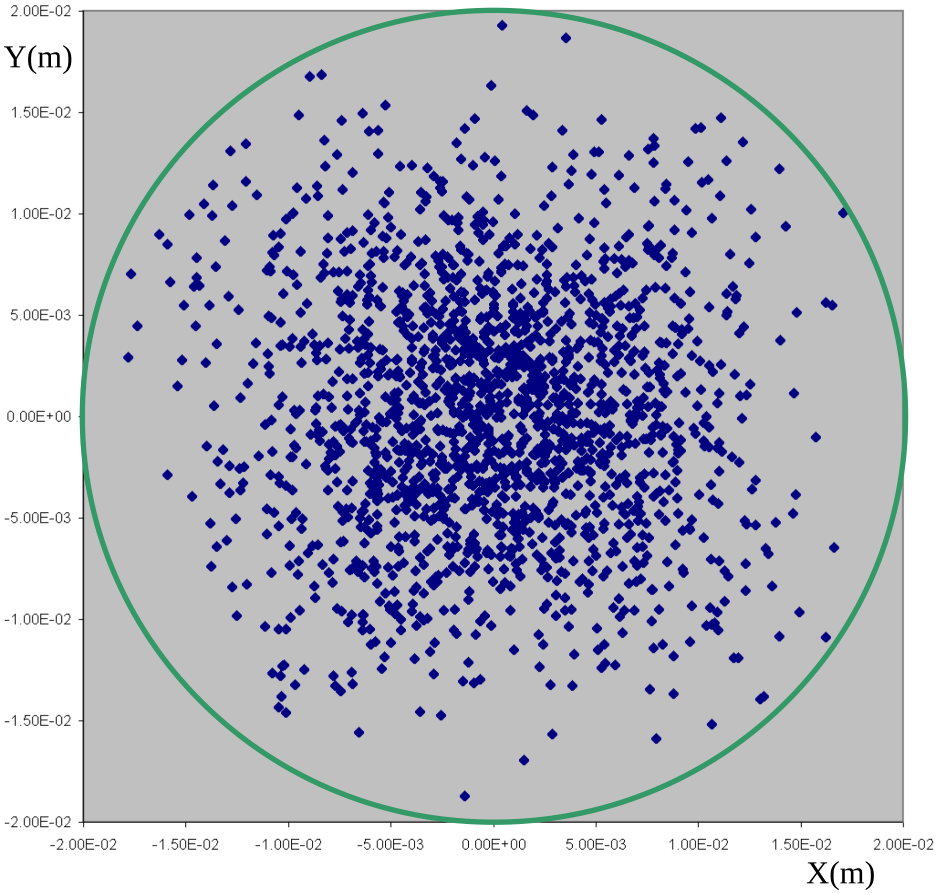


- Flow following particles.

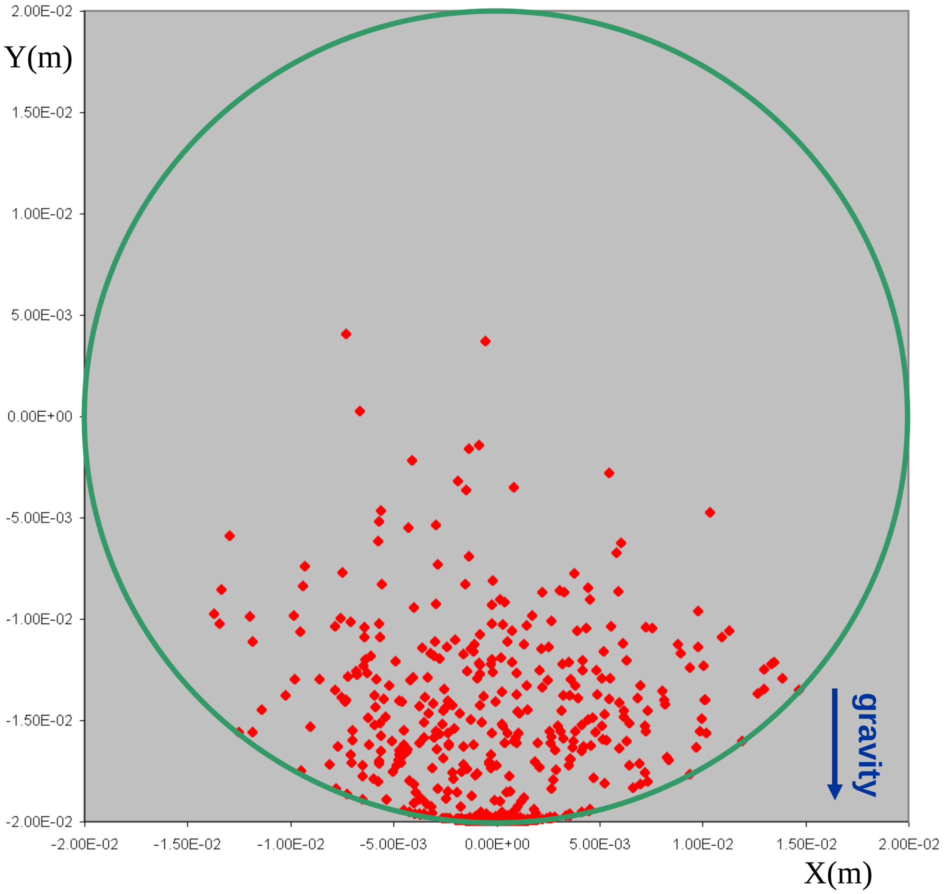


Effect of particle properties

- Flow following particles.
- Sand particles (in water).



Particles from small center inlet



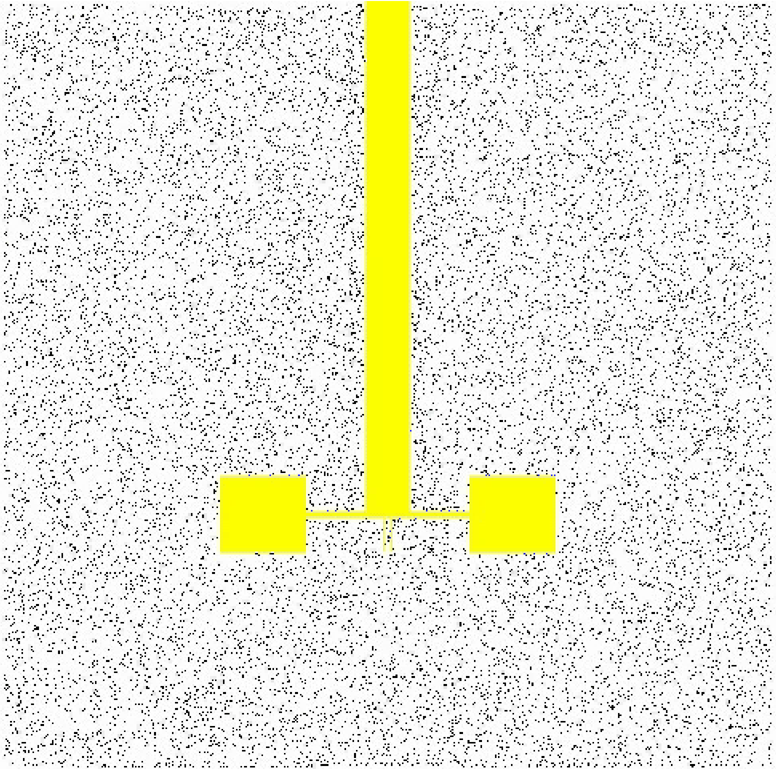
Particles from small center inlet.

Massive particle tracking

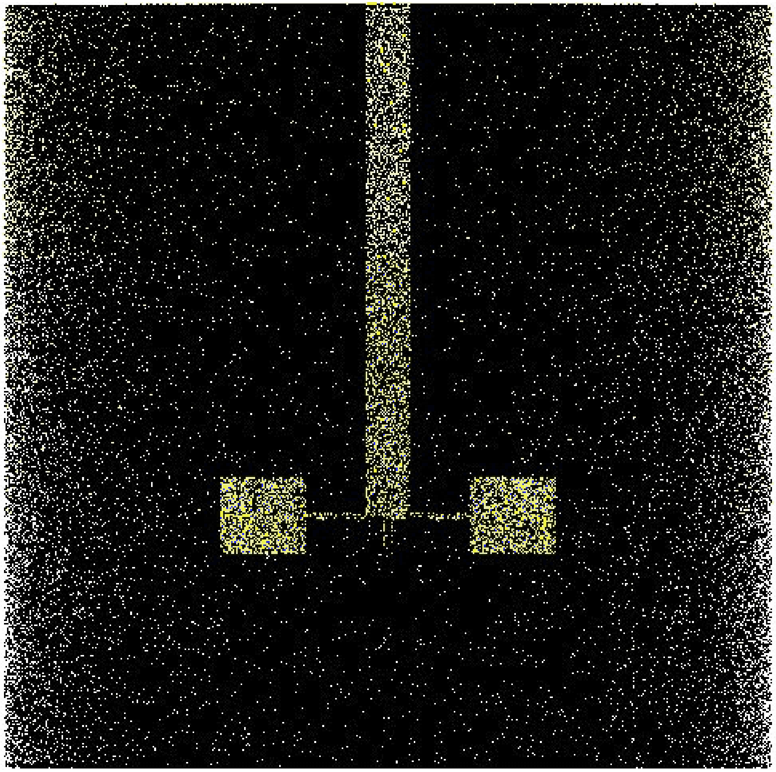
- Massive particle tracking refers to analyses where tens of thousands to millions of particles are tracked to visualize flows or to derive statistics of the flow field.
- Examples:
  - An unbaffled mixing tank with a Rushton turbine.
  - An unbaffled mixing tank with four A310 impellers.
  - A static mixer.

Lattice-Boltzmann Method

- Calculations by Jos Derksen, Delft University, 2003.
- Unbaffled stirred tank equipped with a Rushton turbine.



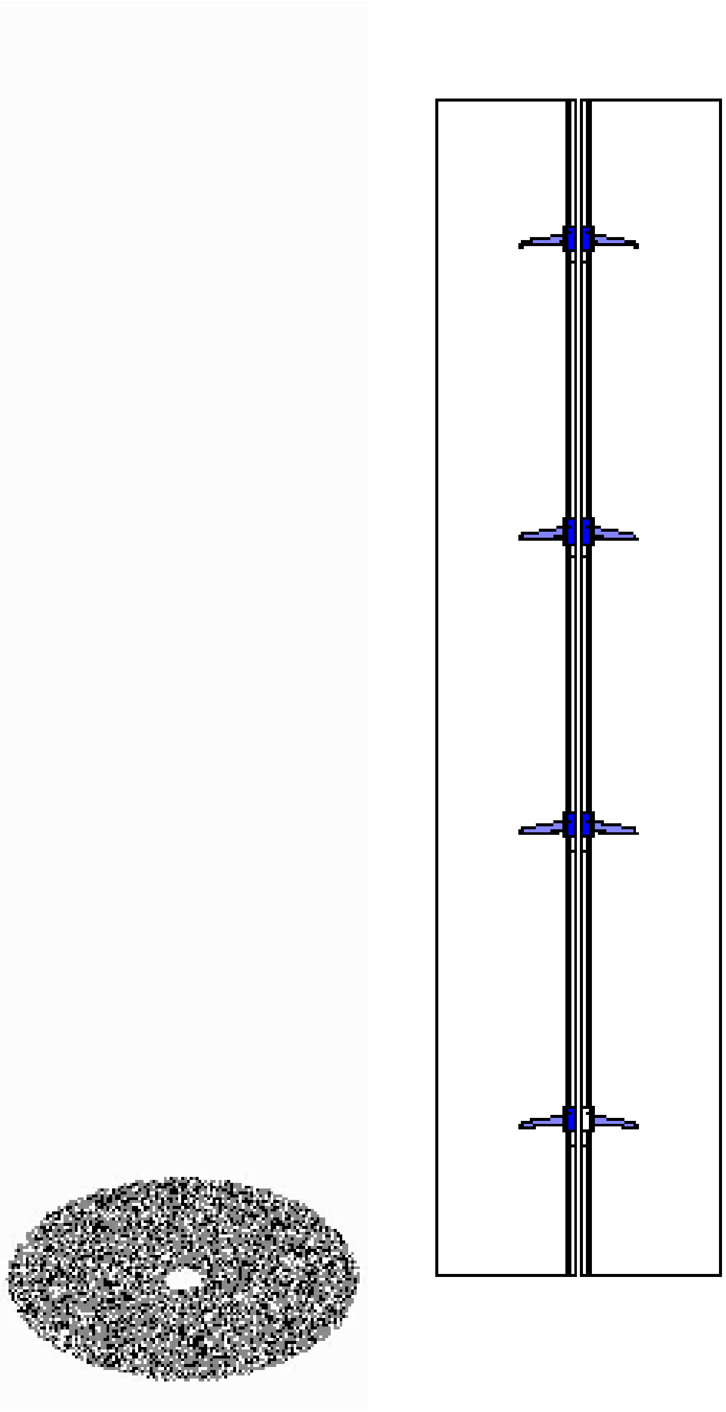
Cross Section



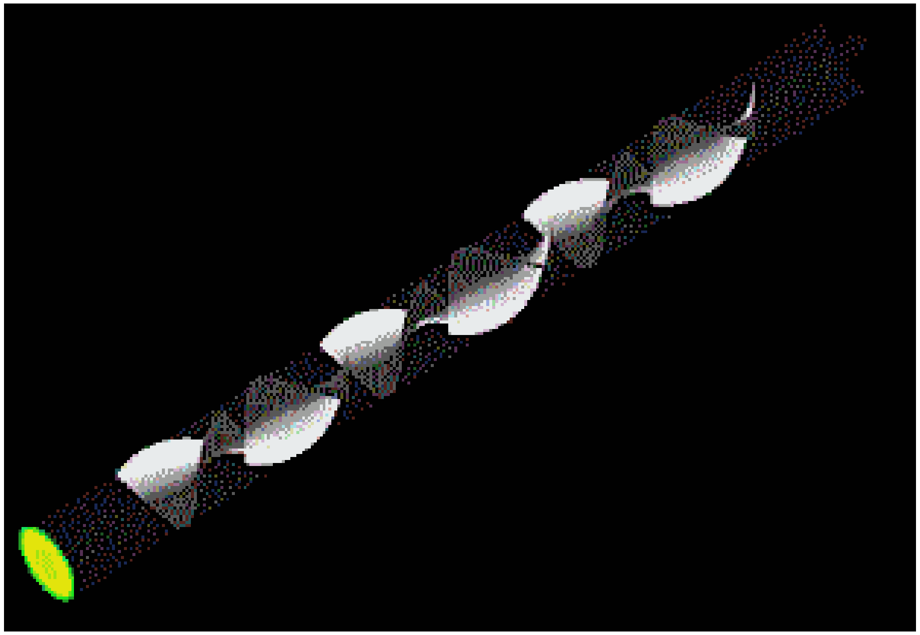
Vessel Wall

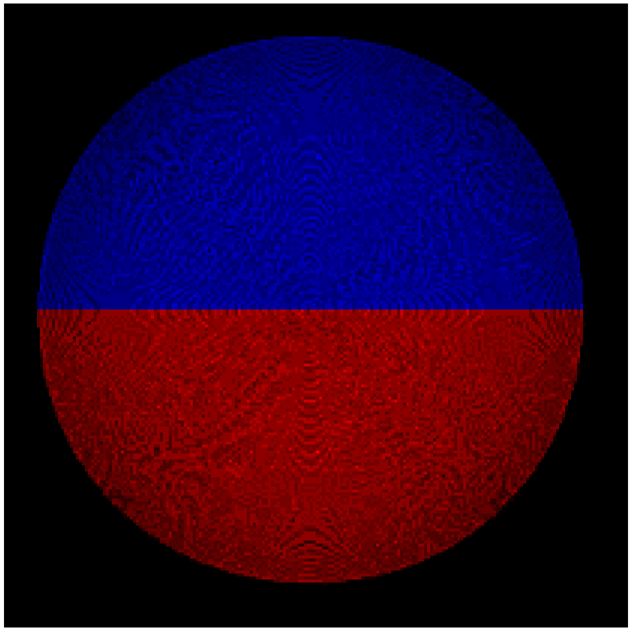
Lattice-Boltzmann Method

- Calculations by Jos Derksen, Delft University, 2003.
- Unbaffled stirred tank equipped with four impellers.



Particle tracking animations





Particle tracking accuracy

- There are three types of errors: discretization, time integration, and round-off.
- Research has shown that in regular laminar flows the error in the particle location increases as t^2, and in chaotic flows almost exponentially.
- Errors tend to align with the direction of the streamlines in most flows.
- As a result, even though errors multiply rapidly (e.g. 0.1% error for 20,000 steps is $1.001^{20,000}$ = 4.8E8), qualitative features of the flow as shown by the deformation of material lines can be properly reproduced. But the length of the material lines may be of by as much as 100%.
- Overall, particle tracking, when properly done, is less diffusive than solving for species transport, but numerical diffusion does exist.

Summary

- There are different main ways to model material transport:
  - Multiphase flow: multiple momentum equations.
  - Species flow: one set of momentum equations.
  - Discrete phase modeling (DPM; particle tracking): one set of momentum equations for the fluid flow. Additional force balance for the individual particles.
- Species mixing:
  - Material distribution, mixing parameters.
  - Basis for chemical reaction calculations.
- DPM:
  - Heat and mass transfer from particles.
  - Mixing analysis.
  - Unlike species, do not necessarily follow fluid flow exactly.