Stochastic models for turbulent particle dispersion in general inhomogeneous flows

A. Dehbi
Paul Scherrer Institut
Switzerland

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Outline

- Background. Why stochastic models?
- Discrete random walk model (DRW). Shortcomings
- Continuous random walk (CRW) based on the Langevin equation
  - Standard Langevin equation
  - Non-dimensional Langevin equation
- Sample results of the CRW model
  - Isothermal flows
  - Flows with thermal gradients (active thermophoresis)
- Concluding remarks

Particles-turbulence: applications

- Particle-turbulence interactions play a crucial role in wide range of applications
  - Atmospheric dispersion of pollutants
  - Sediment transport in rivers
  - Drug delivery in human airways
  - Combustion
  - Fouling in compressor and turbine blades
  - Chemical pulping
  - Nuclear fission products transport

- “Turbulence has a strong influence on plankton contact rate, which is a crucial parameter for plankton ecology”. ☺

Recent paper in J. Marine Systems

Background

- CFD method increasingly successful in prediction of turbulent flows in general geometries
- Particle dispersion in CFD codes predicted using:
  - Eulerian two-fluid methods
    - Particles regarded as continuous phase with own averaged equations (mass, momentum, etc)
    - Better suited for denser suspensions when particle-particle interactions important
    - Main challenges: defining interphasial exchange terms, boundary conditions
  - Lagrangian particle tracking (LPT)
    - One solves first for the continuous phase (Eulerian)
    - Then: one follows paths of a “large” sample of particles by integration of Newton’s 2nd Law

Lagrangian methods: Pros & Cons

- Pros:
  - Rigorous and intuitive inclusion of all relevant forces on particle (e.g. drag, gravity, thermophoretic force, etc)
  - Rigorous and intuitive treatment of boundary conditions
  - More appropriate for dispersed flows, with low particle loading

- Cons:
  - Computational expense: Necessary to track a large number of particles until stationary statistics are achieved

Background

- CFD with LPT successful in predicting laminar flows
- In turbulent flows, DNS and LES coupled to LPT offer most rigorous way of treating particle dispersion in Euler/Lagrange frameworks. However:
  - Very time consuming
  - Difficult (sometimes impossible) to apply in general geometries
  - Want quick answers with “good enough” accuracy using today’s CFD codes
- In past, CFD-LPT treatment in turbulent flows has showed unsatisfactory accuracy due to:
  - Inappropriate modeling of turbulence seen by particles
  - Rather rough assumptions e.g. turbulence isotropic in whole domain
- Recent advances in stochastic models and coupling to CFD codes offer hope for a good compromise between accuracy and computer expense

Particle-Turbulence interactions in LPT

- Supposing drag is the only significant force on the particle. The particle path is extracted from:

$$\frac{dU_p}{dt} = F_D(U - U_p), \quad F_D = \frac{18\mu}{\rho_p d_p^2} C_D \frac{\text{Re}}{24}, \qquad \text{Re} = \frac{\rho_p d_p |U - U_p|}{\mu}$$

- A major issue in Lagrangian particle tracking: modeling fluid turbulence.

$$U = \overline{U} + u$$

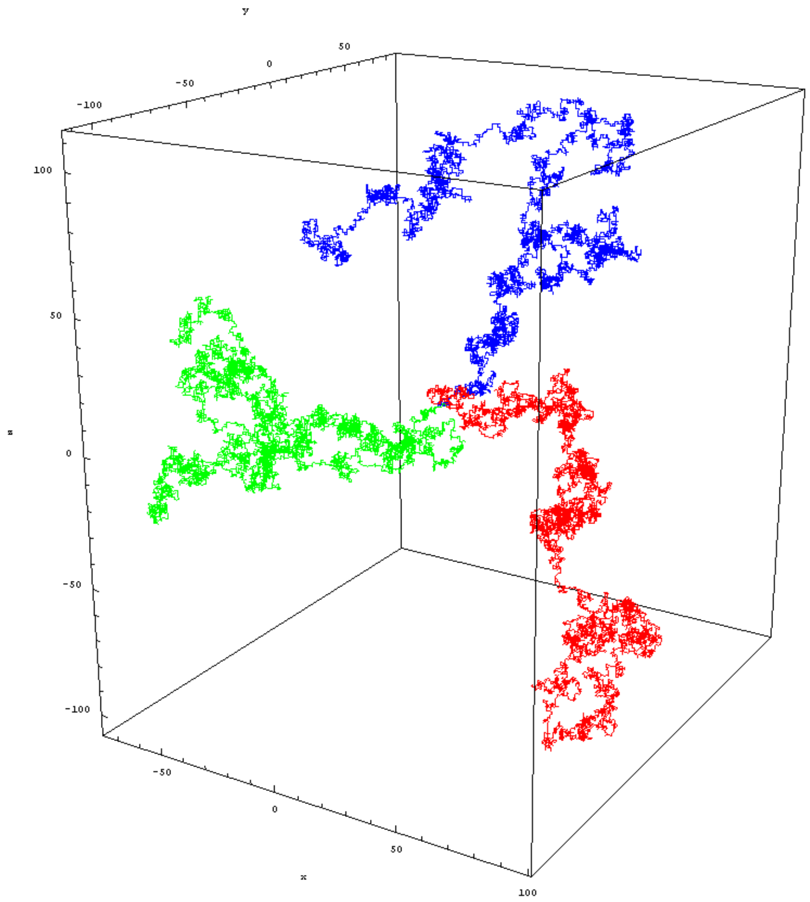
u ← To be modeled

$\overline{U}$ ← *CFD*

- RANS turbulent models in CFD produce *averaged* fluid field quantities
- How to extract instantaneous fields from averaged fields? **Stochastic models**

Random Walk Models: preview

- Premise:
  - A random walk model consisting of a large number of statistically independent steps is suitable to represent the chaotic nature of turbulent diffusion
- The mean flow equations solved analytically/numerically (CFD-RANS)
- Turbulence modeled with a random walk model
  - Discrete Random Walk
  - Continuous Random Walk



Discrete Random Walk (DRW) Model

- Also known as Eddy Interaction Model (EIM). Due to Gosman et al., 1983
- Particle interacts with turbulence in “Discrete Random Walks”
  - Particle is “trapped” by an eddy during an “eddy lifetime”

$$\tau_e = 2 \cdot \tau_L = 2 \cdot C_L \frac{k}{\varepsilon}$$

  - During the lifetime of the eddy:
    - The mean fluid velocities seen by the particle are those of the fluid
    - The fluctuating fluid components are randomly distributed Gaussian variables whose rms value are equal and deduced from the turbulent kinetic energy *k*:

$$\sqrt{\overline{u'^2}} = \sqrt{\overline{v'^2}} = \sqrt{\overline{w'^2}} = \sqrt{2k/3}$$

    - The instantaneous fluid velocity seen by a particle is: $u_i' = \lambda_i \sqrt{\overline{u_i'^2}}$
    - λ’s are Gaussian random variables with 0 mean and standard deviation 1

Discrete Random Walk (DRW) Model

- Integrate trajectory until eddy life is over
- When the eddy lifetime is over, generate another eddy with random rms of velocity
- The particle trajectory is determined by the Lagrangian tracking

$$\frac{d\mathbf{x}_p}{dt} = U_p$$

$$m_p \frac{dU_p}{dt} = \mathbf{f} = \mathbf{f}_{Drag} + \mathbf{f}_{Gravity} + \mathbf{f}_{thermophoresis} + \mathbf{f}_{lift} + ...$$

- In 3D: trajectory obtained by integrating 6 coupled ODE's
- Tacking is continued until particle is hits the wall or leaves domain

Typical Discrete Random Walk Trajectory

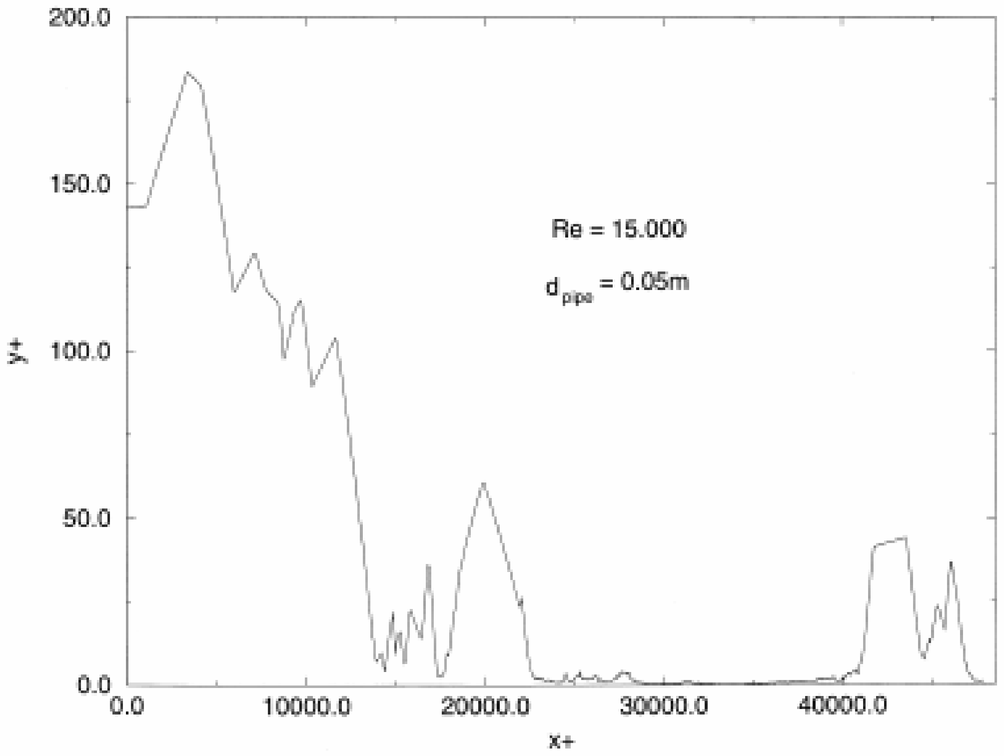
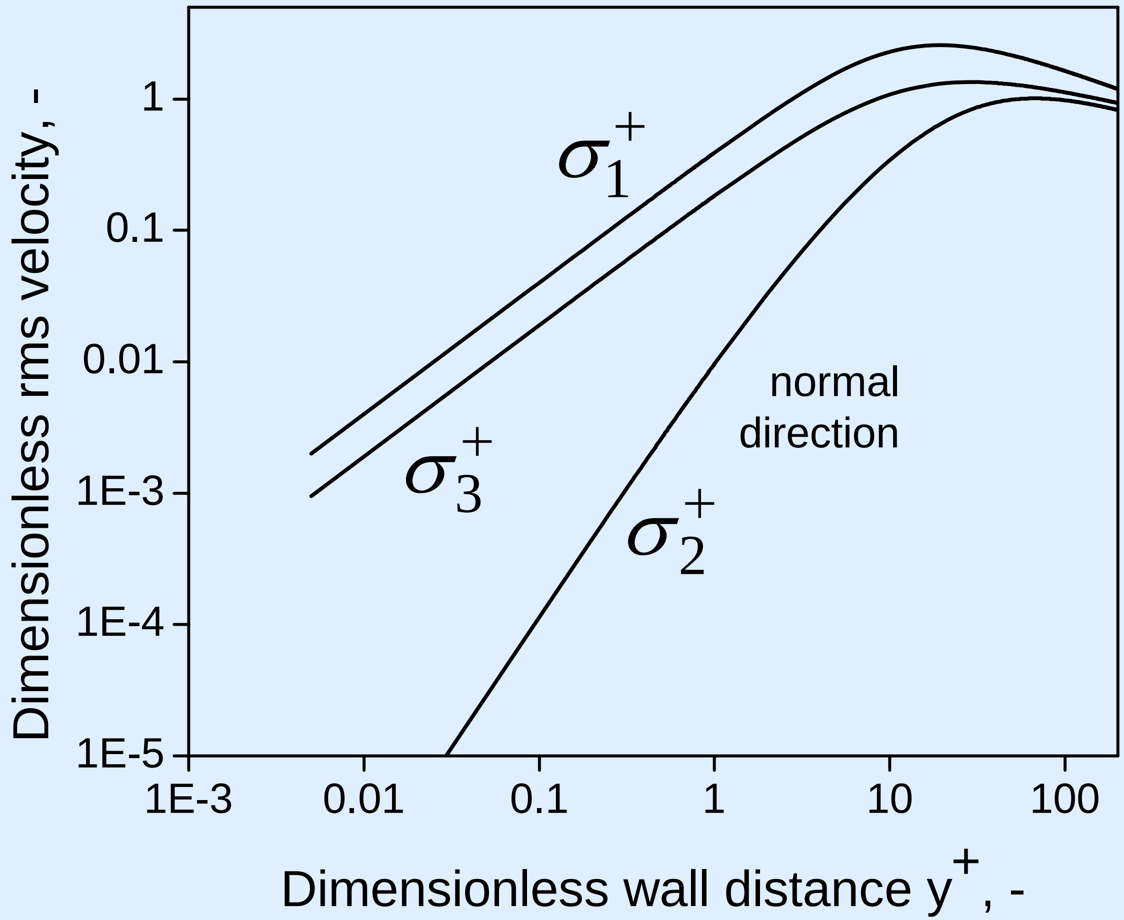


Fig. 1. Typical particle trajectory in the boundary layer of turbulent pipe flow: $\tau_p^+ = 0.02$; initial velocity $u_x^+ = 18$, $v_x^+ = 12$.

Shortcomings of original DRW model

- Many practical flows can be approximated as having isotropic turbulence in the *bulk*
- However: turbulence is very anisotropic in boundary layers
- In presence of walls, particle deposition dictated by phenomena in boundary layer
- Thus: Original DRW prediction of deposition is poor even in simple geometries (always strong over-prediction of deposition)
- Better treatment of boundary layer effects is required because of:
  - Anisotropy
  - Different time scales

Turbulent velocity scales in boundary layer



DNS fits in channel flows at Re=2100. (Courtesy Marchioli & Soldati, 2007)

Improvement of DRW: boundary layer model

- Keep default model as is as long as particle in the bulk ($y^+ > 100$)
- If particle in boundary layer ($y^+ < 100$) introduce rms values of gas velocities obtained from curve fits of DNS data in channel flow:

$$\sigma_1 \equiv \sqrt{\overline{u'^2}} = \frac{0.40 \cdot y^+}{1 + 0.0239 (y^+)^{1.496}} \cdot u^*$$ (streamwise direction)

$$\sigma_2 \equiv \sqrt{\overline{v'^2}} = \frac{0.0116 \cdot (y^+)^2}{1 + 0.203 \cdot y^+ + 0.00140 (y^+)^{2.421}} \cdot u^*$$ (normal direction to wall)

$$\sigma_3 \equiv \sqrt{\overline{w'^2}} = \frac{0.19 \cdot y^+}{1 + 0.0361 (y^+)^{1.322}} \cdot u^*$$ (spanwise direction)

with the friction velocity $u^* = \sqrt{\frac{\tau_w}{\rho}}$

Times scales

- Lagrangian time scale of fluid particle defined as:

$$R_{u_i}(\tau) = \frac{\overline{u_i(t)u_i(t+\tau)}}{\overline{u_i(t)u_i(t)}}$$

← Computed from LPT-DNS of fluid particles & ensemble averaging

$$\tau_L = \int_0^\infty R_{u_i}(\tau)d\tau$$

← τ_L: typical time before particle loses memory of its history. Velocities are

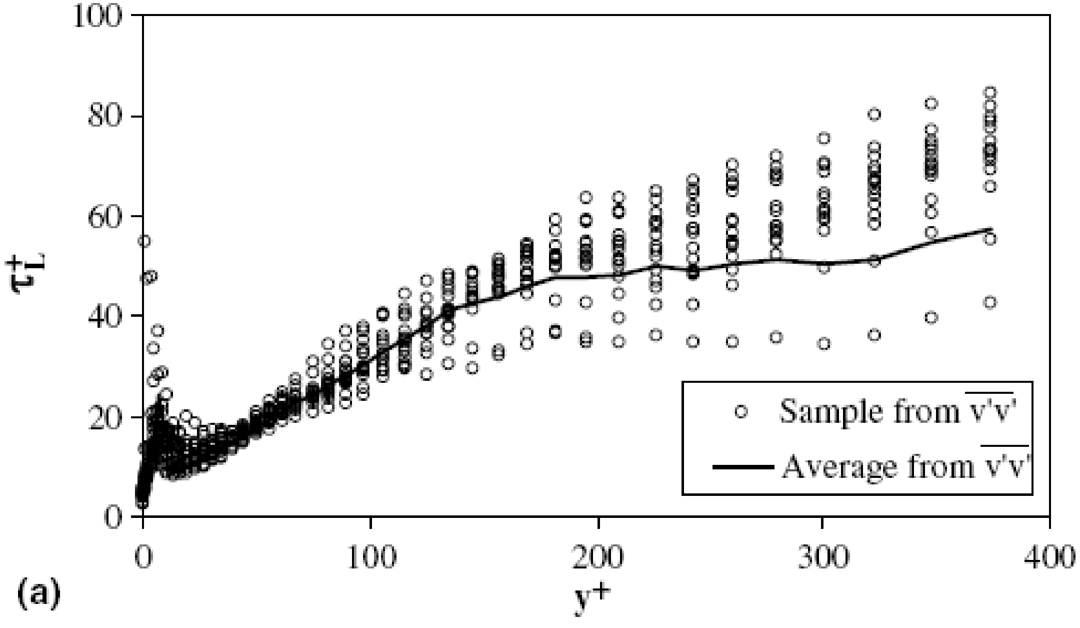
-Correlated in time intervals O(τ_L)

-Uncorrelated for greater time intervals

Times scales

➢ From Bocksell & Loth (2006): LPT tracking of fluid particles in DNS channel flow done by integration of $a_i \equiv \frac{dU_j}{dt} = U_j \frac{\partial U_i}{\partial x_j}$

$$\tau_L^+ = \tau_L \cdot \frac{(u^*)^2}{\nu}$$



Times scales, fits

- DNS computed scales reasonably approximated by wall function fits given by Kallio & Reeks (1989)

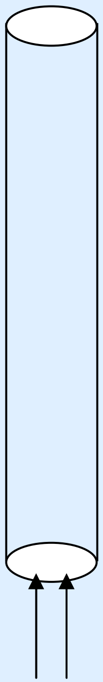
$$\tau_L^+ = 7.122 + 0.5731 \cdot y^+ - 0.00129 \cdot y^{+2}$$ for 5.0 < y^+ < 100

$$\tau_L^+ = 10.0$$ for y^+ <= 5.0

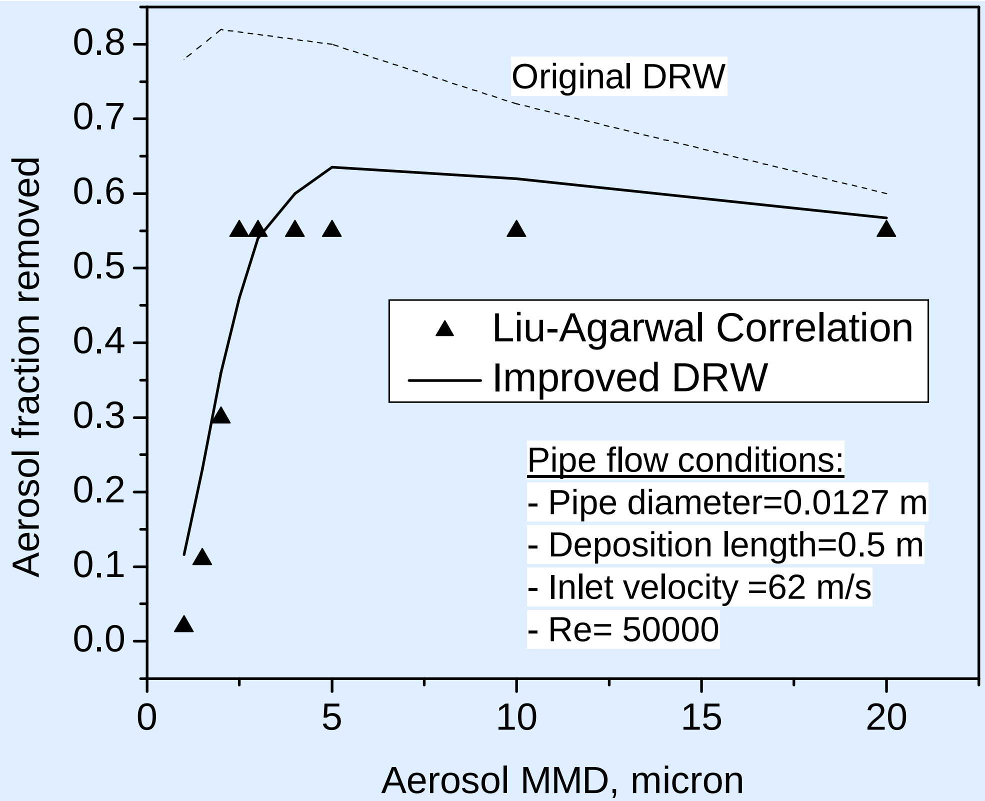
- with the Lagrangian time scale τ_L obtained from

$$\tau_L^+ = \tau_L \cdot \frac{(u^*)^2}{\nu}$$

Results: Liu deposition in pipe experiments ('74)



Particle flow



- Unphysical deposition is significantly reduced compared to original model

Shortcomings of DRW Model

- Still suffers from inherent deficiencies:

  - Modeled turbulence too synthetic

  - In limit of massless particles, DRW still predicts some concentration build-up near the wall (“spurious drift”), with as a result:

    - Non-vanishing deposition velocity in the tracer limit
    - Over-prediction of particle deposition when external forces are present (e.g. thermophoresis)

  - A good dispersion model should obey the “well-mixed criterion” (Thompson 1987) i.e.:
    - If initially well mixed, tracer particles should remained well mixed in the domain as time evolves

Beyond DRW: CRW

- Continuous random walk (CRW) offers a more physically sound way of modeling particle dispersion
- Fluid velocity seen by particles continuously fluctuates with time
- Original Langevin equation (ca. 1910) used by Langevin to model Brownian velocity fluctuations
- The stochastic Langevin equation applied for homogeneous turbulence (Obukhof 1959)

Langevin equation in homogeneous turbulence

- A spherical particle moves in a Eulerian flow domain according to:

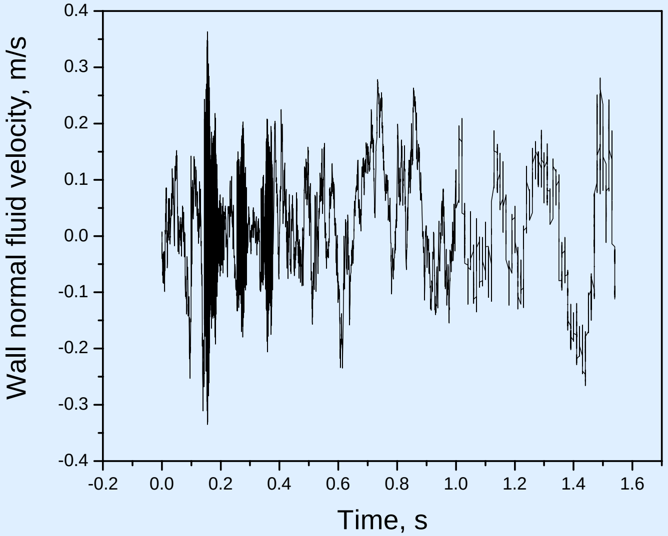
$$\frac{dU_p}{dt} = F_{Drag}(U - U_p) \qquad F_{Drag} = \frac{18\mu}{\rho_p d_p^2} C_D \frac{\text{Re}}{24}$$

- In turbulent flows, the carrier gas velocity: $U = \overline{U} + u$
- Mean velocity *U* from CFD. How to model the fluctuating velocity *u* ?
- The Langevin equation tries to mimic turbulence:

$$du_i = \underbrace{-\frac{u_i(t)}{\tau_i} \cdot dt}_{\text{Damping}} + \underbrace{\sigma_i \sqrt{\frac{2}{\tau_i}} \cdot d\omega_i}_{\text{Stochastic}}$$

Damping · **Stochastic** · **Lagrangian time scale** (τ_i) · **rms of velocity** (σ_i) · **Random number with variance dt** ($d\omega_i$)

Radial fluid velocity *v* seen by particle



Classical Langevin equation: a few words

- Langevin equation has intuitively the right physics
- Produces velocity fluctuations which are “credible”
- However:
  - Equation is a postulate i.e. is not derived from first principles
  - Only comparison with experiments will allow us to conclude to its usefulness or lack thereof
  - Does not obey, in its original format, the “well-mixed criterion” (Thompson, 1987). It leads to non-physical accumulation of small particles in regions of high kinetic energy (in laminar sublayer). Luckily one can correct for this.

Corrections for inhomogeneous turbulence

- Sampling from rms of velocity values introduces “spurious drift”, i.e. unphysical migration of small, fluid-like particles from bulk to walls
- Correction: start with acceleration of fluid particle:

$$a_i = U_j \frac{\partial U_i}{\partial x_j}$$

- Write velocity as mean + fluctuation: $U_i = \overline{U}_i + u_i$

Plugging 2nd equation in first above, and averaging in time, while using continuity, one gets after algebra:

Due to mean flow (CFD)

Due to inhomogeneous turbulence

$$\overline{a}_i = \overline{U}_j \frac{\partial \overline{U}_i}{\partial x_j} + \overline{u_j \frac{\partial u_i}{\partial x_j}}$$

Tracer limit corrections

- Physics dictates what terms are dominant in the turbulent acceleration
- Example: DNS statistics are used to close the drift correction in boundary layers:

$$\overline{a}_i' = \overline{u_j \frac{\partial u_i}{\partial x_j}}$$

- Finally, the correction velocity in inhomogeneous turbulence:

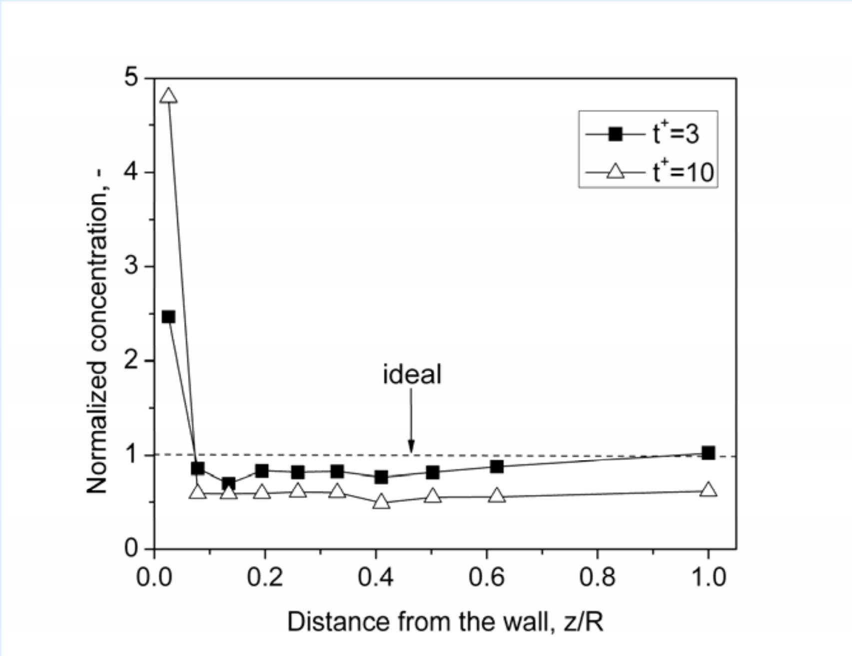
$$\overline{\Delta u_i} = \overline{a}_i' \Delta t = \Delta t \cdot \overline{u_j \frac{\partial u_i}{\partial x_j}}$$

- With correction, “spurious drift” and deposition of tracer particles significantly reduced. Periodic pipe flow of Re=10000

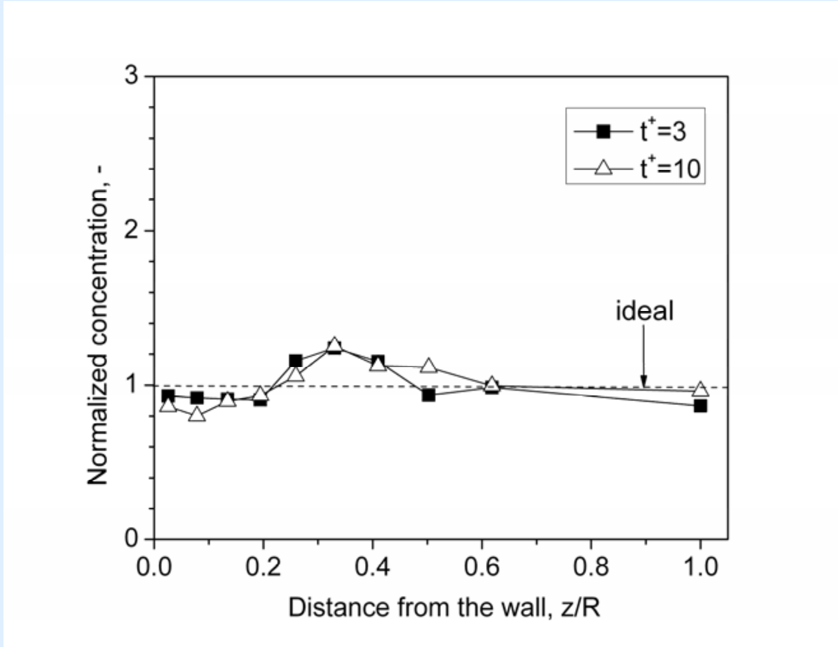
Tracer particles

Injected uniformly

Tracer limit corrections, pipe flow, Re=10000



Particle concentration. No drift correction



Particle concentration. With drift correction

Correction for arbitrary inertia

- Inertia particles "sees" different fluid turbulence than would a fluid particle
- Bocksell & Loth (2006) have extended the drift correction to inertial particles with arbitrary Stokes number *Stk (*measure of particle relaxation vs flow scales*)*
- The correction is given by:

$$\overline{\Delta u_i} = \frac{1}{1+Stk} \cdot \left(\overline{\Delta u_i}\right)_{fluid} \qquad Stk \equiv \frac{\tau_p}{\tau_L}$$

- Expression has correct limits:
  - Very low inertia particles (Stk=0) have correction of fluid particles
  - Very high inertia particles (Stk $\to \infty$) have no correction. Particle motion and turbulence increasingly decoupled
- Expression is a significant finding

Classical Langevin with corrections: assessment

➢Classical Langevin equation with drift correction reads:

Damping — Stochastic — Drift correction

$$du_i = \underbrace{-\frac{u_i(t)}{\tau_i}\cdot dt}_{\text{Damping}} + \underbrace{\sigma_i\sqrt{\frac{2}{\tau_i}}\cdot d\omega_i}_{\text{Stochastic}} + \underbrace{\frac{1}{1+Stk}\cdot \overline{u_j\frac{\partial u_i}{\partial x_j}}\cdot dt}_{\text{Drift correction}}$$

➢Yields reasonable predictions of particle dispersion in mildly inhomogeneous flows. Well-mixed criteria met.

➢Not accurate enough in strongly inhomogeneous flows such as boundary layers

Non-dimensional Langevin equation for boundary layers

- In recent years: many improvements to Langevin equation to tackle inhomogeneous turbulence (e.g. pipe). Transported quantity in inhomogeneous turbulence is
  - No longer *u* but *u*/σ
- One writes the so-called non-dimensional Langevin equation in boundary layer:

$$d\left(\frac{u_i}{\sigma_i}\right) = -\left(\frac{u_i}{\sigma_i}\right)\cdot\frac{dt}{\tau_i} + d\eta_i + A_i dt$$

Damping — Stochastic — Drift correction

$$\overline{d\eta_i^2} = \left[\frac{2}{\tau_i}\right]\cdot dt$$

$$A_i = \frac{\partial\left(\frac{\overline{u_2 u_i}}{\sigma_i}\right)}{\partial x_2}\cdot\frac{1}{1+Stk}$$

x_2 is wall normal

- Requires Eulerian statistics from DNS databases. Readily available.
- Can couple CFD mean flow with Langevin fluctuating flow to predict more accurately particle motion in general flows

Non-dimensional Langevin equation outside boundary layer

- Outside boundary layer in bulk: turbulence roughly isotropic:

$$\sigma = \sigma_1 = \sigma_2 = \sigma_3 = \sqrt{\frac{2}{3} \cdot k}$$

- It can be shown (my paper Int. J. Multiphase Flows, 2008) that the drift correction in the bulk takes the form:

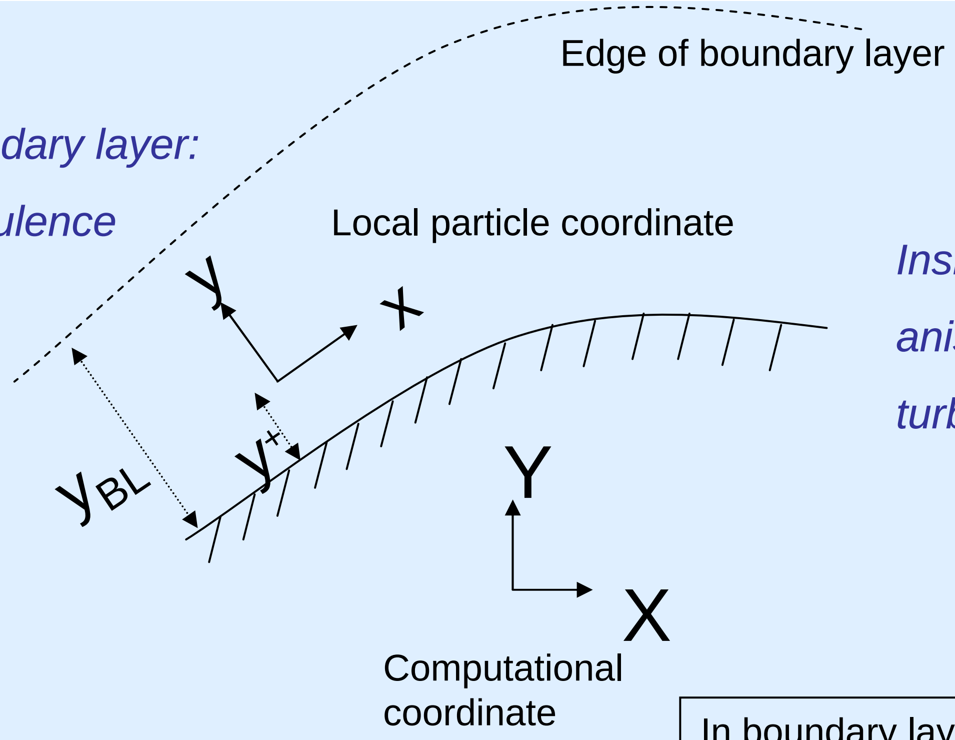
$$A_i dt = \delta(\frac{u_i}{\sigma_i}) = \overline{u_j \frac{\partial(\frac{u_i}{\sigma_i})}{\partial x_j}} \cdot \frac{dt}{1+Stk} \cong \frac{1}{3\sigma} \frac{\partial k}{\partial x_i} \cdot \frac{dt}{1+Stk}$$

- CFD codes solve for *k*, so drift correction readily computed in CFD

Non-dimensional Langevin equation in & outside boundary layer

Outside boundary layer:

isotropic turbulence



Inside boundary layer:

anisotropic

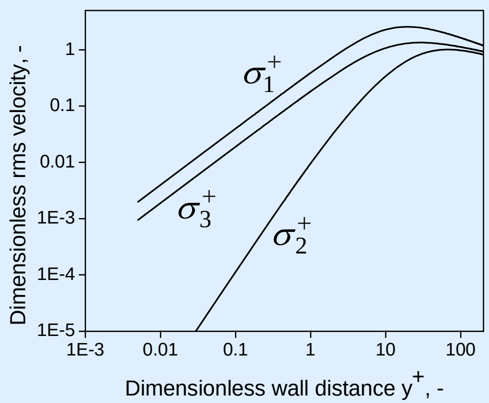
turbulence

In boundary layer

1-Streamwise

2- Wall normal

3- Span



Langevin equation in inhomogeneous media

- Langevin equations:

Boundary layer

$$d\left(\frac{u_1}{\sigma_1}\right) = -\frac{1}{\tau_L}\left(\frac{u_1}{\sigma_1}\right)\cdot dt + \sqrt{\frac{2}{\tau_L}}\cdot d\omega_1 + \frac{\partial\left(\frac{\overline{u_1 u_2}}{\sigma_1}\right)}{\partial x_2}\cdot\frac{dt}{1+Stk}$$

$$d\left(\frac{u_2}{\sigma_2}\right) = -\frac{1}{\tau_L}\left(\frac{u_2}{\sigma_2}\right)\cdot dt + \sqrt{\frac{2}{\tau_L}}\cdot d\omega_2 + \frac{\partial\sigma_2}{\partial x_2}\cdot\frac{dt}{1+Stk}$$

$$d\left(\frac{u_3}{\sigma_3}\right) = -\frac{1}{\tau_L}\left(\frac{u_3}{\sigma_3}\right)\cdot dt + \sqrt{\frac{2}{\tau_L}}\cdot d\omega_3$$

Bulk

$$d\left(\frac{u_1}{\sigma}\right) = -\frac{1}{\tau_L}\left(\frac{u_1}{\sigma}\right)\cdot dt + \sqrt{\frac{2}{\tau_L}}\cdot d\omega_1 + \frac{1}{3\sigma}\cdot\frac{\partial k}{\partial x_1}\cdot\frac{dt}{1+Stk}$$

$$d\left(\frac{u_2}{\sigma}\right) = -\frac{1}{\tau_L}\left(\frac{u_2}{\sigma}\right)\cdot dt + \sqrt{\frac{2}{\tau_L}}\cdot d\omega_2 + \frac{1}{3\sigma}\cdot\frac{\partial k}{\partial x_2}\cdot\frac{dt}{1+Stk}$$

$$d\left(\frac{u_3}{\sigma}\right) = -\frac{1}{\tau_L}\left(\frac{u_3}{\sigma}\right)\cdot dt + \sqrt{\frac{2}{\tau_L}}\cdot d\omega_3 + \frac{1}{3\sigma}\cdot\frac{\partial k}{\partial x_3}\cdot\frac{dt}{1+Stk}$$

- Time scales τ_i in boundary layer: roughly equal in all directions (DNS findings by Bocksell & Loth, 2006):

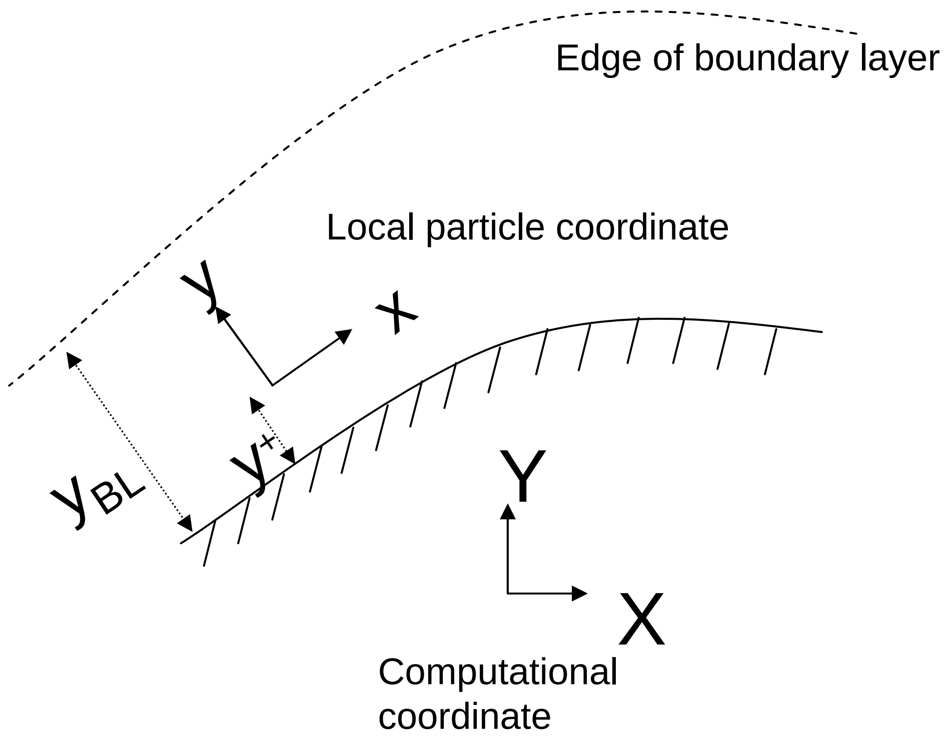
$$\tau_L^+ = 10 \qquad y^+ \le 5$$

$$\tau_L^+ = 7.122 + 0.5731\cdot y^+ - 0.00129\cdot y^{+2} \qquad 5 \le y^+ \le 100$$

$$\tau_L = \frac{2}{C_o}\cdot\frac{k}{\varepsilon}, \qquad C_o = 14$$

Algorithm of CFD model implementation

- Note: need to know "local" coordinate system at any particle position
  - Requires knowing location of "closest" wall to particle at any time.
  - Computation done once at post process. Not trivial, especially in complex geometry.
  - Shuttling between local and computational coordinate systems at every Δt



Benchmarking model: deposition in turbulent flows

- Benchmarking of the model in isothermal flow
  - Particle dispersion data from recent DNS computations (2007)
  - Deposition: Comparison with particle deposition data in:
    - 2D: pipe flow (Liu-Agarwal correlation)
    - 3D flow
      - 90º bend (Pui correlation)
      - Mouth-throat geometry (Stahlhofen data fit, Grgic et al. data)
- Benchmarking of the model with active thermophoresis
  - TUBA tests (Dumaz, 1993)
  - Tsai tests (2004)

Comparison with DNS database statistics

- Extensive DNS database for particle dispersion statistics assembled by Marchioli, Soldati et al. (IJMF, 2007).

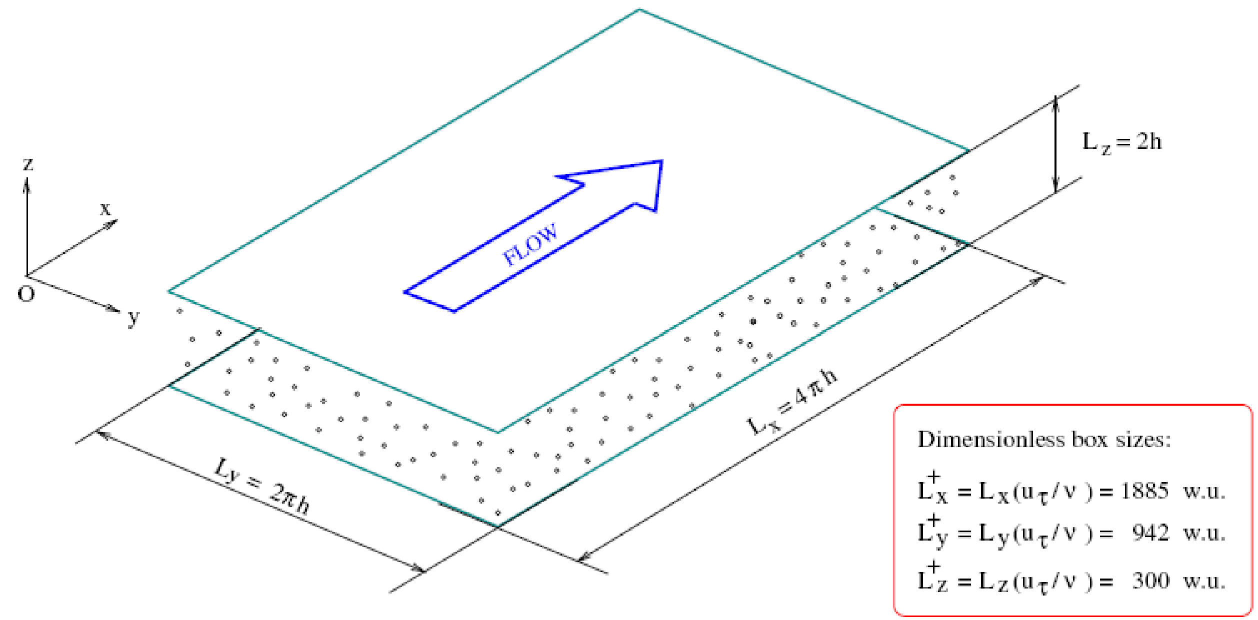


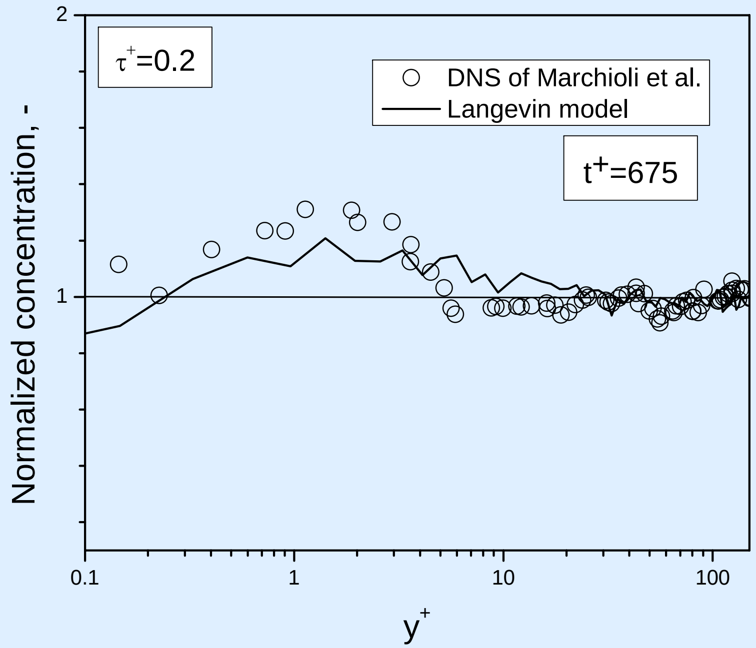
Fig. 1. Particle-laden turbulent gas flow in a flat channel: computational domain.

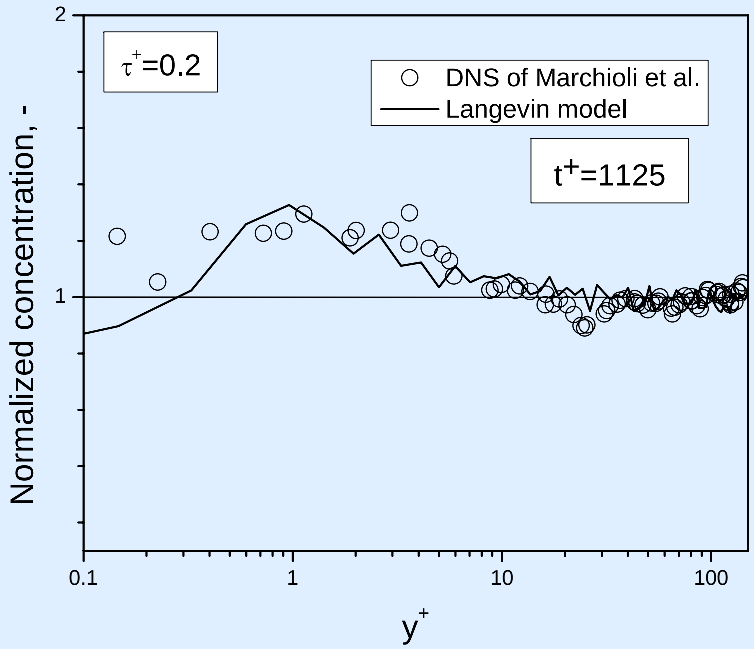
Comparison with DNS database statistics

- Re_τ=150, Re_h=2100. Periodic boundary condition in 2 directions
- 6 classes of particles, with τ^+=0.2,1, 5, 15, 25, 125
- Database spans Δt^+=1200, i.e. about 10 channel transit times
- Statistics:
  - Particle concentration profiles at two times, t^+=675,1125
  - Mean and rms of axial and normal velocities between t^+=742 & t^+= 1192

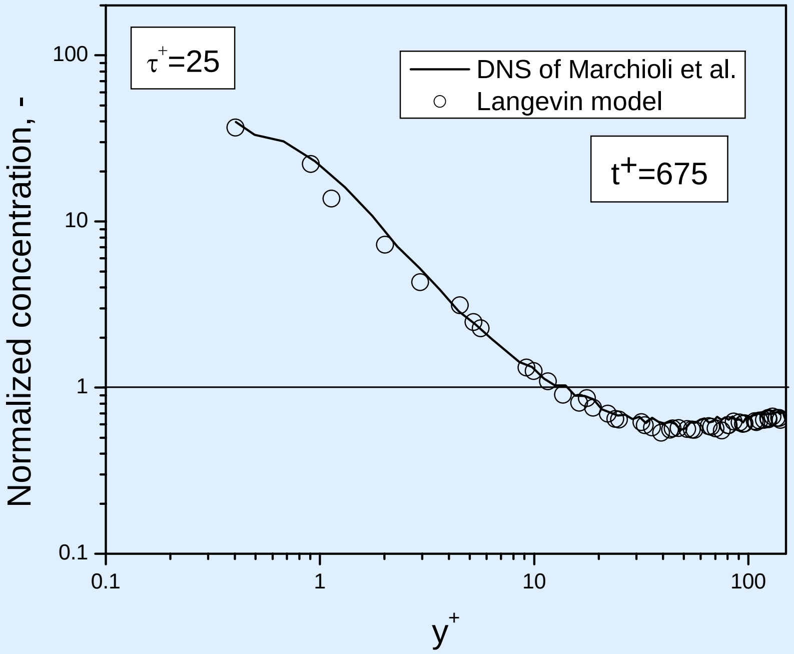
- Investigation studies effects of: drag, lift, gravity
- Here we compare against results with drag only with particles with τ^+=0.2, 25, 125
- Boundary conditions: particles reflect elastically on impact with wall

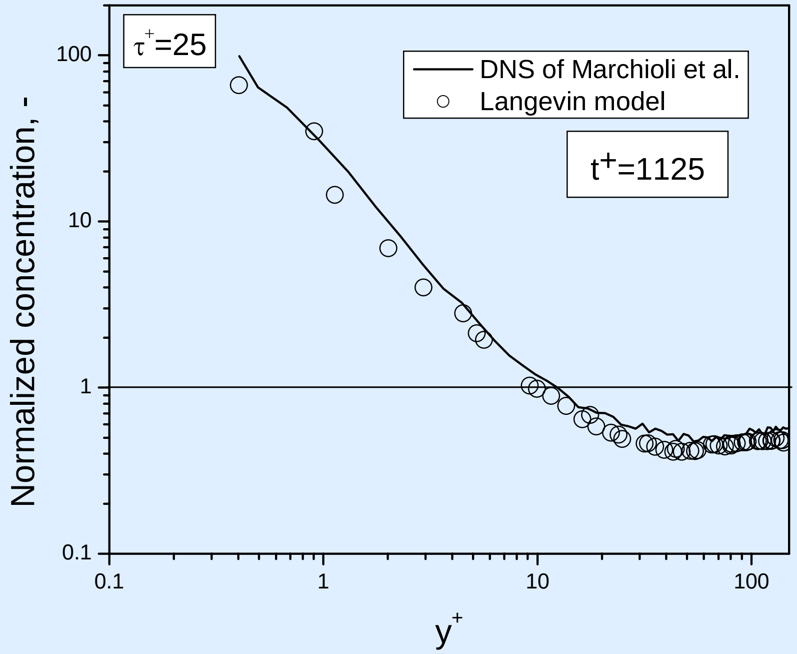
Concentrations, tracer particles $\tau^+=0.2$



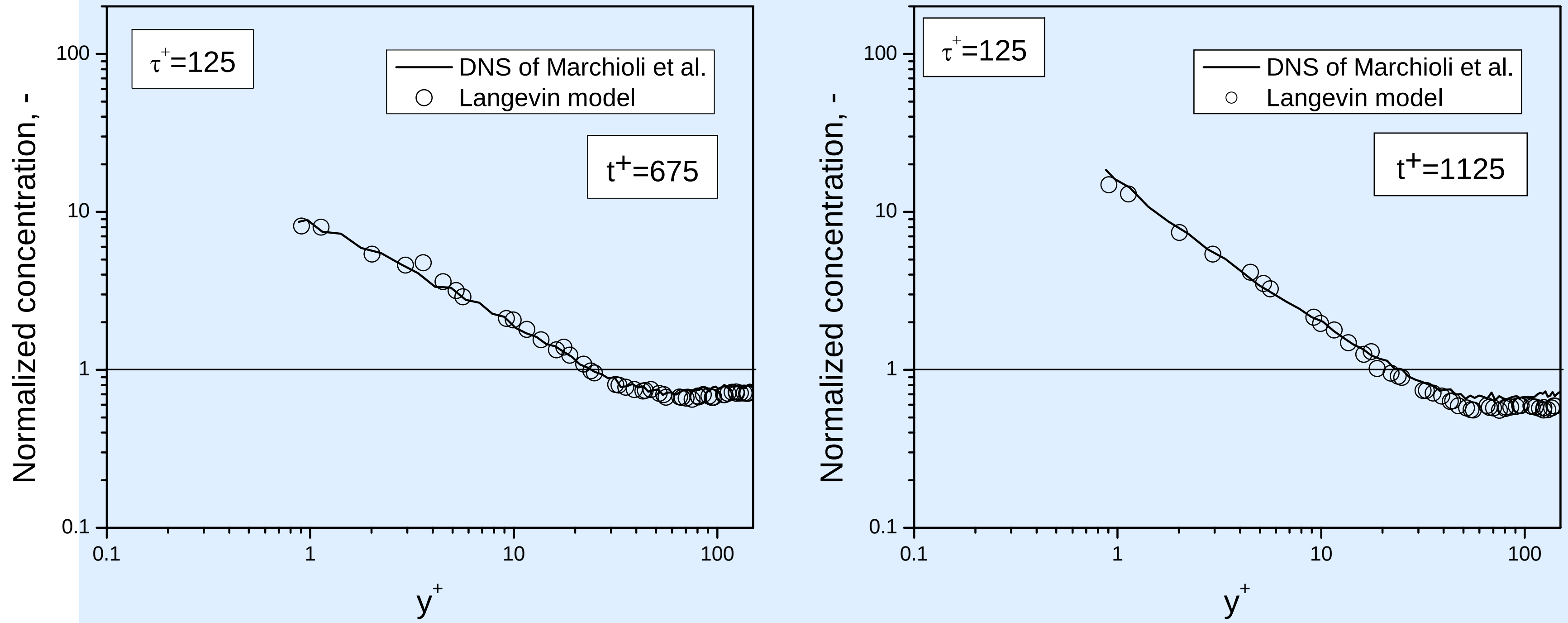


Concentrations, mid-inertia τ^{+}=15

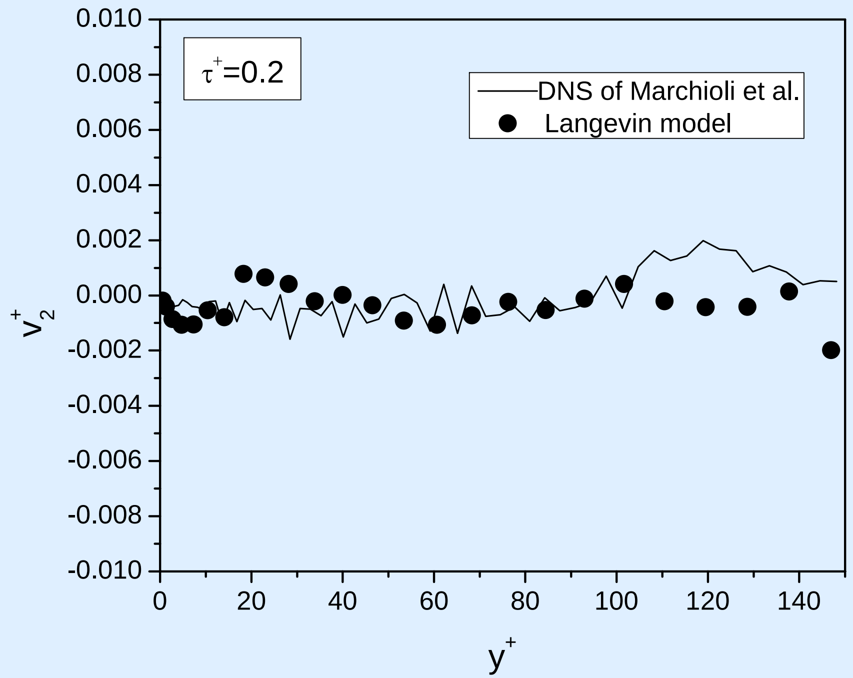


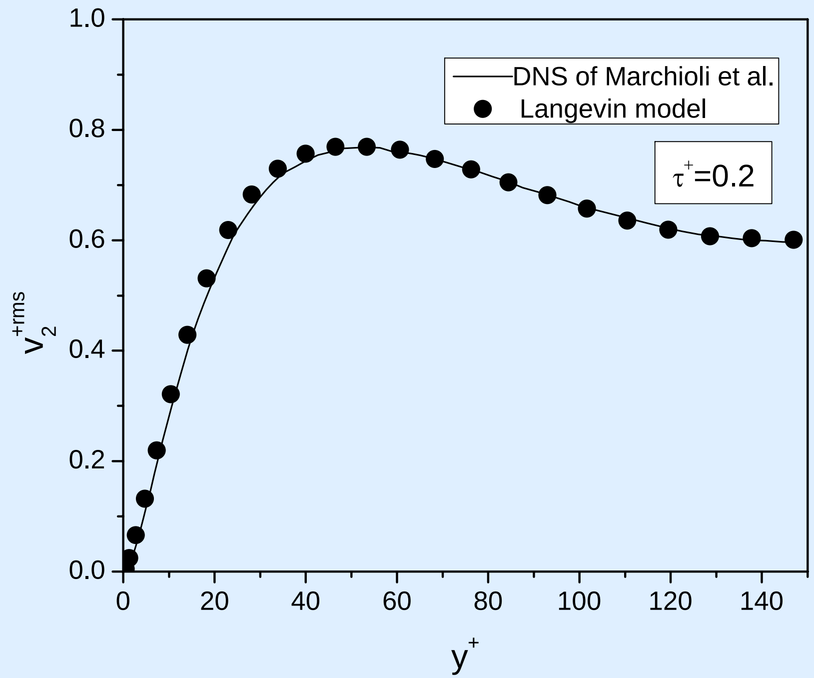


Concentrations, heavy particle τ^+=125

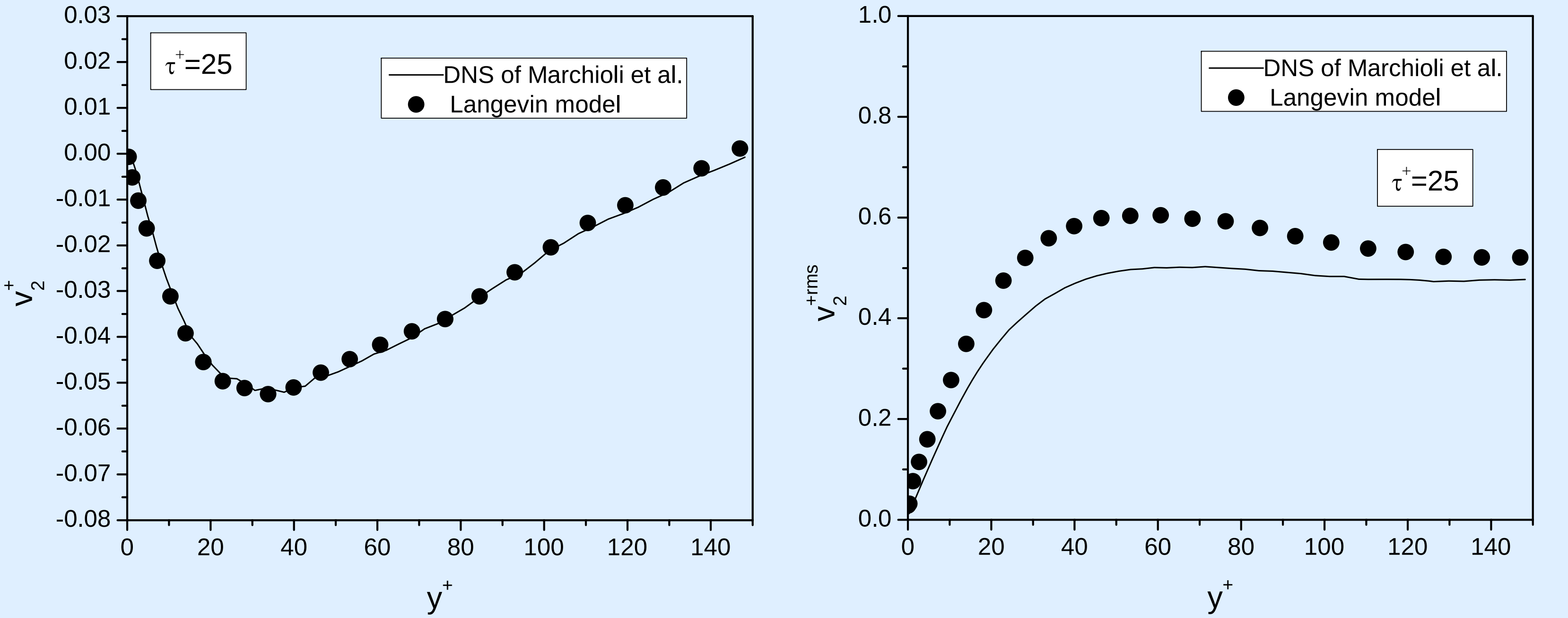


Normal mean velocity and rms, tracer particle τ^+=0.2

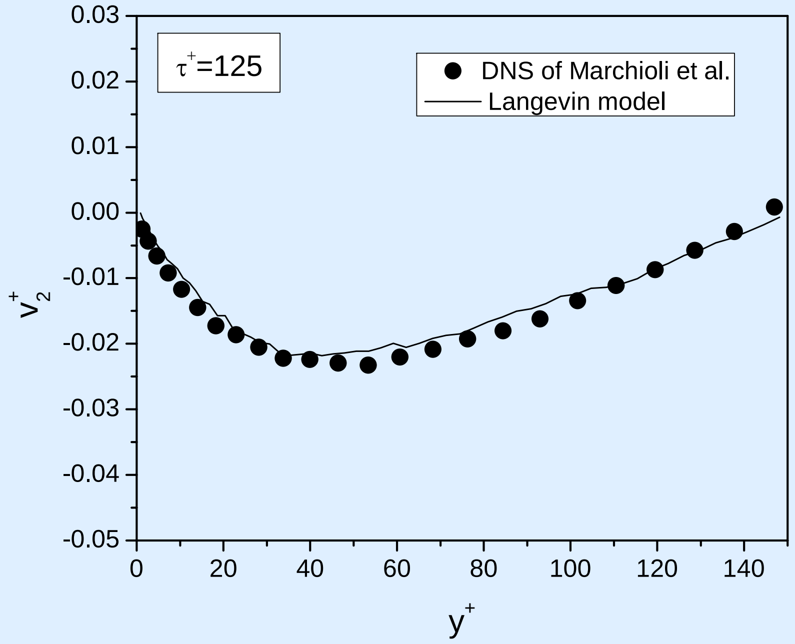


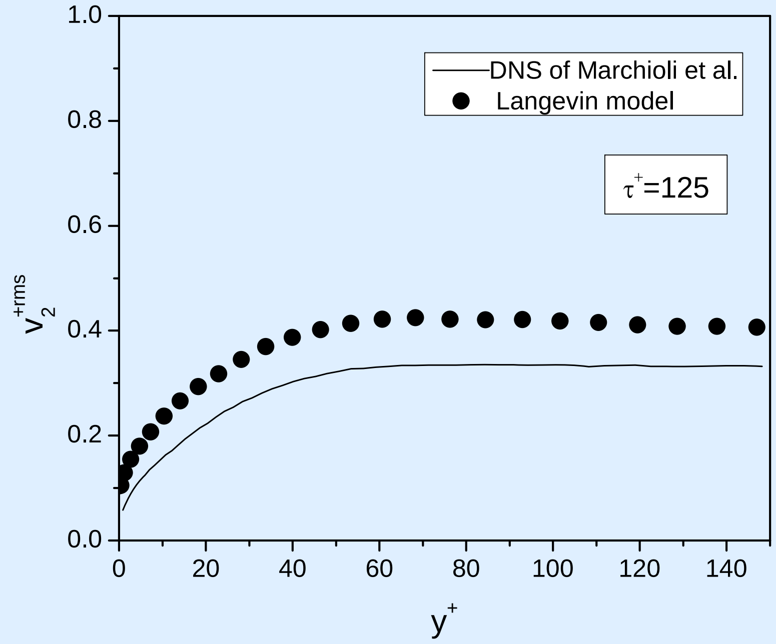


Normal mean velocity and rms, mid-inertia τ^+=25



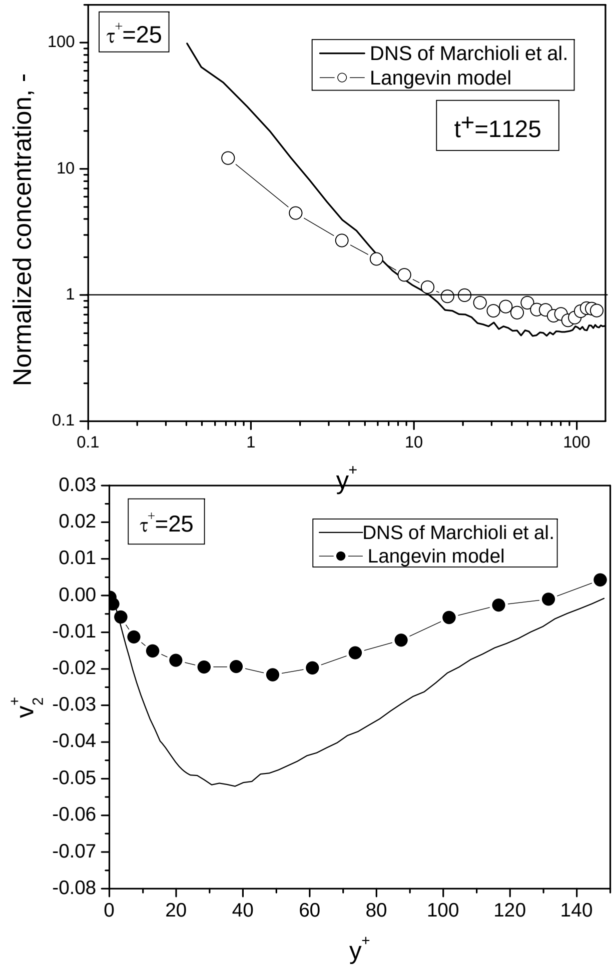
Normal mean velocity and rms, heavy particle τ^+=125





Conclusions from comparison with DNS

- Model predictions of particle dispersion surprisingly good
  - Concentration
  - Velocity profiles (deposition rates)
- rms values of velocity slightly larger. Due to assumption of Gaussin distribution for the turbulent fluctuations.
- Every term in non-dimensional Langevin equation counts e.g. not including the Stokes correction factor



Typical heat transfer correlation graph: Δ= ±30%

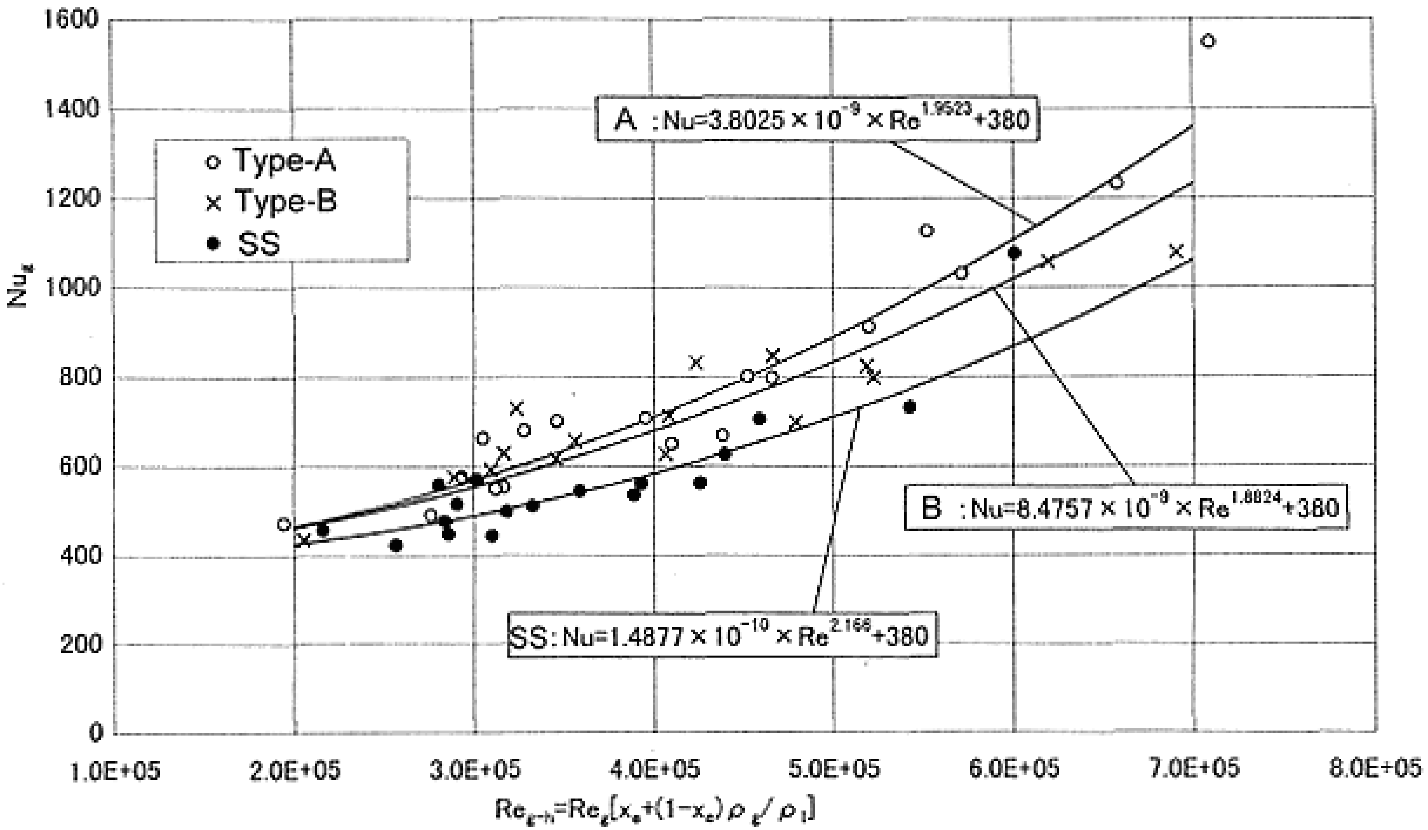
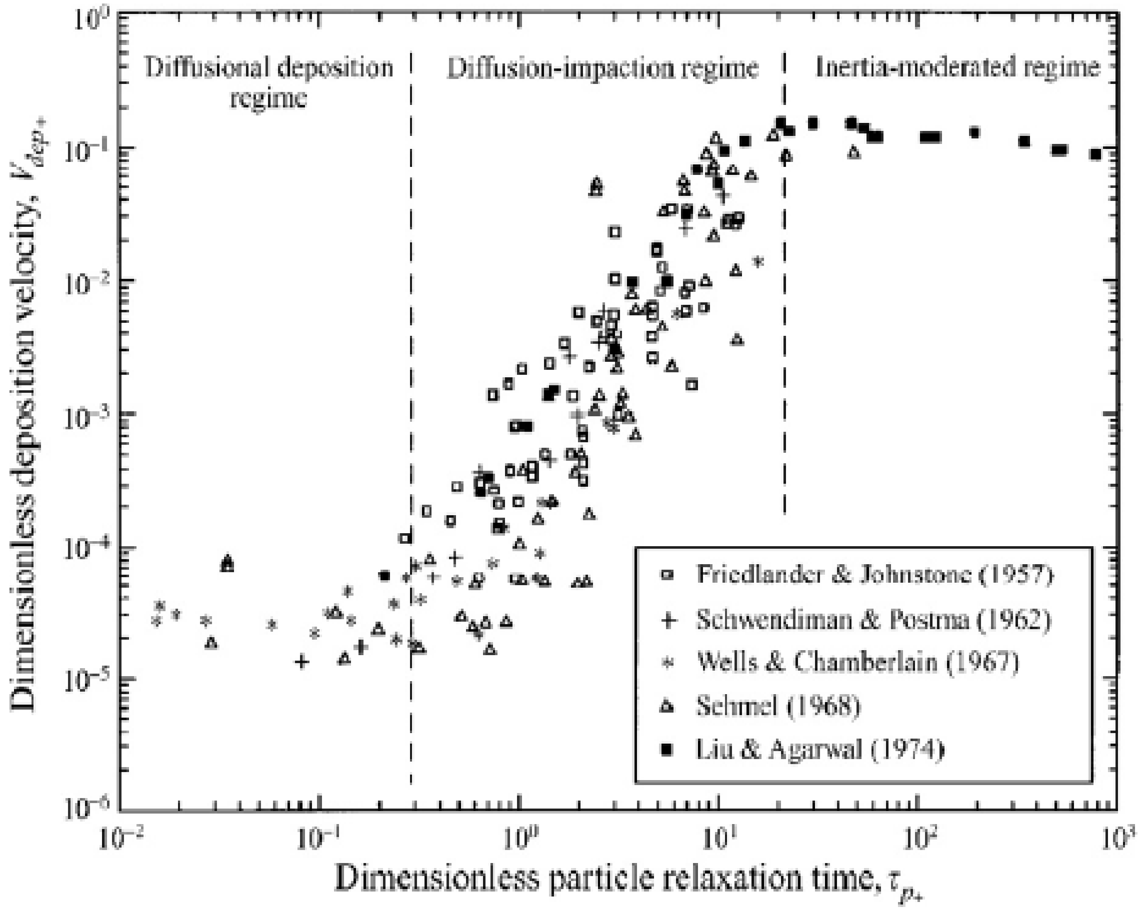


Fig.7 Effect of grid spacer type, Type-A/Type-B and SS, on film boiling heat transfer

Deposition in pipe flow: experimental data. Δ= ± 100-1000%!



$$V^+ = \frac{1}{4}\frac{D}{L}\frac{\overline{U}}{u^*}\ln(\frac{C_{in}}{C_{out}})$$

$$\tau_p^+ = \frac{\tau_p u^{*2}}{\nu}$$

Pause: Why particle deposition so uncertain?

- Standard way of measuring particle deposition rates:
  - Assume particle profiles are fully developed after a few 10's of L/D's
  - Draw a sample from somewhere in the bulk, and filter it.
  - Assume concentration profile is flat because "turbulence mixes up things" (counterpart to temperature/velocity profiles in turbulent flows)

- Recent DNS show procedure above is seriously flawed:
  - Preferential concentration in boundary layer. Assuming fully mixed profiles in sampling may induce large errors!
  - Very long times needed for particles to reach fully developed profiles, several 1000's of L/D! Get different deposition rates depending on where deposition is measured.
- Recent measurements confirm phenomena of preferential concentration
- Turbulence actually de-mixes particles!

Particle flow over plate. Tests Wang ‘07

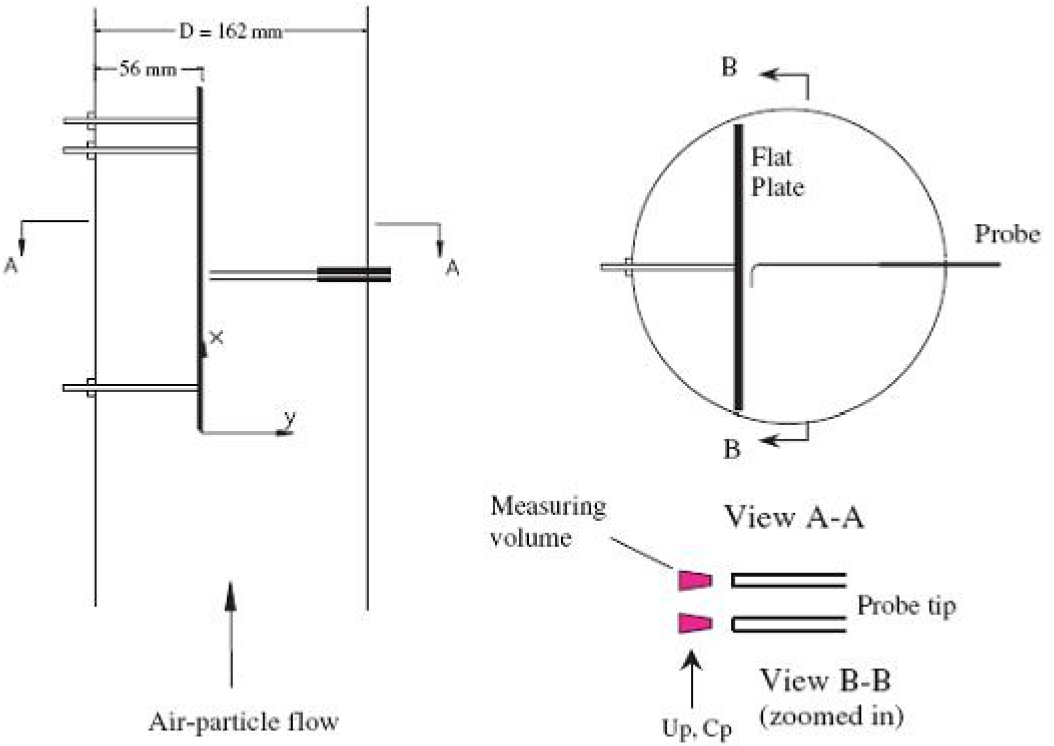
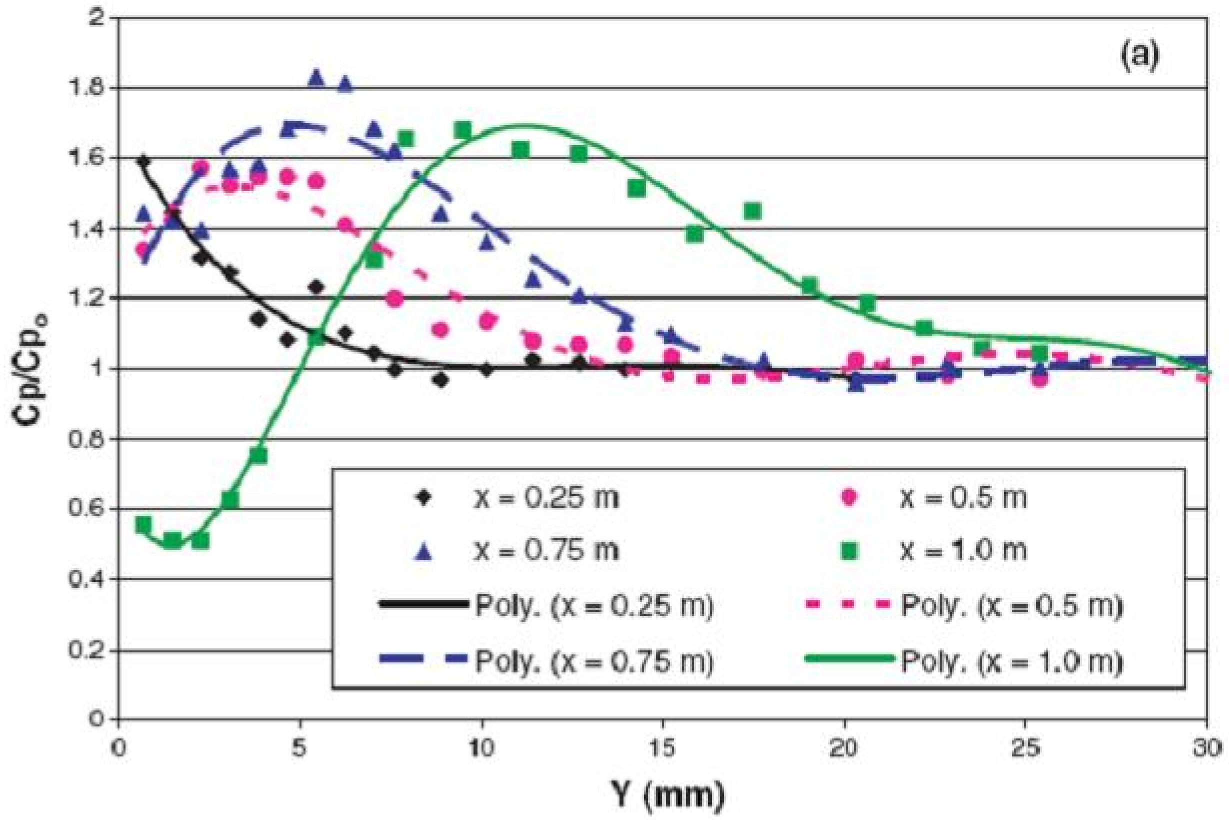
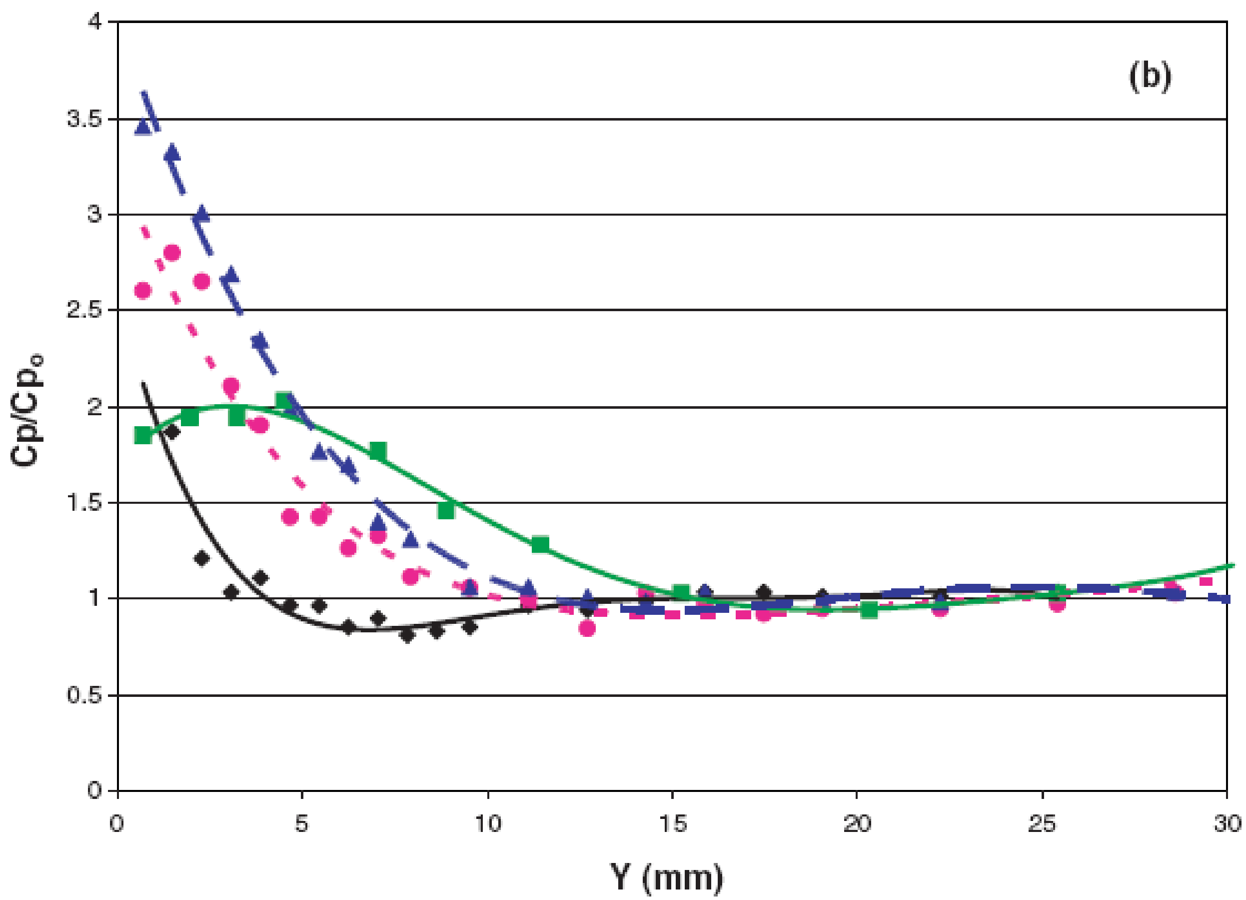


Fig. 2. Sketch of the test section.

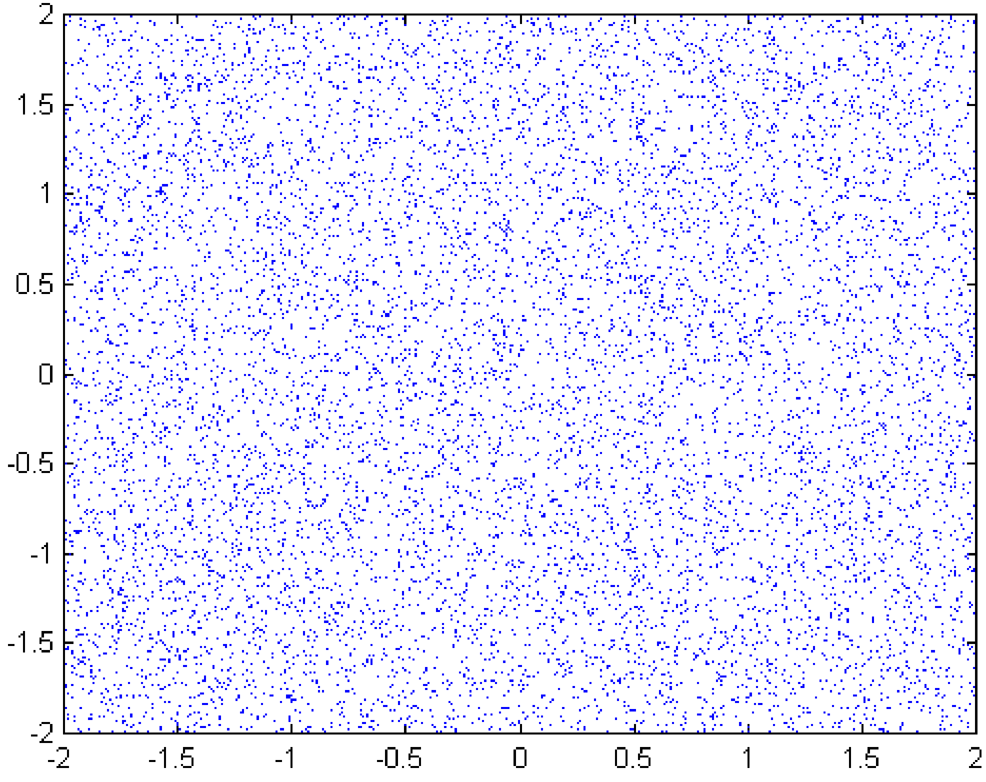
Particle concentration. Diameter= 60 μm



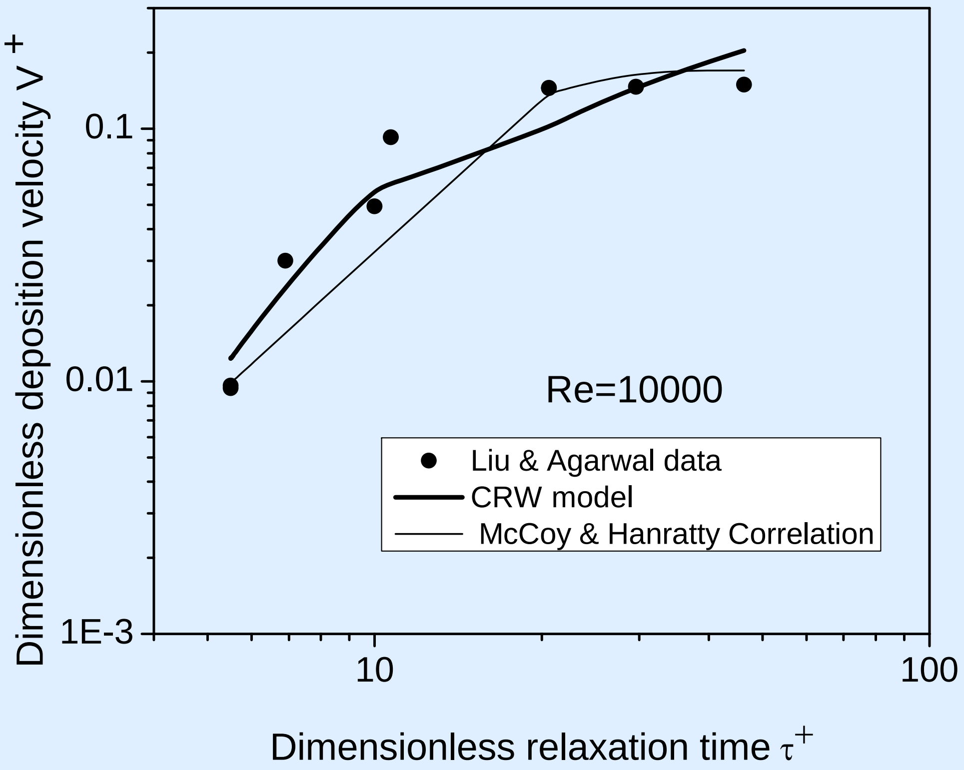
Particle concentration. Diameter= 200 μm

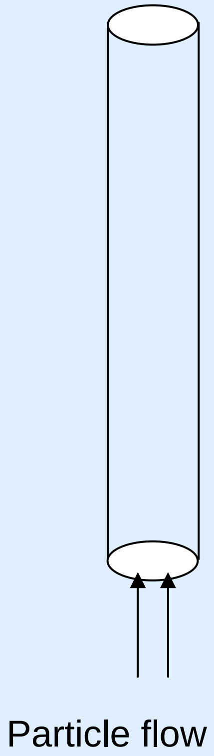


Synthetic turbulence. Particles demixing



Model assessment vs pipe flow data, low turbulence (Re =10000)

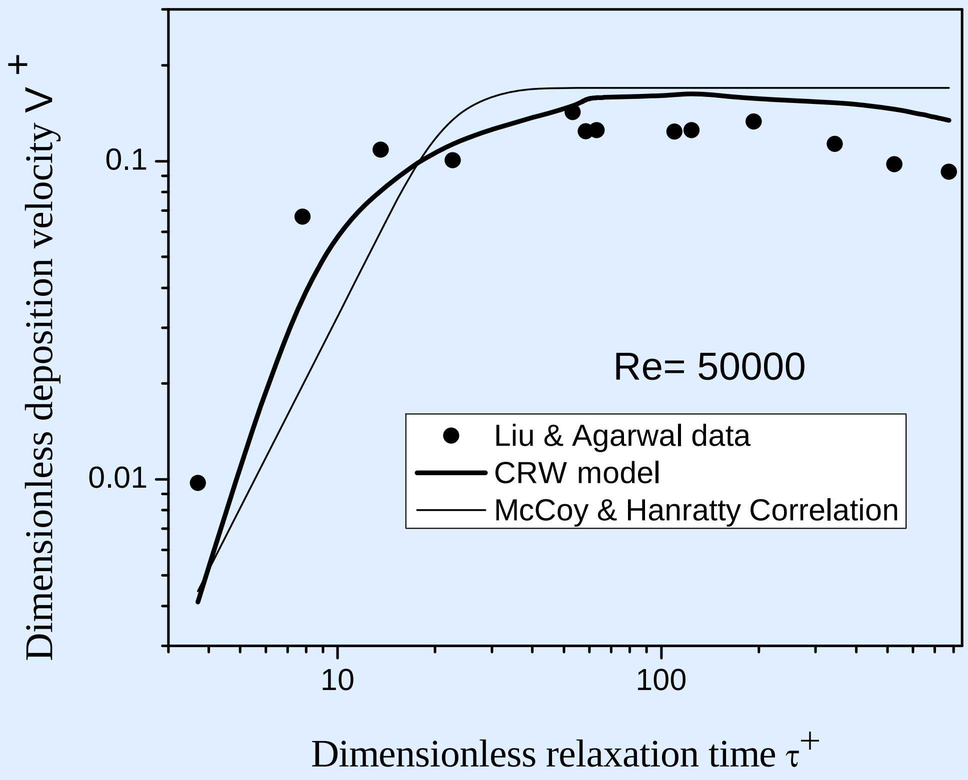




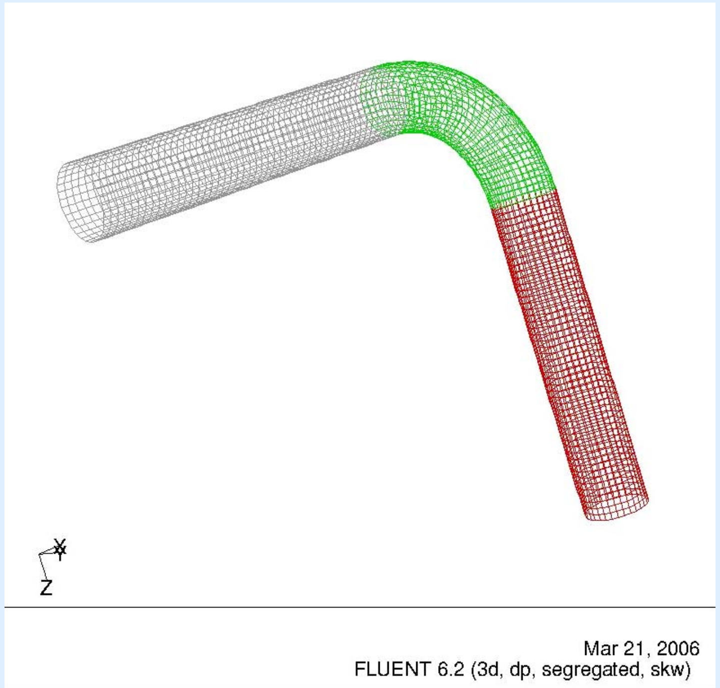
$$V^+ = \frac{1}{4}\frac{D}{L}\frac{\overline{U}}{u^*}\ln\left(\frac{C_{in}}{C_{out}}\right)$$

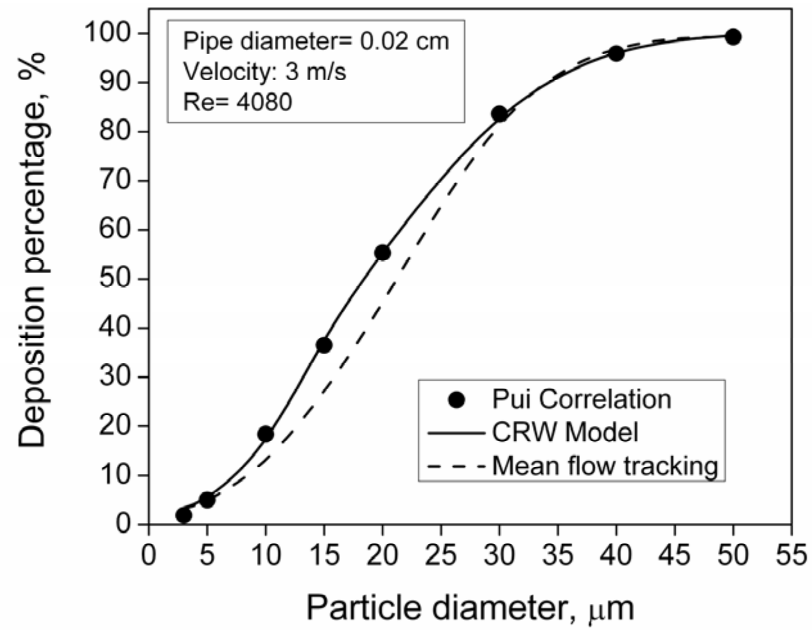
$$\tau_p^+ = \frac{\tau_p u^{*2}}{\nu}$$

Model assessment vs pipe flow data, high turbulence (Re=50000)



Model assessment: deposition in 90° bend flow



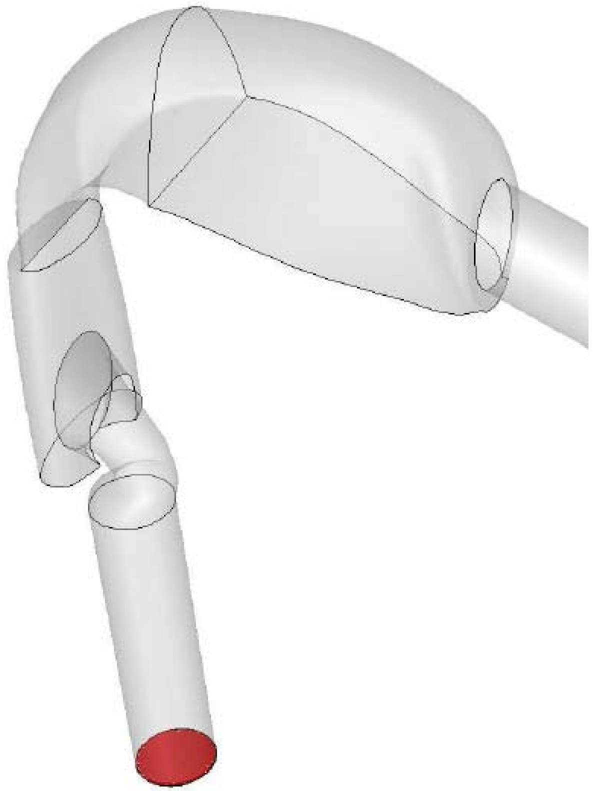


Model assessment in 3D flows: deposition in mouth-throat geometry (MTG)

CAD files of MTG:

Courtesy: professor W. Finlay,

University of Alberta



Deposition in mouth-throat (Finlay et al.)

- Research by Prof. Finlay's group Uni. of Alberta

- Deposition of DEHS particles obtained by
  - Gravimetry
  - Gamma scintigraphy

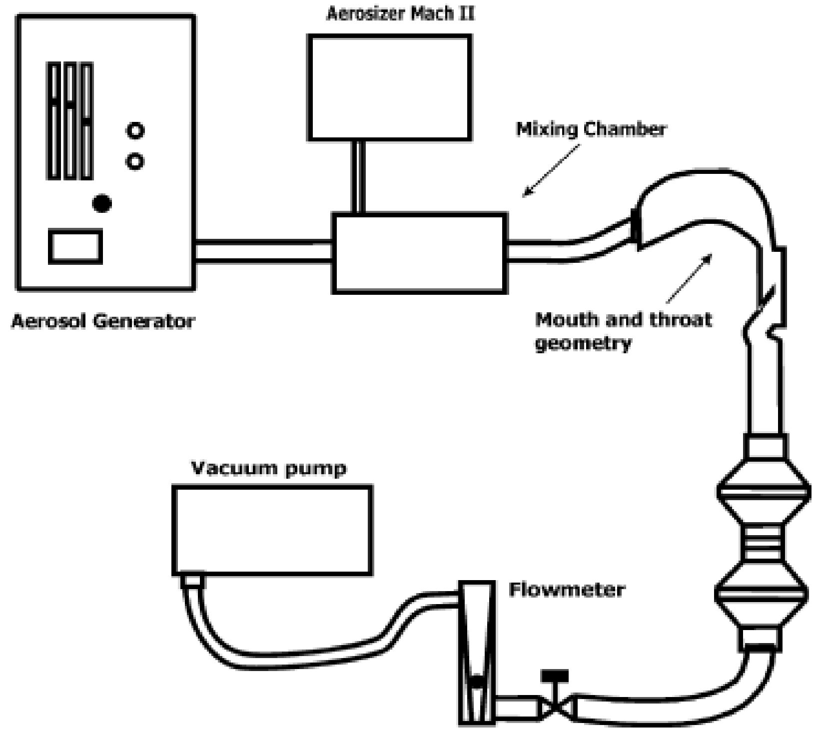


Fig. 1. Schematic of experimental setup.

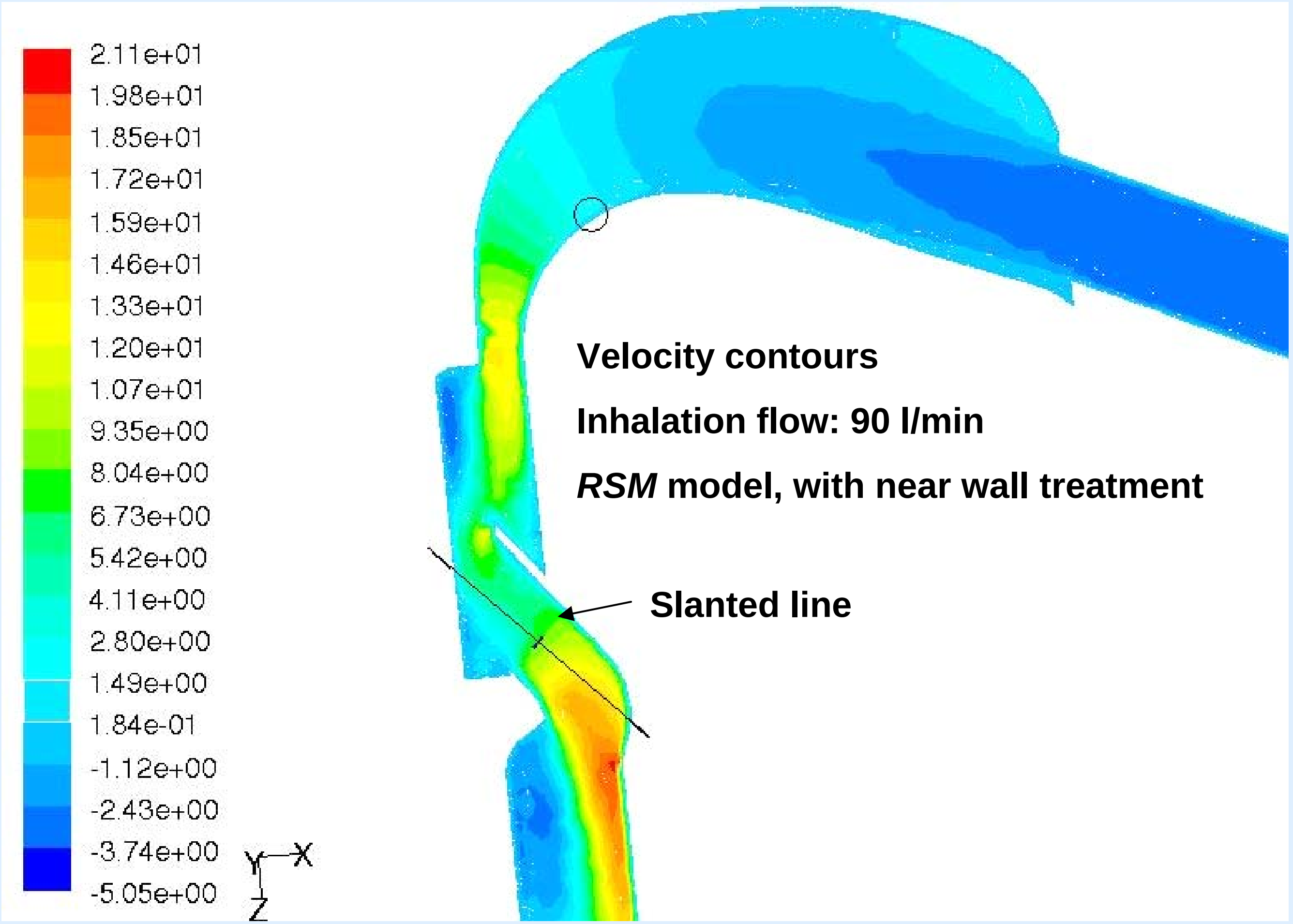
Quality assurance of MTG CFD computations

- Before using dispersion model, need to have confidence that the computed flow field is free of user-induced errors
- Best practice guidelines (BPG) followed to ensure in particular:
  - Grid-independence of results
  - Required grid resolution in the boundary layer
- For mouth-thoat geometry
  - Reynolds Stress Model (RSM, 7 equations) used
  - RSM considered the “best” CFD turbulence model for general flows

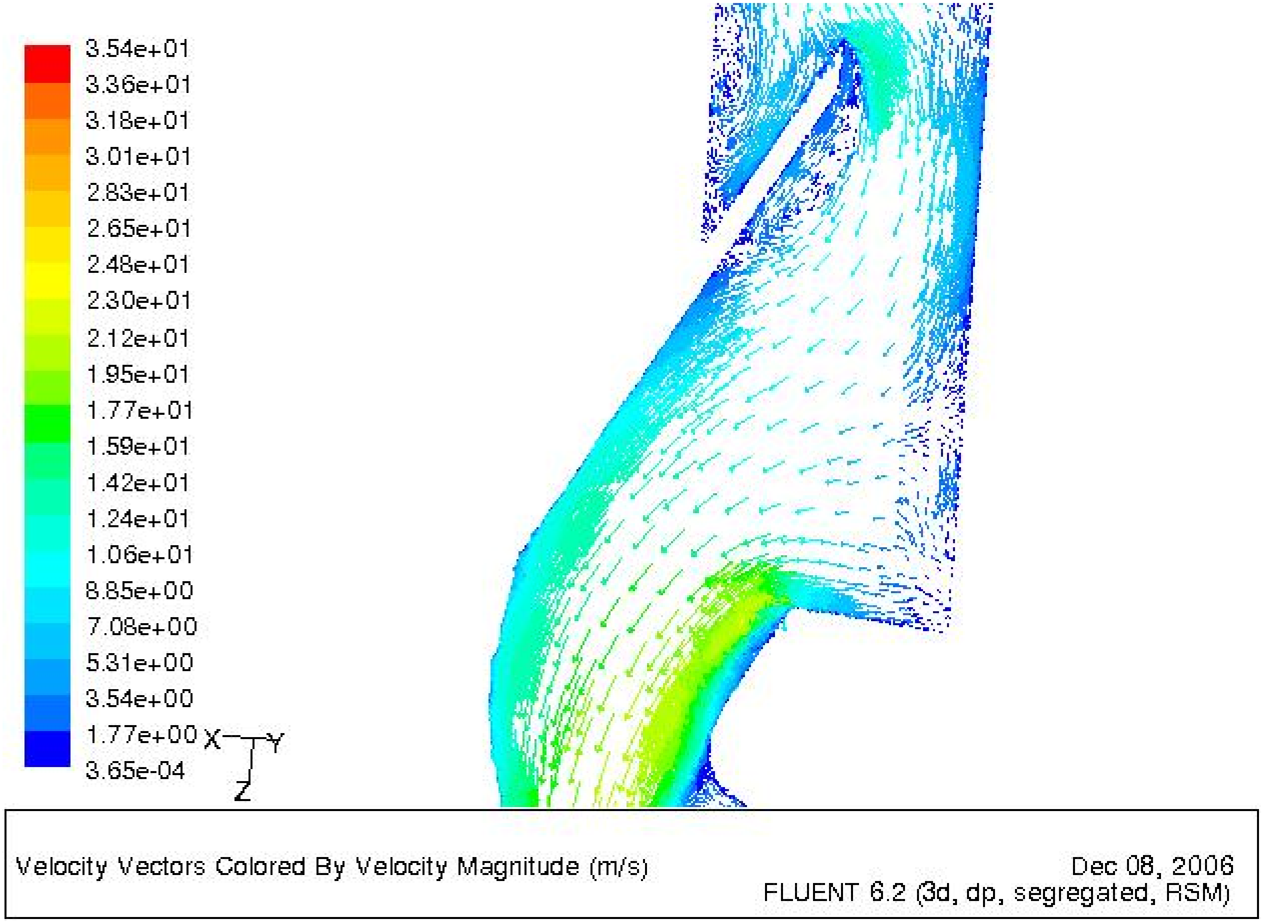
Best Practice Guidelines for mouth-throat simulation

- Hybrid mesh: hex in boundary layer & tet elsewhere
- Fine enough to ensure y+ order 1 in wall adjacent cells (
- 3 grid levels
- Second order accuracy

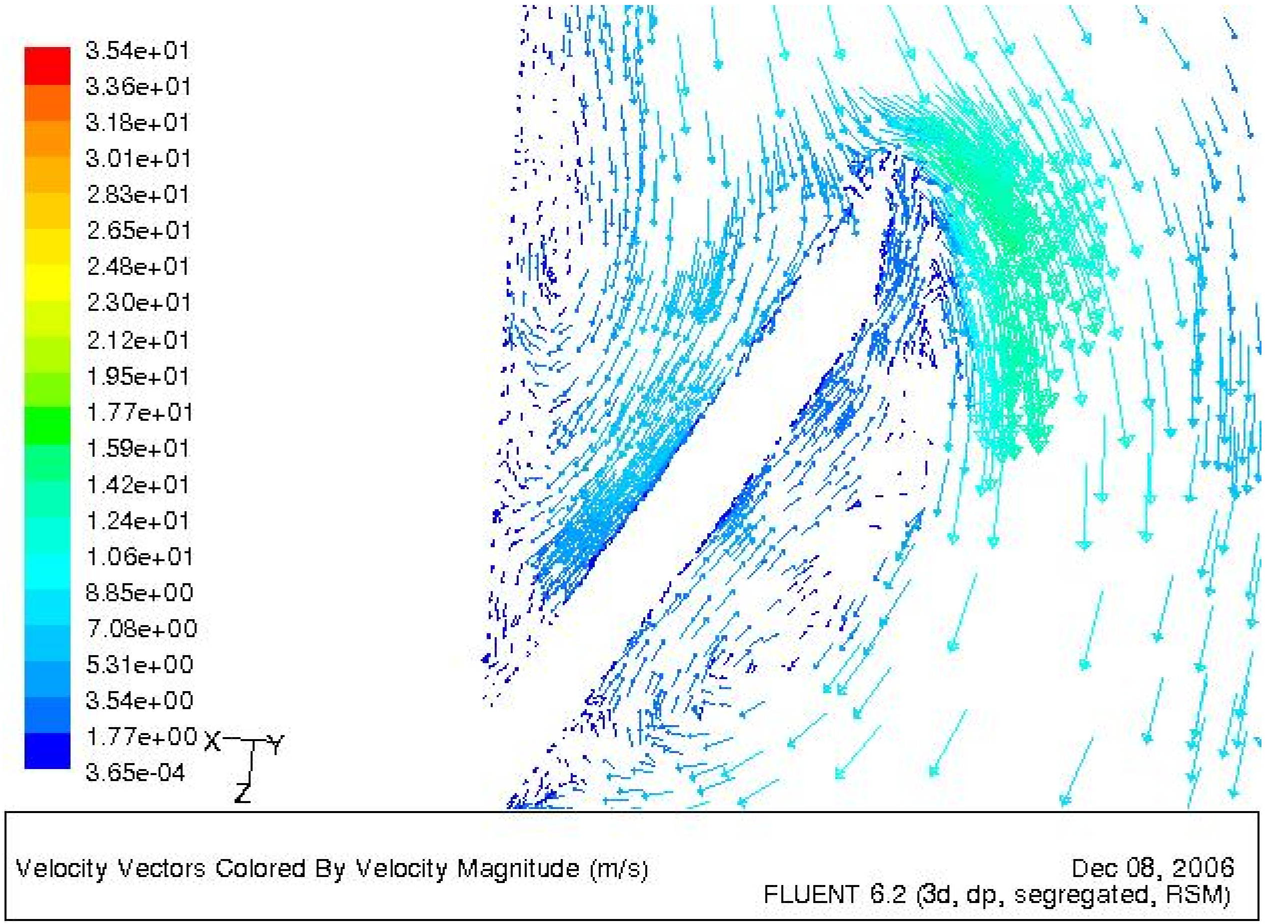
Sample velocity contours



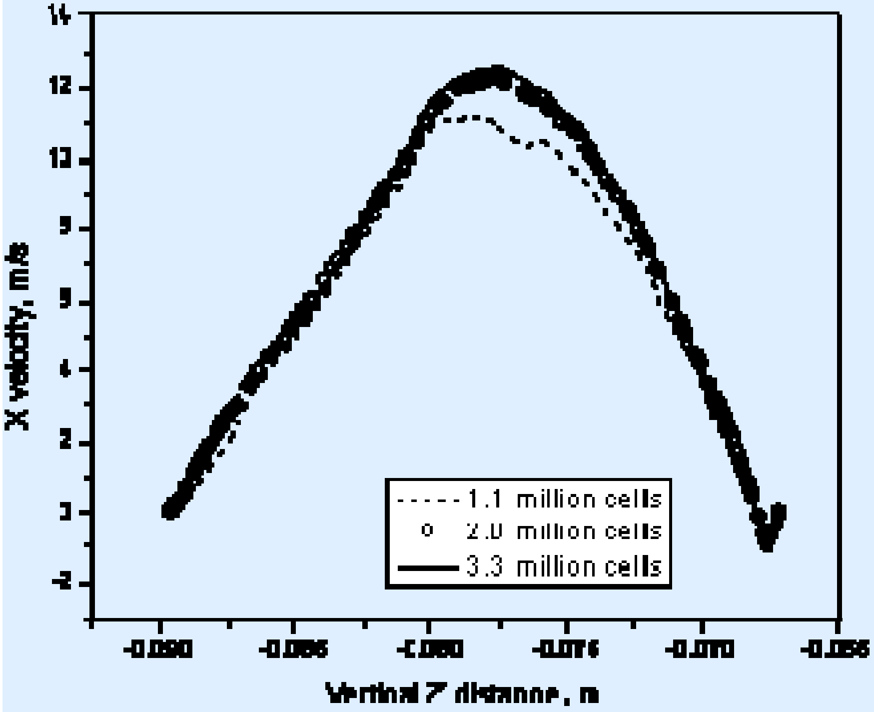
Flow in throat section

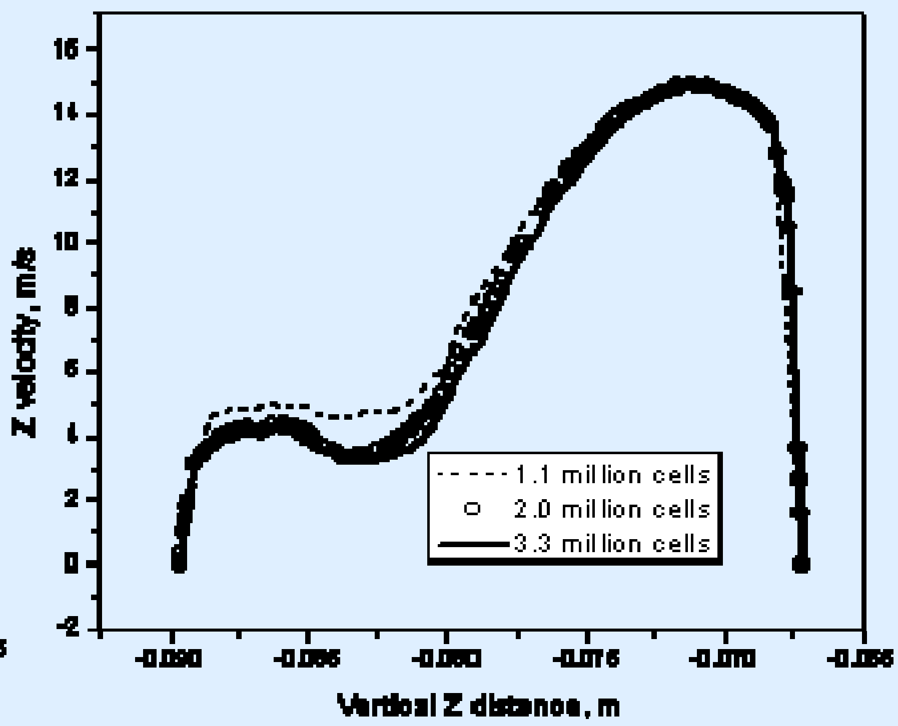


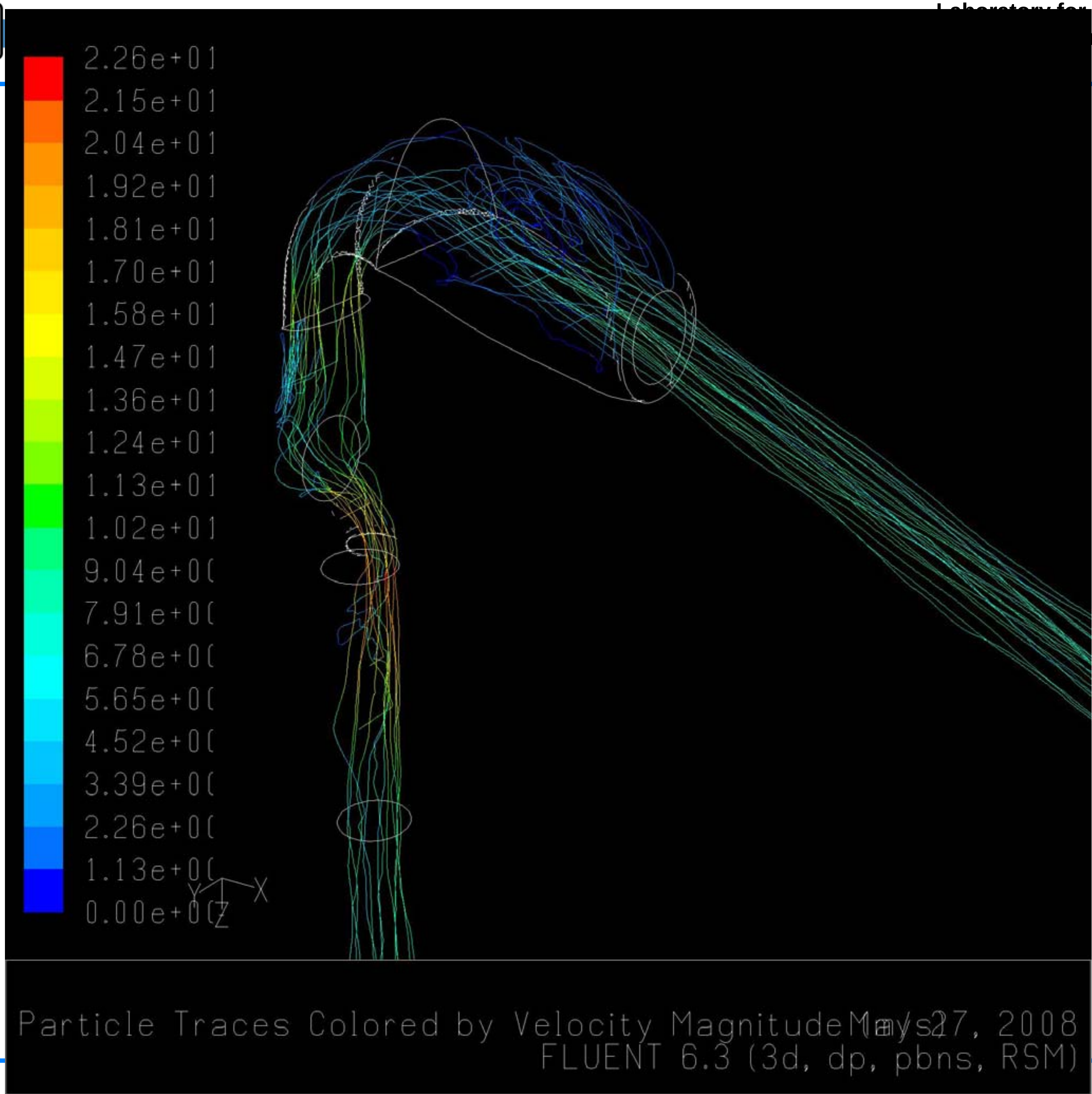
Close-up view of flow in throat



Sample velocity profiles



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2.15e+01
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1.36e+01
1.24e+01
1.13e+01
1.02e+01
9.04e+0
7.91e+0
6.78e+0
5.65e+0
4.52e+0
3.39e+0
2.26e+0
1.13e+0
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Y
X
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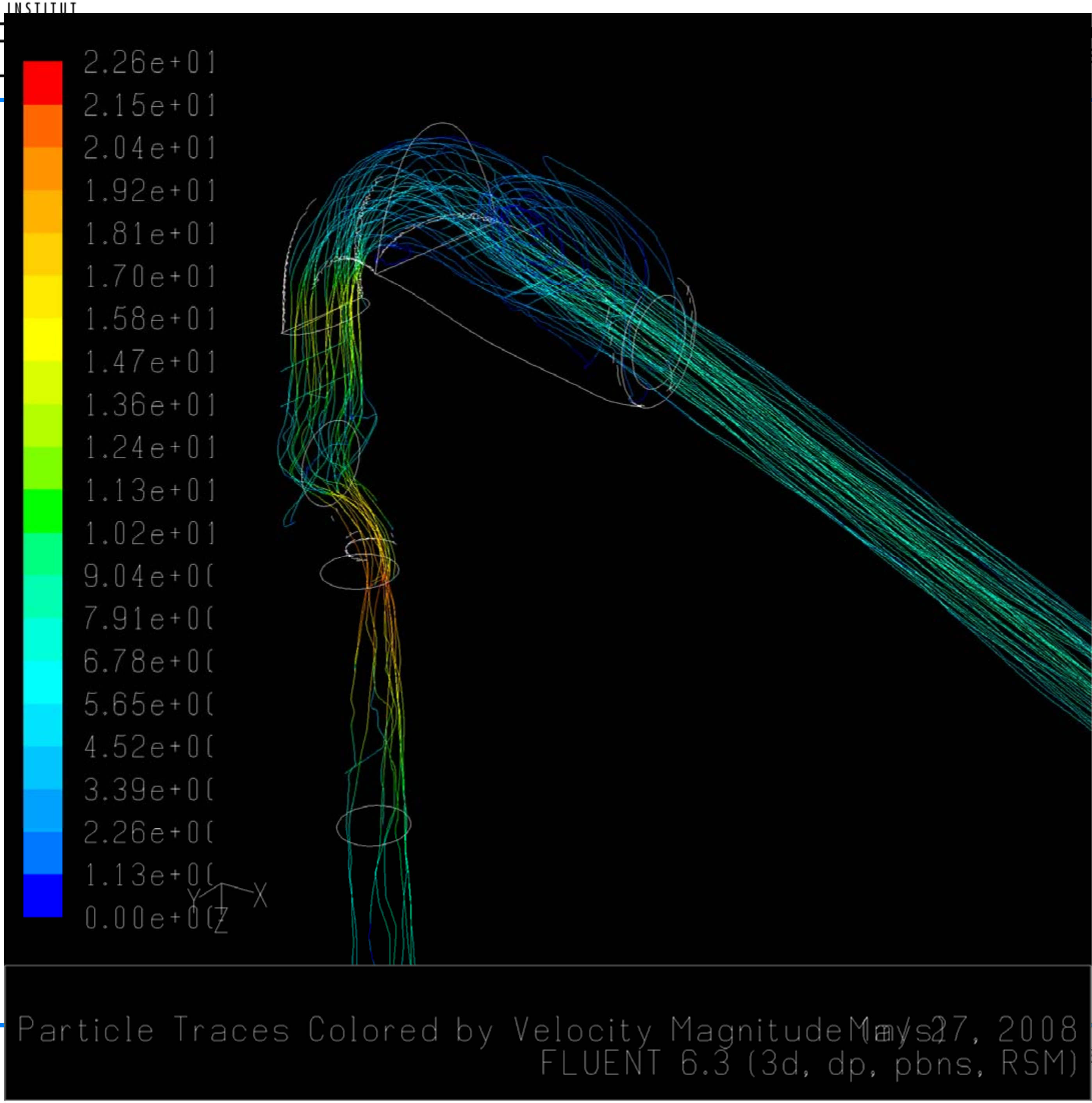
Particle Traces Colored by Velocity Magnitude (m/s)
May 27, 2008
FLUENT 6.3 (3d, dp, pbns, RSM)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1.36e+01
1.24e+01
1.13e+01
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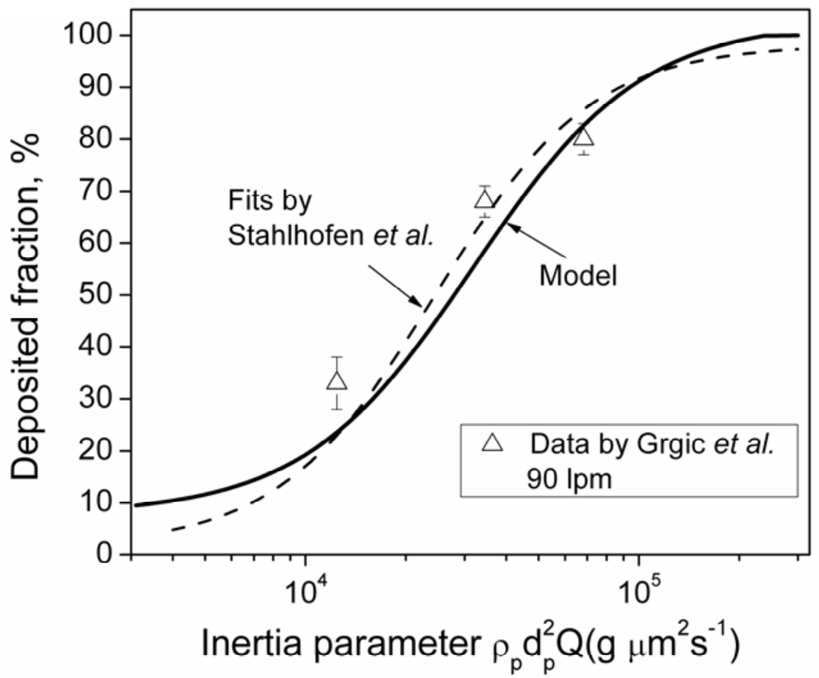
0.00e+00
Y
X
Z
Particle Traces Colored by Velocity Magnitude (m/s)
May 27, 2008
FLUENT 6.3 (3d, dp, pbns, RSM)

Particle deposition in mouth-throat geometry



Percent deposited, 90 l/min

Particle diameter µm	Data by Grgic et al.	CRW Model	Mean flow tracking
3.0	33 ± 5	23.4	4.0
5.0	68 ± 3	59.5	17.2
6.5	78 ± 3	80.1	33.0

Percent deposited, 30 l/min

Particle diameter µm	Data by Grgic et al.	CRW Model	Mean flow tracking
3.0	2 ± 2	6.4	4.4
5.0	11 ± 3	11.8	4.1
6.5	32 ± 3	21.6	5.8

Particle dispersion in presence of thermophoresis

- Thermophoresis: Force that drives particles from hot to cold regions of fluid
- A spherical particle moves in a Eulerian flow domain according to:

$$\frac{dU_p}{dt} = F_{Drag}(U - U_p) + F_{Thermo}$$

$$F_{Drag} = \frac{18\mu}{\rho_p d_p^2} C_D \frac{\mathrm{Re}}{24}$$

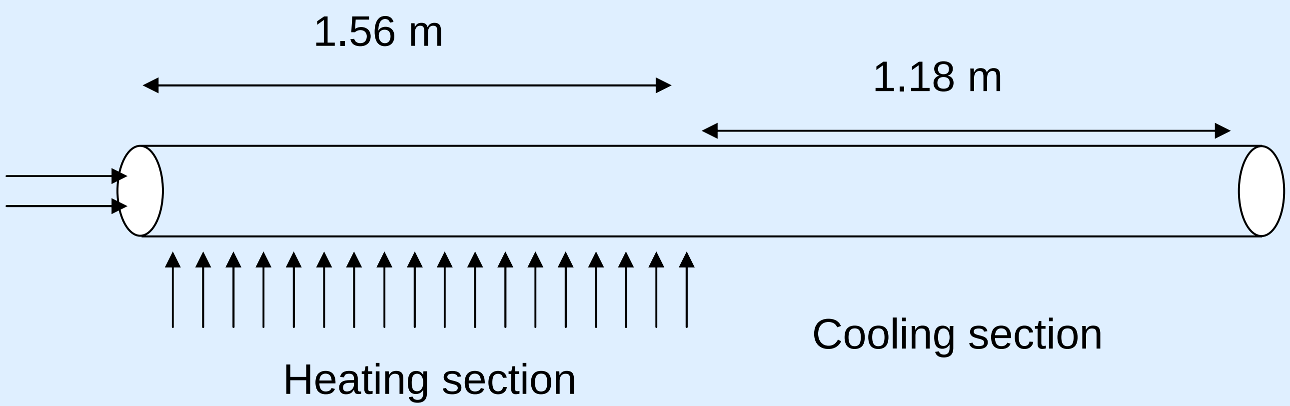
$$F_{Thermo} = C \frac{1}{T} \nabla T$$

Thermophoresis: Tests by Tsai (2004)

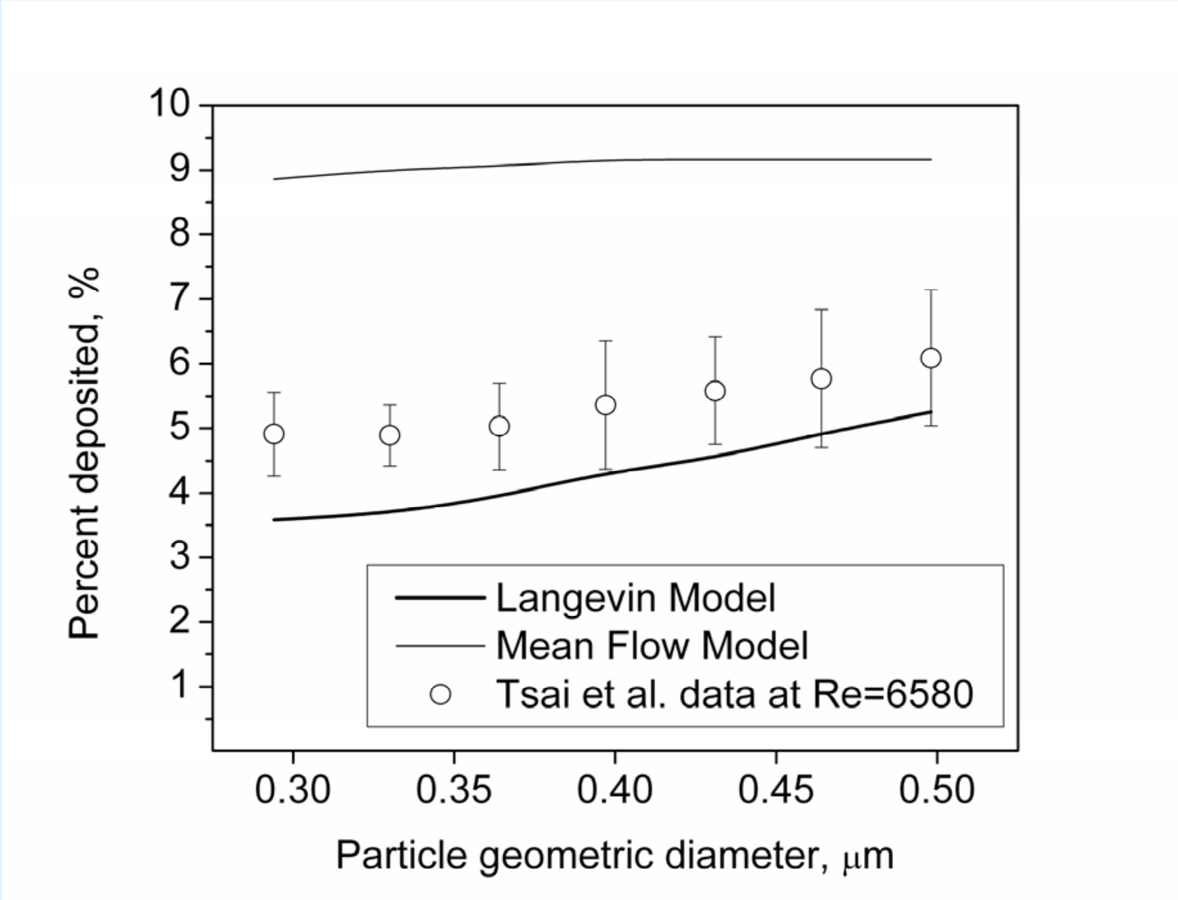
Pipe diameter= 4.3 mm
Pipe length= 1.18 m
Air @ 343 K
Wall @ 296 K
U=23.2 m/s
Re=6600

Integral deposition measured

Aerosol: NaCl
Monodisperse = 0.04-0.5 μm



Thermophoresis: Tests by Tsai (2004)



Thermophoresis: TUBA tests (Dumaz, 1993)

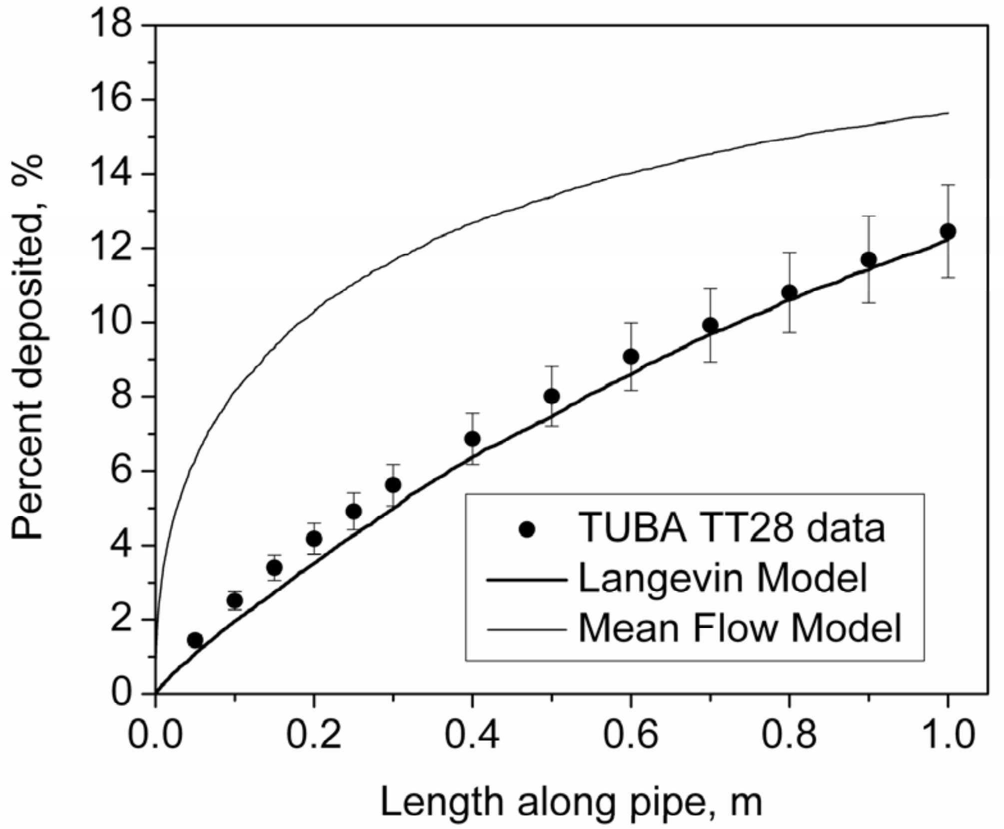
Pipe diameter= 18 mm
Pipe length= 1 m
Air @ 641 K
Wall @ 312 K
U=14.2 m/s
Re=4200

Aerosol: CsI
AMMD= 1.19 μm
GSD=1.86

Local deposition measured
Error: + or - 10 %

Laboratory for Thermal Hydraulics
Nuclear Energy and Safety

Thermophoresis: TUBA tests (Dumaz, 1993)



Turbulence and thermophoresis for tracer particles

- In isothermal flows, small inertia (tracer) particles
  - Don't deposit
  - Tend to remain fully mixed
- If thermophoresis acts on them: particles go towards the wall ***but***
  - They do have a chance to reflect back to the bulk because they respond very quickly to random turbulence bursts (unlike high inertia particles)
- Hence: tracer particles that go to the wall will ***not*** all deposit there
- Therefore: turbulence actually *reduces* thermophoretic deposition of very low inertia particles
- This explains why if one ignores radial fluctuating fluid velocities, the model will over-estimate thermophoretic deposition

Conclusions

- Non-dimensional Langevin based CRW model offers the best hope for accurate predictions of practical CFD-based particle dispersion
- Model relies heavily on DNS statistics
- Hence DNS research is of great importance to help produce better dispersion models
- Best chance of success in predicting dilute particle dispersion in turbulence flows with CFD:
  - Accurate mean flow
  - Good stochastic model
- Further benchmarking still necessary, but goal within reach