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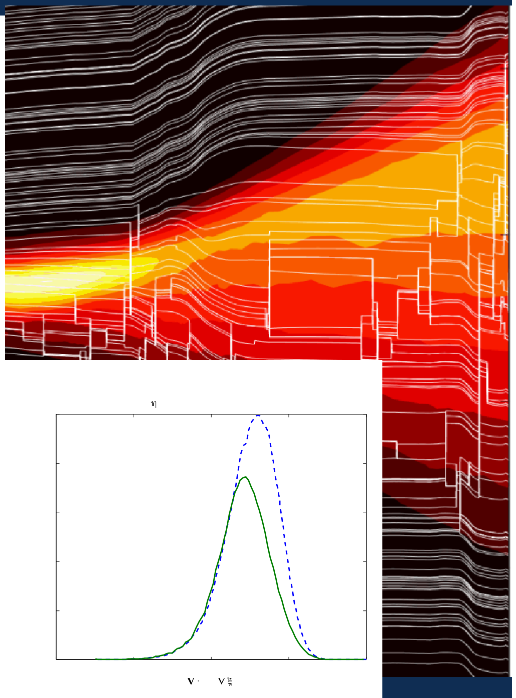

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Statistics of Particle Time-Temperature Histories in Turbulent Reacting Flows

Award Number: HDTRA-11-4503I

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DTRA Basic Research Technical Review
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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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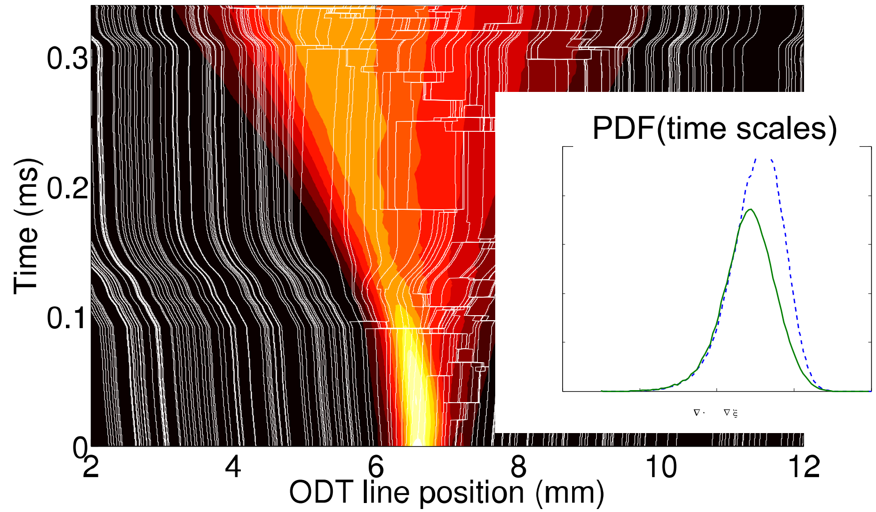
Statistics of Particle Temperature-Time Histories in Turbulent Reacting Flows; Award Number: HDTRA-11-4503I

PI: John Hewson, Sandia National Labs; Co-PI: David Lignell, Brigham Young Univ

Objective: Predict particle time-temperature history statistics through high-fidelity stochastic approach. Use statistical results to determine modeling requirements for probability of release, rare events.

Method: High-fidelity low-dimensional stochastic approach, 1D-turbulence or ODT, resolves fine scale with sufficient statistics to identify low probability events. Interpret ODT results by relating to quantities obtainable through RANS/LES.



Status of effort: Substantial progress has been made toward improving and characterizing particle transport in the context of ODT. Early predictions of particle interactions with temperature fluctuations show the broad range of scales significant.

Personnel Supported:
1 national lab staff,1 faculty member, 2 graduate students, 3 undergraduate students

Publications & Meetings: 2 peer reviewed publications. 4 conference presentations.

Major goals/milestones Year2

- Task 4: Carry out free-shear flow simulations.
- Task 5: First-stage analysis of free-shear flows.
- Task 6: ODT predictions for particle-wall deposition.

Funding Profile:
Year 1: FY11-$158k, Year 2: FY12-$158, Year 3: FY13-$168k
Contact: PI: John Hewson, jchewso@sandia.gov, 1-505-284-9210; Co-PI David Lignell, davidlignell@byu.edu, 1-801-422-1772.

Background

- Can neutralize agents by exposure to sufficient temperature or chemical insult.
  - Ex: to heat a particle

Objective

$$\frac{dT_p}{dt} = \frac{\left(T_g - T_p\right)}{\tau_h}$$

$$\tau_h\left(\lambda_g, \rho c_p, d_p, D_f, v_p - v_g, \ldots\right)$$

- Environment statistics 'seen' by particle:
  - Probability $T_g > T_{crit}$.
  - Duration over which $T_g > T_{crit}$.

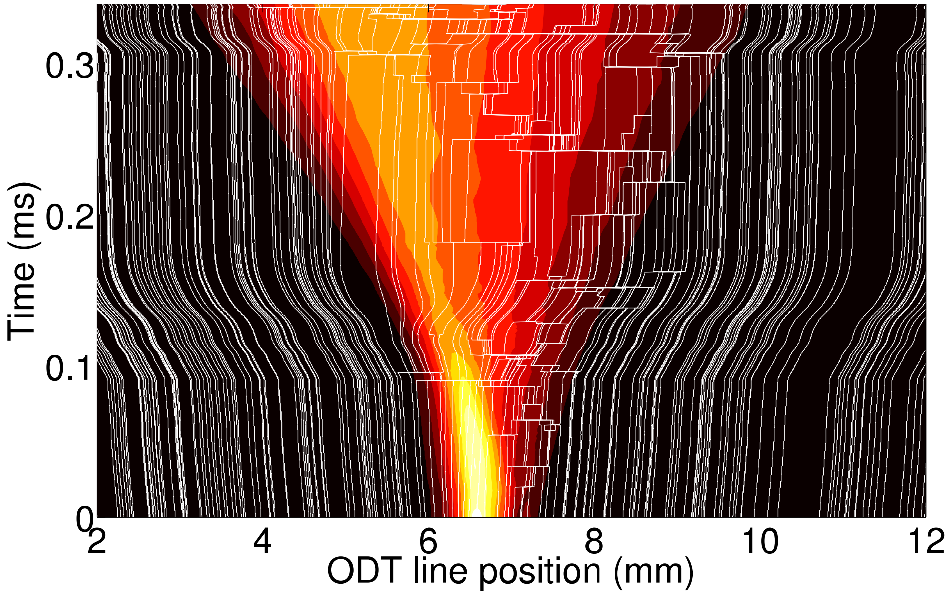
Overview

- Objective:
  - Predict particle time-temperature history statistics through high-fidelity stochastic approach.
  - Use statistical results to determine modeling requirements for probability of release, rare events.
- Relevance:
  - Since any failure to neutralize agent will be a rare event, improved understanding of tails of particle time-temperature history distribution is needed.
- Approach:
  - High-fidelity low-dimensional stochastic approach, 1D-turbulence or ODT, resolves fine scale with sufficient statistics to identify low probability events.
  - Interpret ODT results by relating to quantities obtainable through RANS/LES.

Particle dispersion

Background

- Particle dispersion frequently modeled as random walk.
- Some things are not easy to do with simple dispersion models:
  - Flow history, the cascade and inertial particles.
  - Two-way turbulence coupling.
  - Relative motion of particles and scalars – flame-particle interactions.
- ODT provide an opportunity to intimately tie turbulence evolution and particle dispersion.



- Flame-particle interactions provide an interesting target problem: What is the distribution of interaction times between a particle and flame.

Particle-flame interactions

Background

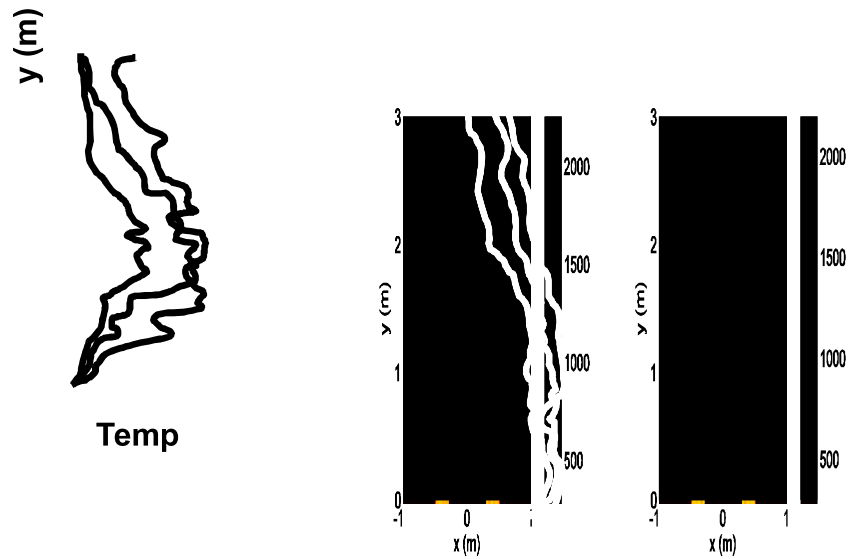
- Particle dispersion is fluid element plus slip velocity:
- Flame dispersion is fluid element plus diffusion velocity.

- This introduces two interaction rates scales:

$$(\Delta t)^{-1} = \left\langle \left(v_p - v_g\right)\nabla\xi \middle| \eta \right\rangle$$

$$(\Delta t)^{-1} = \left\langle \nabla\cdot\left(D\nabla\xi\right) \middle| \eta \right\rangle$$

Predicting particle temperature histories



- What are the statistics associated with each of these interaction scales?
- First, we need to develop a framework for combined particle-flame dispersion.

Outline

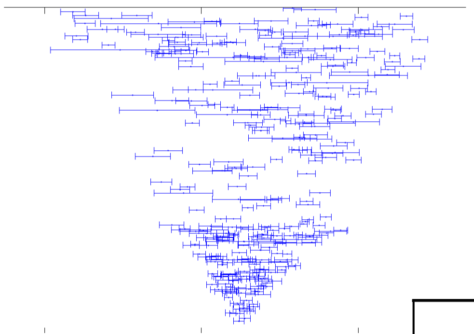
- Background: approaches and relevant time scales.
- Approach: ODT with particles
- Dispersion in jet flows (dilute and dense).
- Shear layer statistics: particle time scales and temperatures.
- Wall-deposition predictions.
- Future directions.

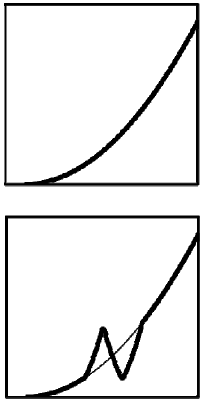
One Dimensional Turbulence (ODT)

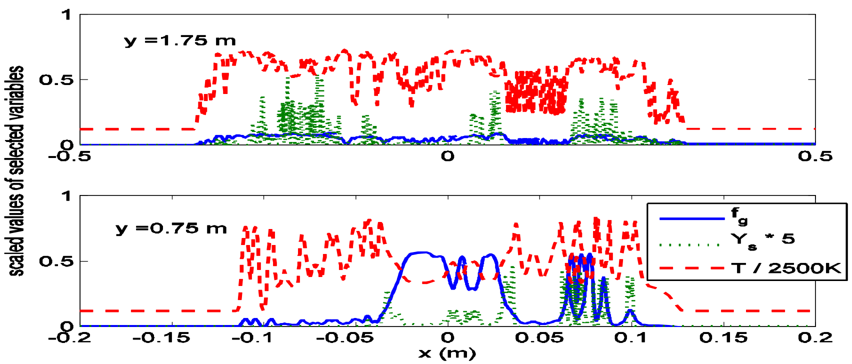
- Resolves diffusive-reactive structures: heat, species, mass, momentum.
- 1-D: line through flame or along dominant gradient
- Turbulent advection modeled via stochastic eddy events.
- Computationally affordable.
  - O(10) min per realization
  - O(100) realizations for statistics

Diffusion and Reaction

Stochastic Advection







ODT Particles – Deterministic diffusion step

- Particles interact with eddies and advance deterministically during diffusion step
- Bassett-Boussinesq-Oseen equation describes deterministic motion of particles in the fluid.

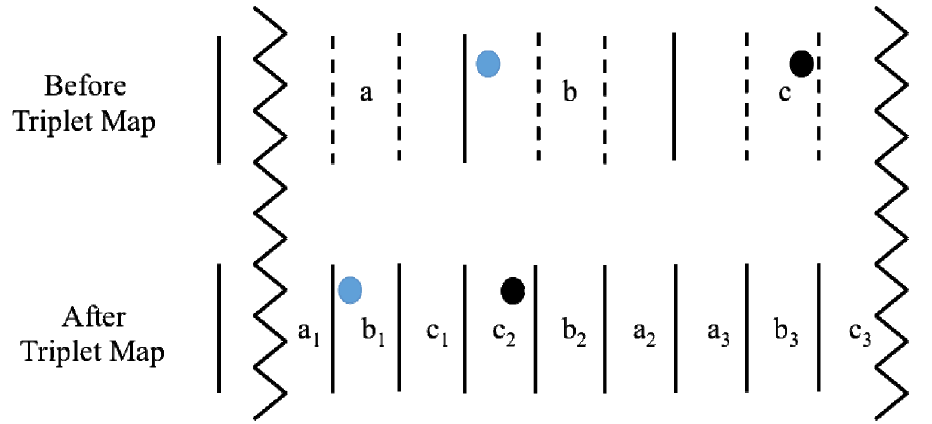
$$\frac{du_{p,i}}{dT} = -\frac{(u_{p,i} - u_{g,i})}{\tau_p} f + \frac{F_i}{m_p} \qquad \frac{dx_p(y_p, z_p)}{dT} = u_{p,i}$$

Particle relaxation time $\tau_p = \frac{\rho_p d_p^2 C_c}{18\mu}$

Triplet mapping particles

- A time developing ODT model with coupled particle tracking

(A) Fluid (tracer) particle in eddy



(B) Inertial particle in eddy: resulting difference with / without eddy

Y

V_p^{old}

Trajectory interaction

Y

V_p^{old}

Δy_p

V_p^{new}

V_p^i

Δy_p

$$\Delta V_p = V_p^i(t_e) - V_p^n(t_e)$$

Trajectory without interaction

V_p^n

Interaction time T

Particle time t

Particle-eddy interaction

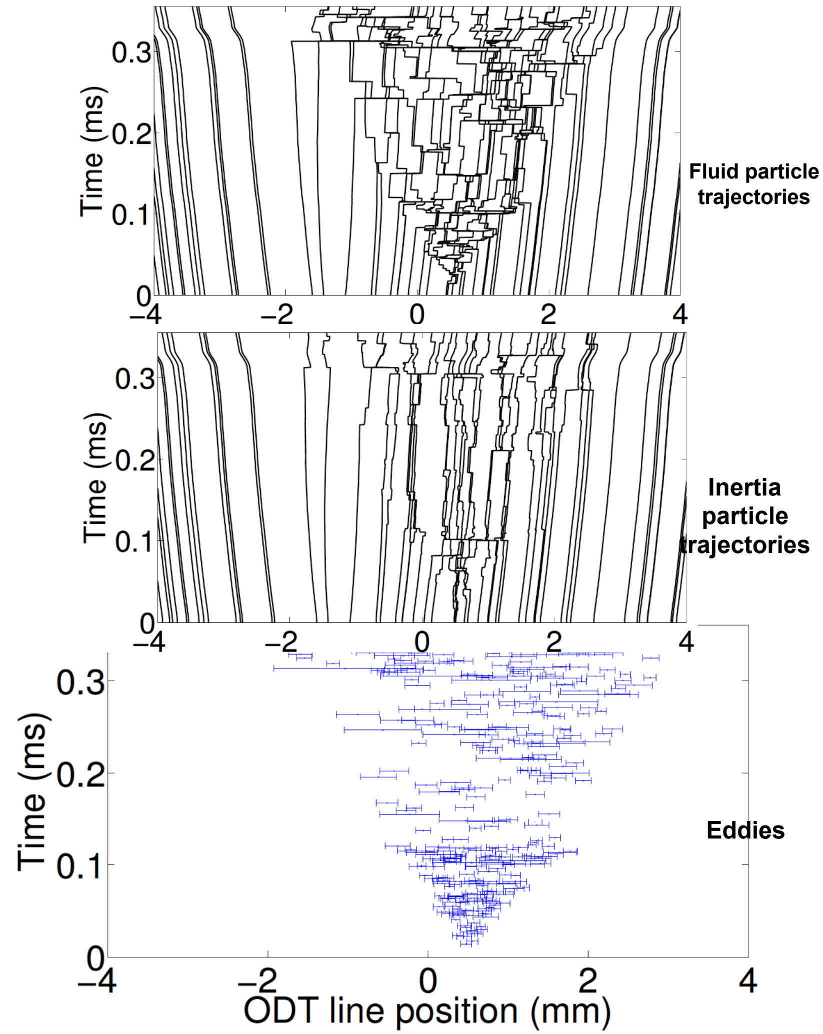
- Eddy interaction time: smaller of eddy lifetime and eddy crossing time.
- Eddy velocity – during eddy events

$$v_{eddy} = \frac{\Delta y_p}{t_e}$$

Eddy-direction velocity from fluid displacement

Eddy lifetime $$t_e = \beta_p \tau(y_0, l; t)$$

Eddy time scale $$\tau(y_0, l; t) = \frac{C}{l^2 \lambda(l)}$$



Particle-eddy interaction – over eddy lifetime

- Two different time coordinates
  - Interaction time coordinate (T)
  - Real time coordinate (t)

Type-I interaction: The particle-eddy interaction is instantaneous in real time t while it exists for finite time in interaction time coordinate T.

Y

V_p^i

Eddy box

Particle path

Eddy lifetime

Interaction time T

Y

V_p^i

Particle path

Instantaneous eddy

Real time t

Type-C interaction:

There is no instantaneous particle displacement;
the eddy exists in real time for eddy lifetime.

Type-I

Y

V_p^i

Eddy

Real time t

Type-C

Y

V_p^i

Eddy

Interaction time T

Real time t

Type-IC interaction

- If a particle has an instantaneous displacement from a type-I interaction at the birth of the eddy, the particle will not have continuous type-C interaction with the same eddy later.

Y

I1 I2 C3

Real time t

Y

C1 I2 C3 C4 C5

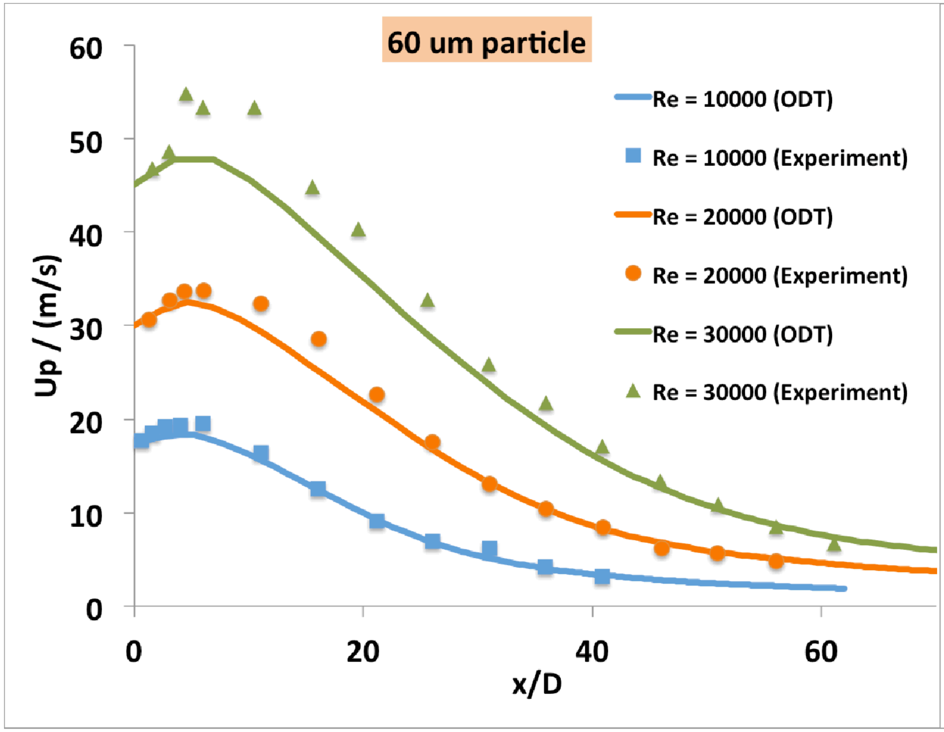
Real time t

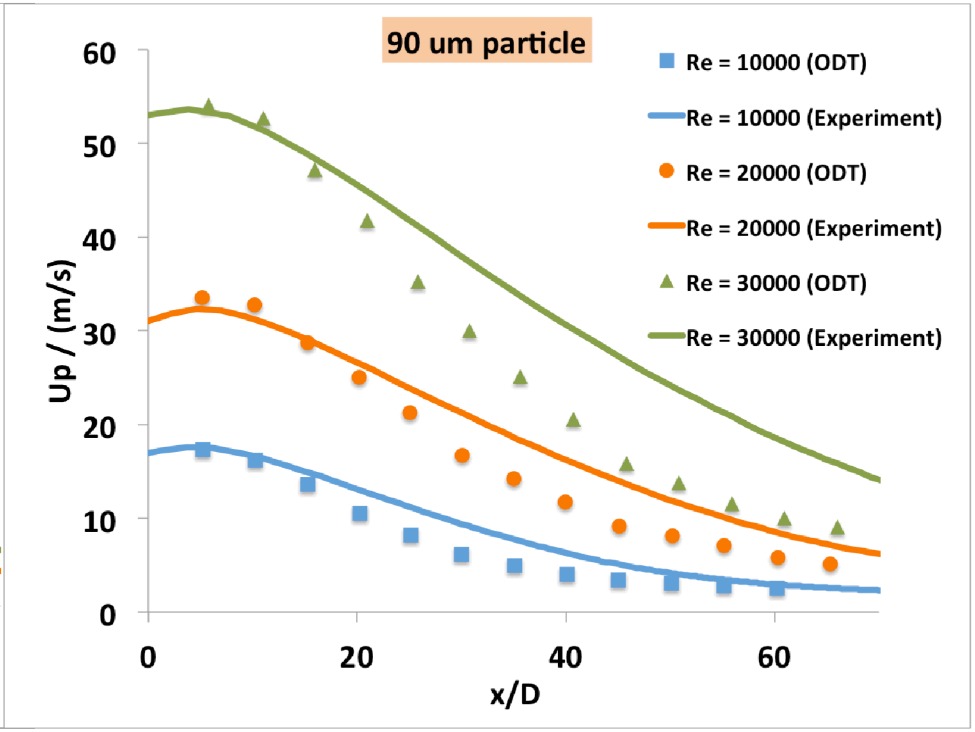
Particle dispersion in a dilute jet

- Experimental measurements from Kennedy and Moody (*Expt. Thermal and Fluid Sci*., 1998).
- Monodisperse hexadecane droplets in
  - 417 pseudo particles, each of which represents 10^6 real particles
- Particle diameter = 60 μm and 90 μm
- Jet diameter = 0.007 m and 0.0126 m
- Reynolds numbers 10000, 20000, 30000.
- ODT parameters (fixed in all the cases):
  - C = 8
  - Z = 50
  - Z_third = 0.32 (large eddy suppression)
  - Beta_p = 1 (particle-eddy interaction time)

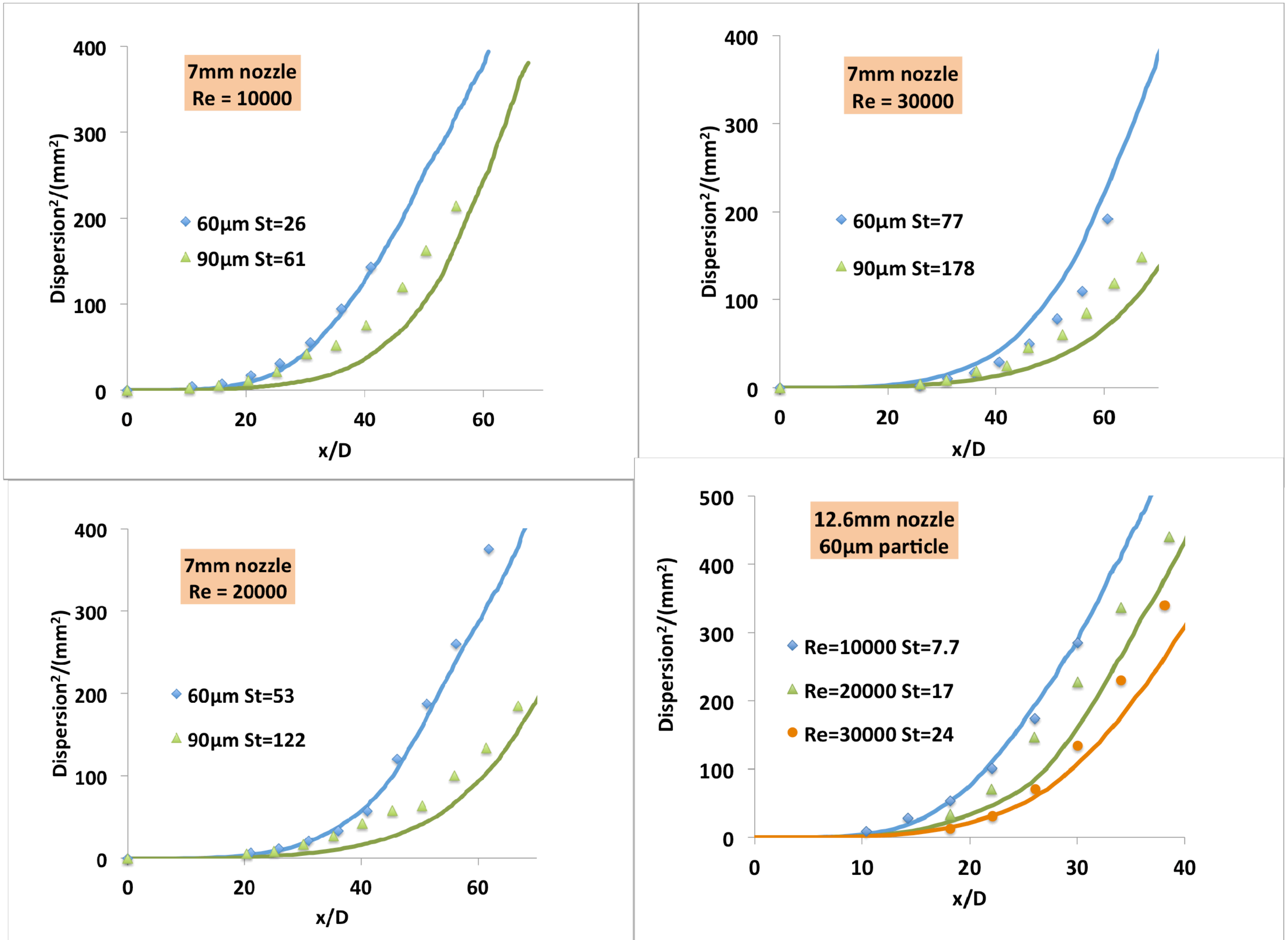
Ambient air at rest

Particle velocities in a dilute jet





Particle dispersion in a dilute jet



Particle dispersion in a dilute jet – sensitivity to $\beta_{\square}$

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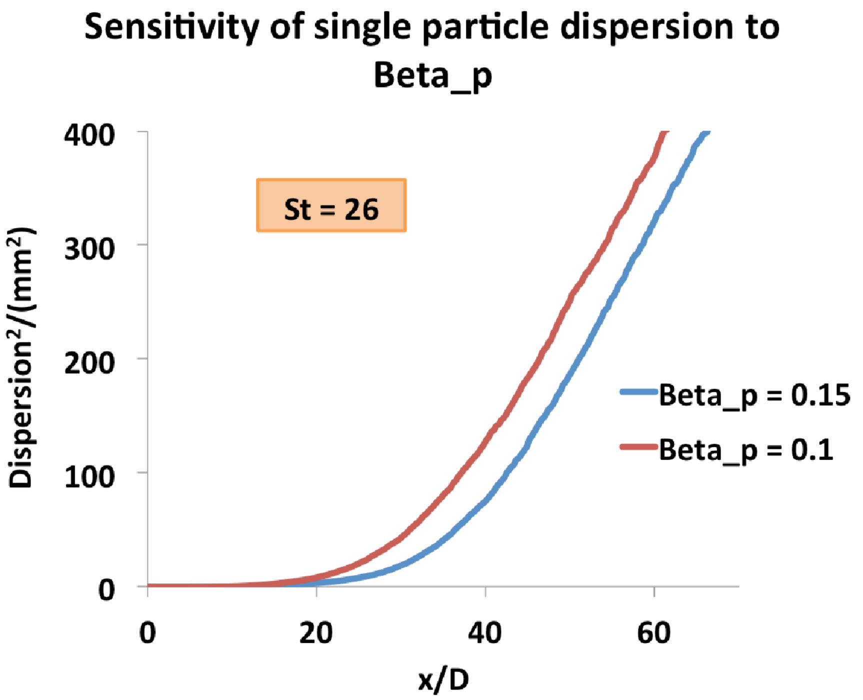
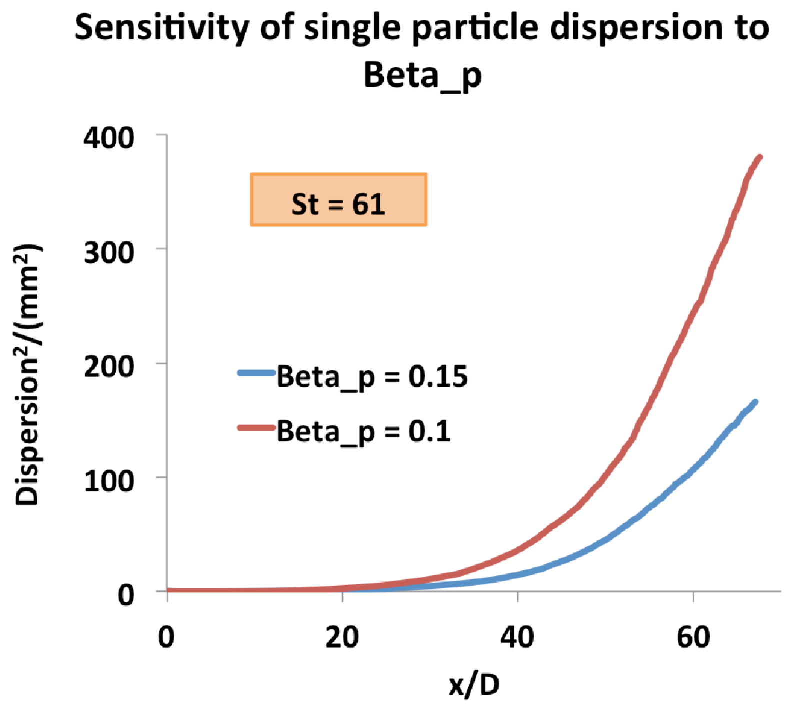




- β_p scales the eddy lifetime and the eddy displacement velocity.
- For large Stokes numbers, smaller β_p leads to greater dispersion.

Particle Implementation: two-way coupling

- Momentum coupling for dense flows

$$S_{p,i} = -\sum_j m_{pj} N_p \frac{du_{pj,i}}{dt}$$

- Momentum coupling incorporated into eddy rate
  - Follows variable density vector ODT formulation.
  - Post triplet map velocity field

$$v_i^{m+1}(y) = v_i\left[f(y)\right] + b_i J(y) + c_i K(y)$$

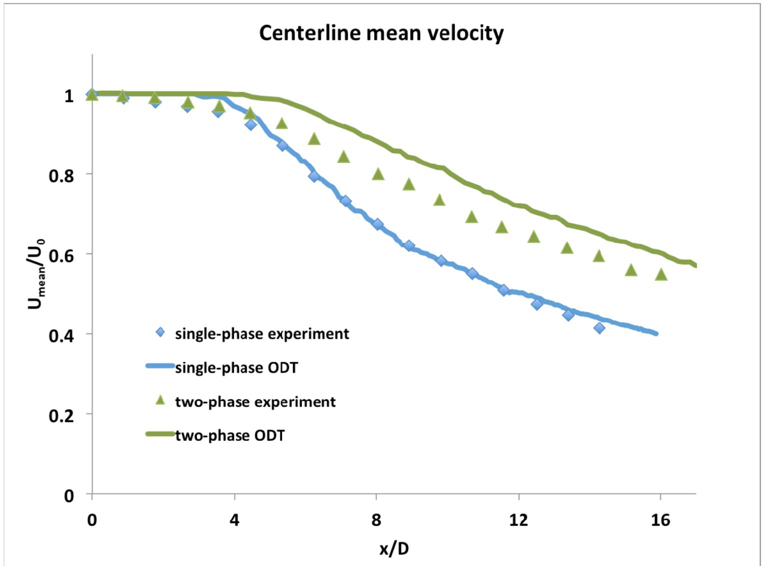
  - $c_i K(y)$ redistributes velocity fluctuations among 3 components – mimics pressure scrambling.
  - $b_i J(y)$ enforces momentum conservation:
    - Particle source.
    - ρv = constant in pressure scrambling model.

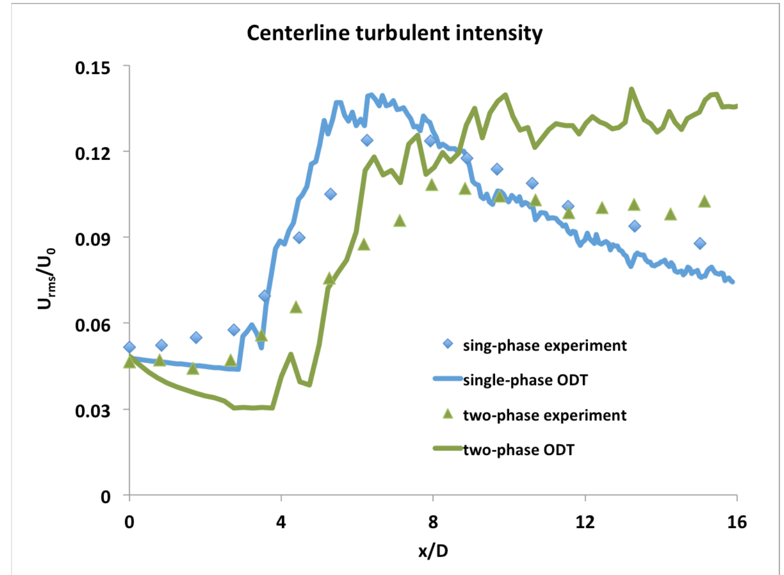
Dense particle-laden jet: overview

- Experimental measurements from Budilarto PhD thesis at Purdue (2003)
- Solid loading = 0.5
  - 417 pseudo particles, each of which represents 10^6 real particles
- Particle diameter = 25 μm
- Stokes number = 3.6
- Jet diameter = 0.0142 m
- Initial gas and particle velocity = 11.7 m/s
- ODT parameters (fixed in all the cases):
  - C = 8
  - Z = 50
  - Z_third = 0.32 (large eddy suppression)
  - Beta_p = 1 (particle-eddy interaction time)
- Three kinds of particle-eddy interactions
  - Type-I, C and IC

Ambient air at rest

Dense particle-laden jet: centerline velocities



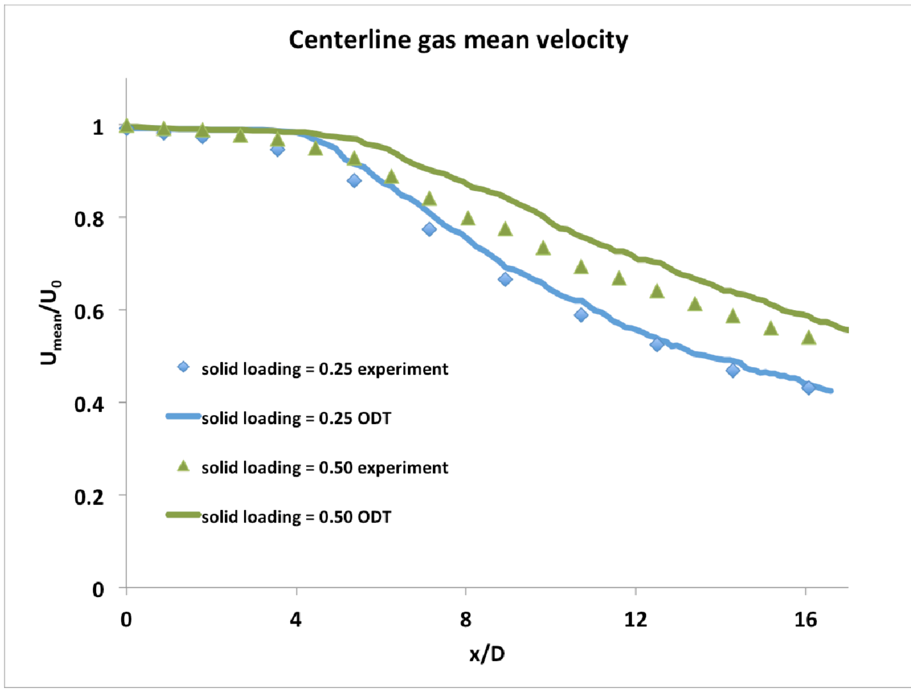


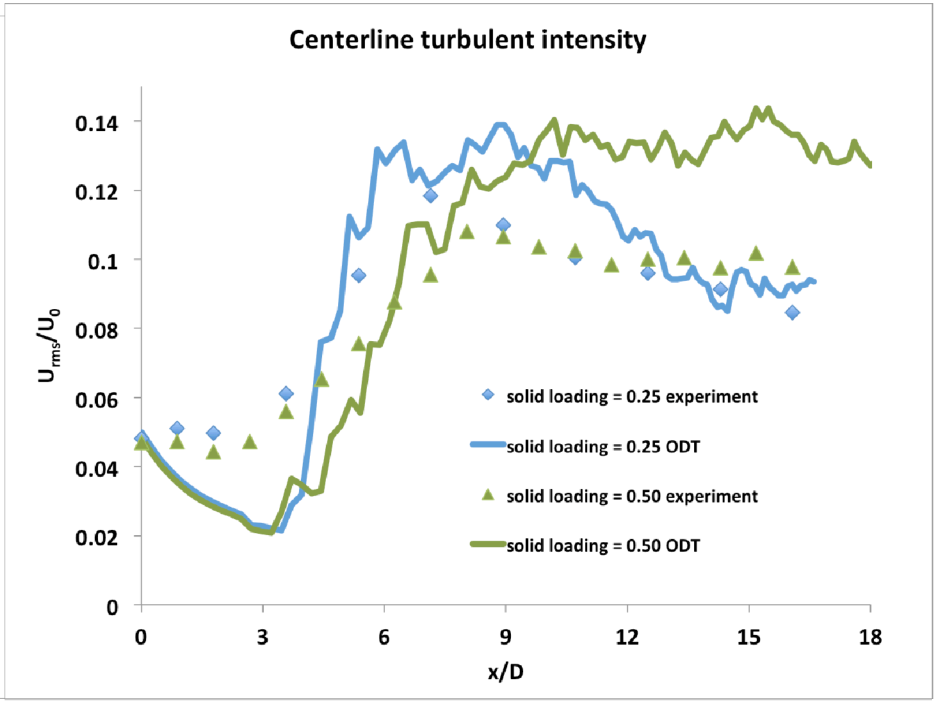
- Centerline mean values are all well predicted.
- Laden jet with greater net density slows more gradually.
- St = 3.6

- Qualitatively similar fluctuation results: particle laden jets develop and decay more gradually.
- ODT fluctuations rise too quickly, too far: from instantaneous nature of eddies?

Dense particle-laden jet: solid-loading fraction

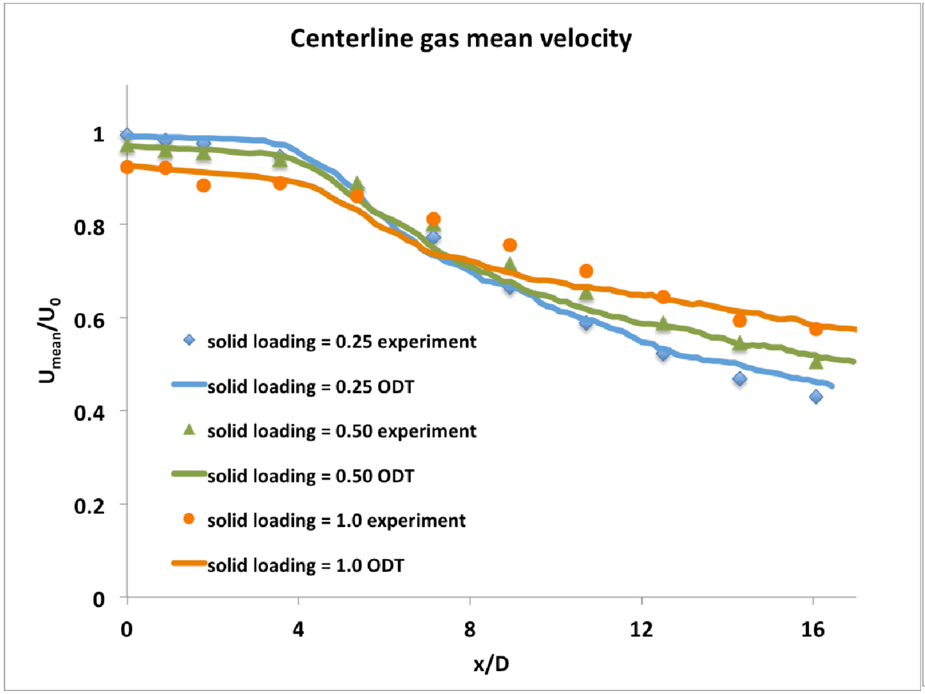
- 25 mm particles (Stoke number = 3.6)
- Solid loadings: 25% and 50%.

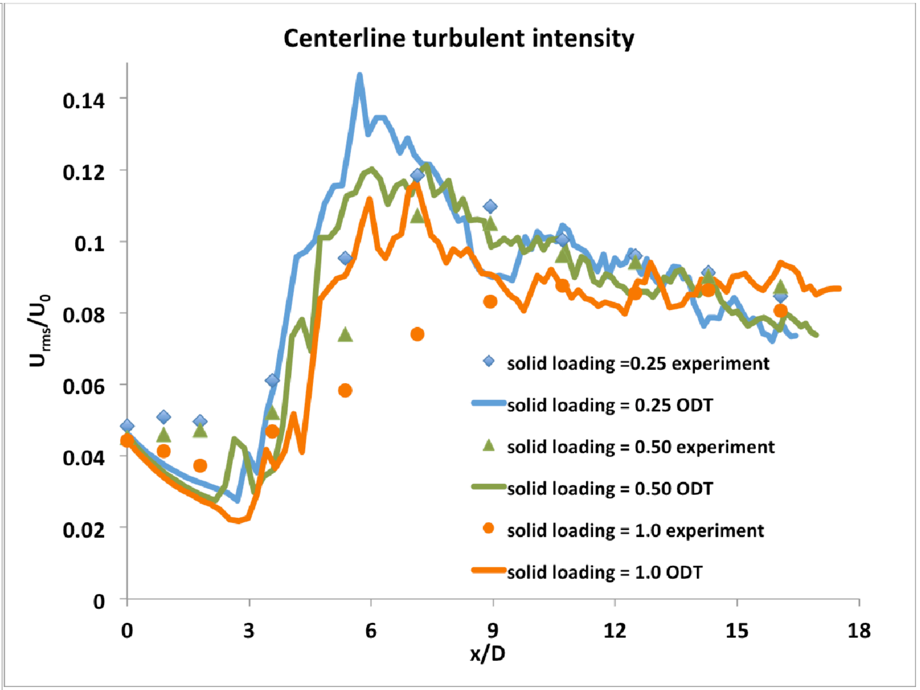




Dense particle-laden jet: solid-loading fraction

- 75 mm particles (Stoke number = 10.8)
- Solid loadings: 25%, 50% and 100%.





Channel flow wall deposition

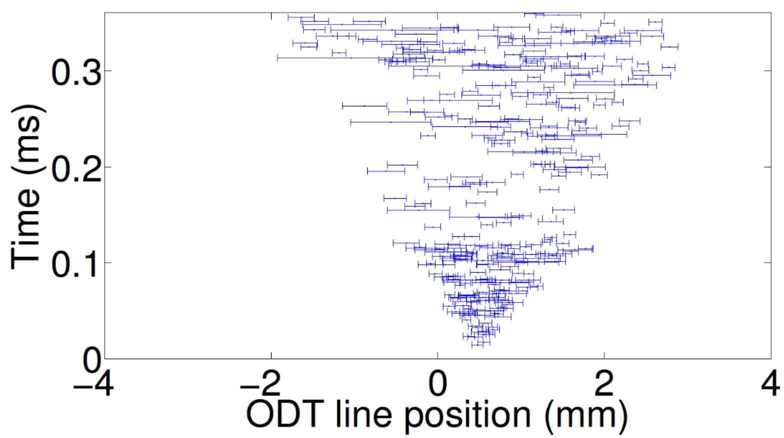
- For intermediate τ_p, turbophoretic deposition dominates.
- For larger τ_p, particles less affected by BL turbulence.

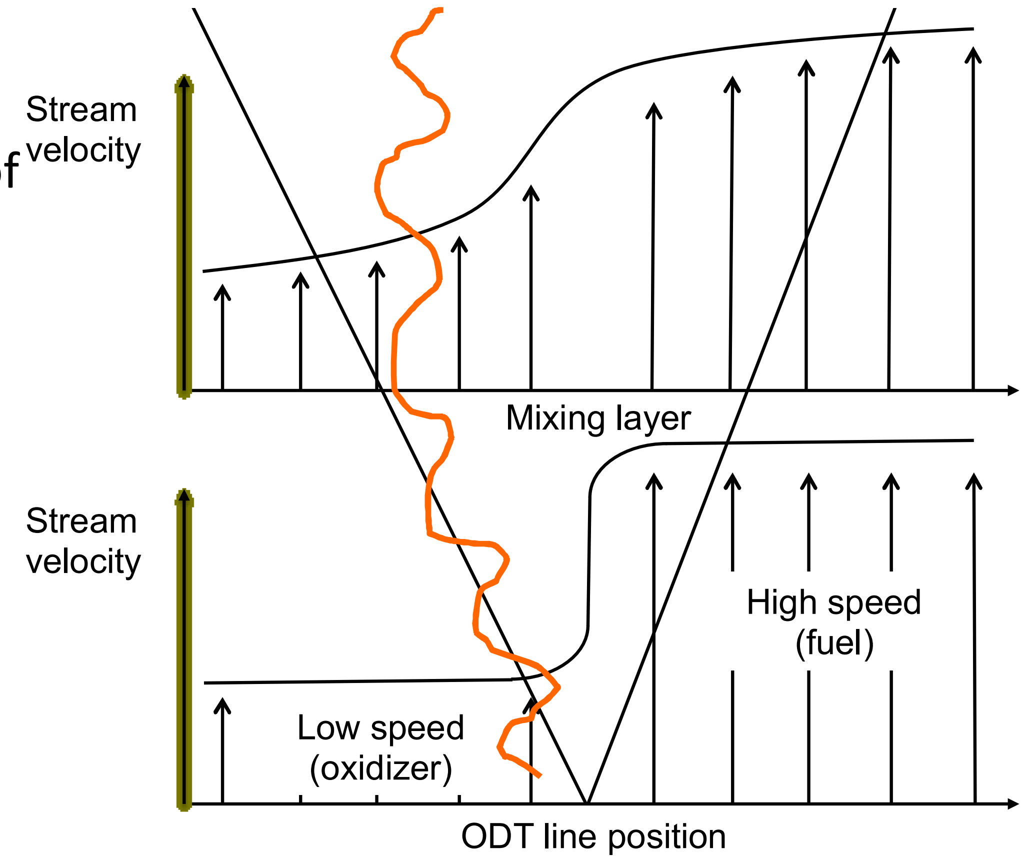
- Note: this comparison motivated some changes in particle-eddy interaction model.

Liu and Agarwal, *Aerosol Science,* 5:145-155, 1974.

Reacting Mixing Layer

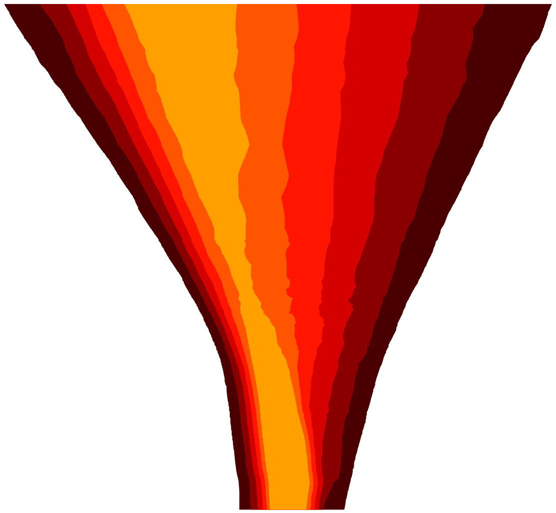
- Temporal ethylene mixing layer.
- 1.5 cm domain, Δv = 196 m/s.
- Streams at 550 K, 1 atm.
- Particle positions across middle of domain.
- Particle time scale 0.5 ms, 5 ms,
  - St = O(10-100's)



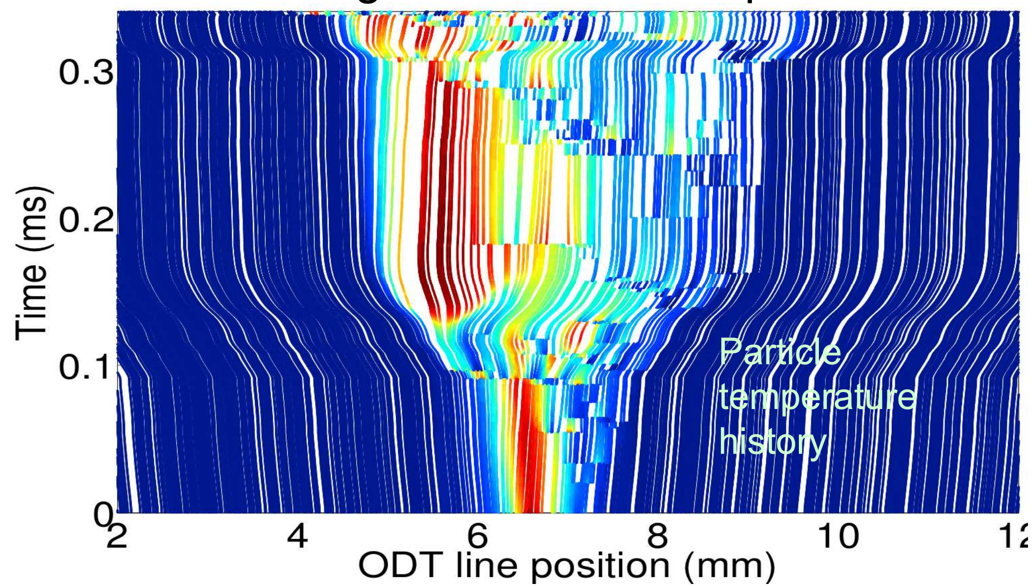


Temperature Histories

average temperature



Single realization temperature



- What are the statistics associated with each of these interaction scales?

Particle slip relative to flame width

$$(\Delta t)^{-1} = \langle (v_p - v_g)\nabla\xi | \eta \rangle$$

Flame diffusion relative to fluid element

$$(\Delta t)^{-1} = \langle \nabla \cdot (D\nabla\xi) | \eta \rangle$$

Shear layer time scales

Conditional average dissipation rate

Conditional average flame diffusion rate

Particle slip relative to flame width

$$(\Delta t)^{-1} = \left\langle \left(v_p - v_g \right) \nabla \xi \middle| \eta \right\rangle$$

Flame diffusion relative to fluid element

$$(\Delta t)^{-1} = \left\langle \nabla \cdot \left(D \nabla \xi \right) \middle| \eta \right\rangle$$

Shear layer time scale distributions

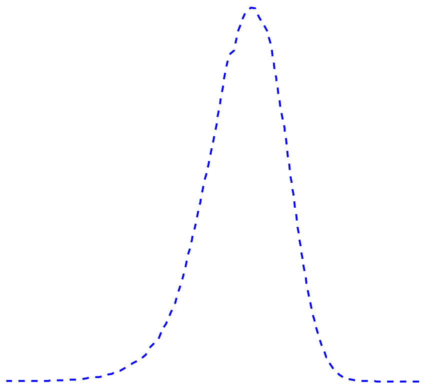
Particle slip relative to flame width

$$\left(\Delta t\right)^{-1} = \left\langle \left(v_p - v_g\right) \nabla \xi \middle| \eta \right\rangle$$

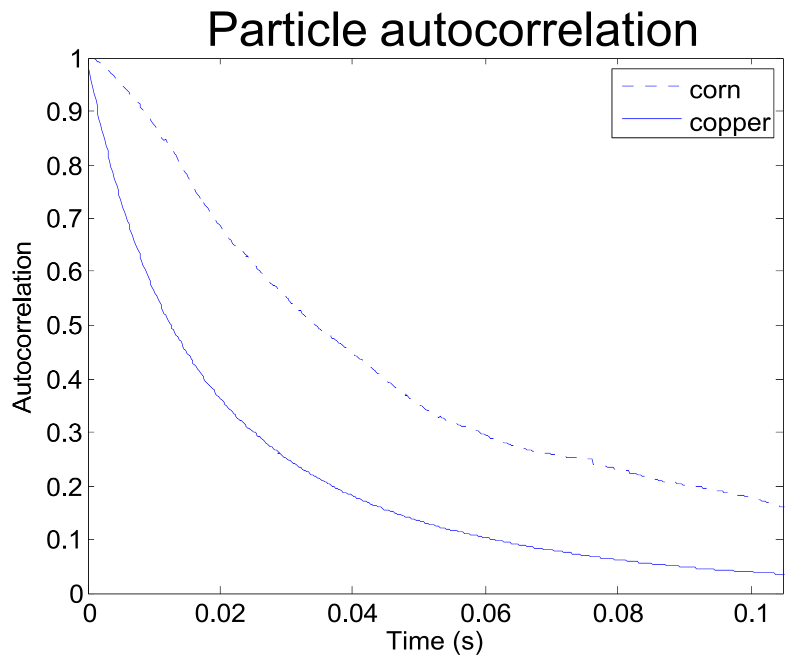
Shear layer time scale distributions

Flame diffusion relative to fluid element

$$\left(\Delta t\right)^{-1} = \left\langle \nabla \cdot \left(D \nabla \xi \right) \middle| \eta \right\rangle$$



Future work – Next steps



- Continued validation of particle-turbulence interactions.
- Particle-wall deposition simulations.
  - First-crossing analysis and turbulent dispersion modeling.
- Further analysis of free-shear flows
  - Crossing frequencies, interaction time scales, correlation time and length scales, particle temperature statistics.
  - Langevin and Fokker-Planck approaches to interpreting correlations between T_p, T_g.

‘Unexpected results’

- Extended ODT model from type-I to type-C and type-IC implementations.
- Two-way particle-turbulence momentum and kinetic energy coupling.
- Strong particle clustering observed in statistically steady channel flow.

Collaborations

- Brigham Young University, David Lignell, Guangyuan Sun.
- ODT code development
  - Alan Kerstein
  - Heiko Schmidt, TU Cottbus.
  - Michael Oevermann, Chalmers University.
- United Technologies Research Center (interactions on water mists).

Dissemination

- Publications
  - ODT jet validation paper: D. O Lignell, D. S. Rappleye, "One-dimensional turbulence simulation of flame extinction and reignition in planar ethylene-jet flames," *Comb. Flame*, 159: 2930-2943, 2012.
  - Methods paper: D. O. Lignell et al., "Mesh adaption for efficient multiscale implementation of one-dimensional turbulence," *Theroretical Computational Fluid Dynamics,* 27:273-295, 2012.
- Presentations
  - AIChE Annual Meeting, Pittsburgh, Nov 2012.
  - APS Division of Fluid Dynamics Meeting, San Diego, Nov 2012.
  - SIAM Numerical Combustion Meeting (2 presentations), April 2012.

Summary

- Continued development of ODT particle-eddy interaction models:
  - Type-C and type-IC to supplement type-I.
  - Momentum coupling for large mass loadings.

- Validation of ODT particle dispersion using dilute and particle-laden jet flows and channel flow.

- Demonstration of particle time-temperature interaction scales in shear layer.

Acknowledgements

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- The investigators appreciate the guidance from Alan Kerstein and John Schmidt regarding the ODT model and implementation of particle transport into the ODT model.

Backup material