Effects of Stirring and Mixing Processes on Reactive Species in Turbulent Flow Environments

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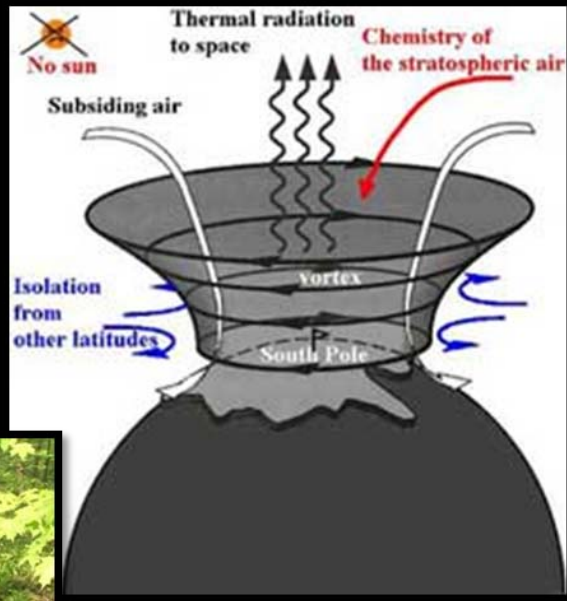
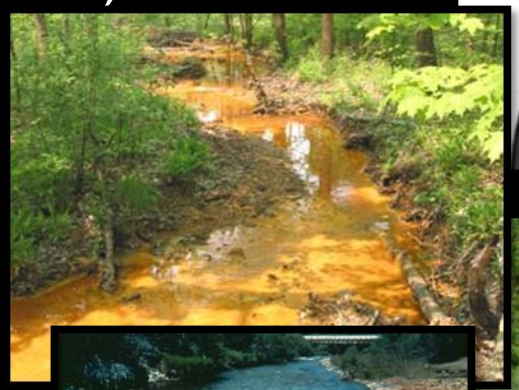
Contaminant Transport Applications



Reactive chemical mixing & stirring in turbulent flows play a crucial role in many fields:

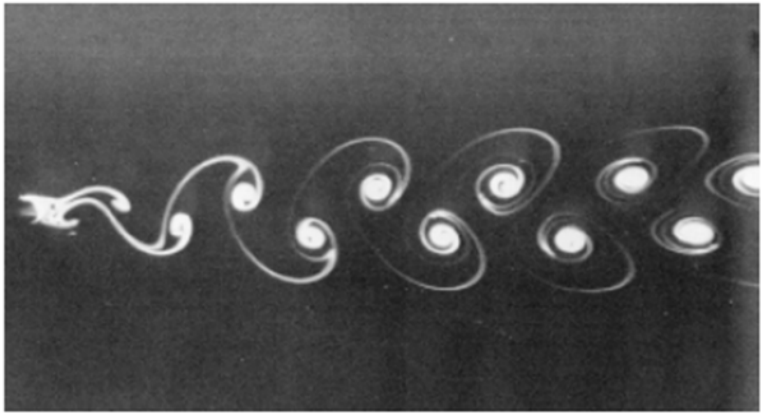
- AMD Plume Dynamics
- Wastewater Treatment
- Spawning
- Atmospheric Chemistry
- Combustion
- Microfluidics



Turbulent Flow Environments

Turbulent ocean flows are made up of multiple vortices (eddies)

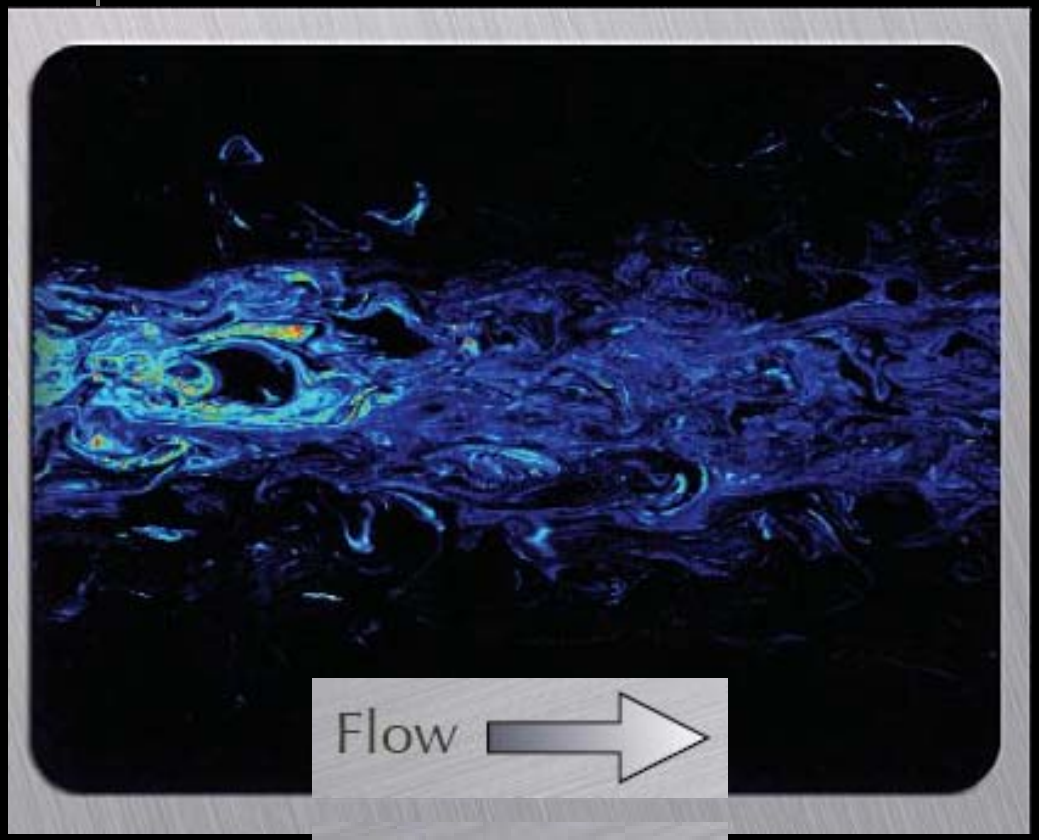
- Large scales: turbulent stirring (stretches patches of contaminants out into filaments)
- Small scales: molecular diffusion (ultimately brings initially distinct contaminants together)



Karman vortex street behind a cylinder placed in uniform flow. Re ~ 300 [Courtesy: Sadotoshi Taneda; from An Album of Fluid Motion by Van Dyke (1982)]

(Source: Dr. Matthew Reidenbach, UC-Berkeley)

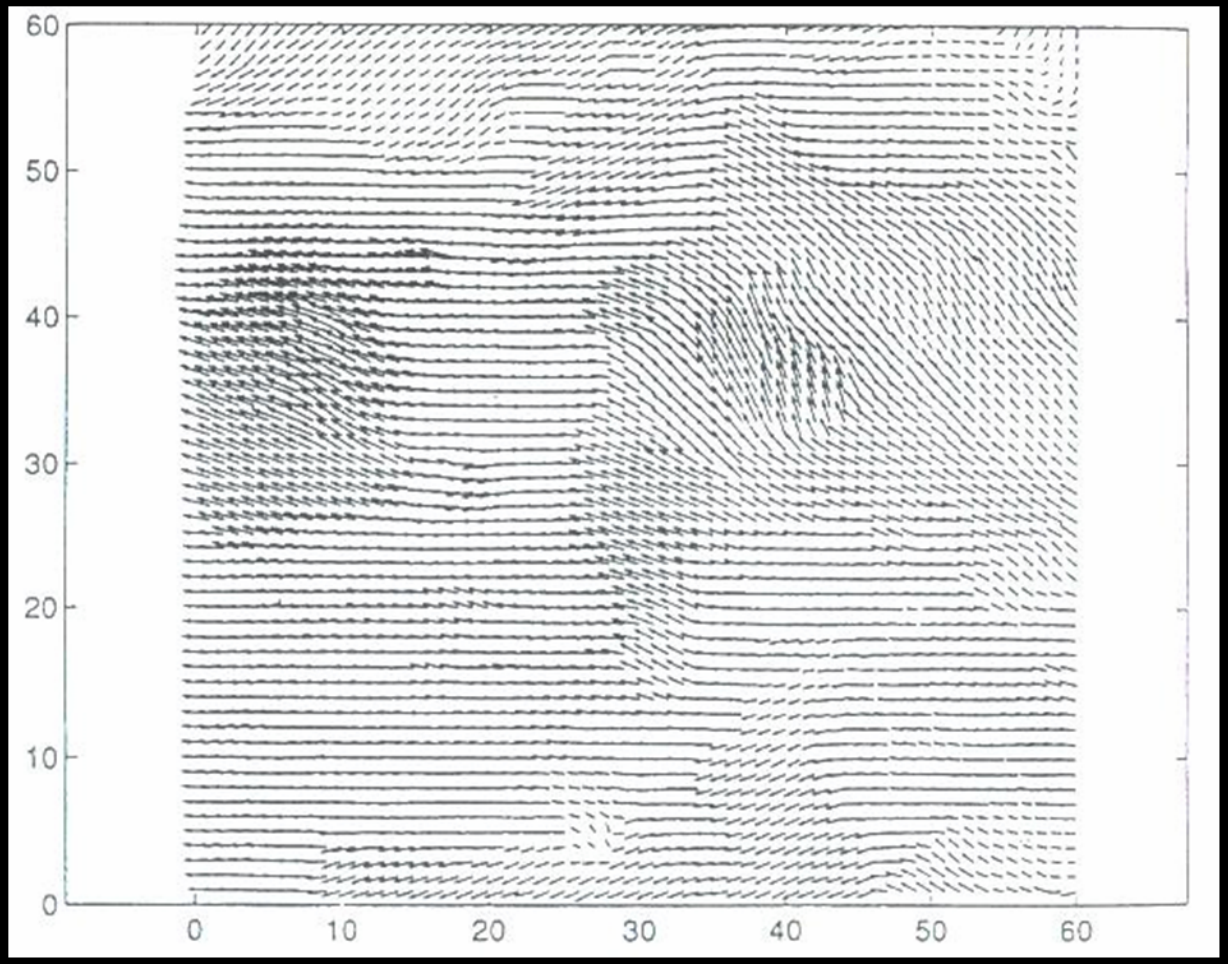
Real Plume Structure



Top View

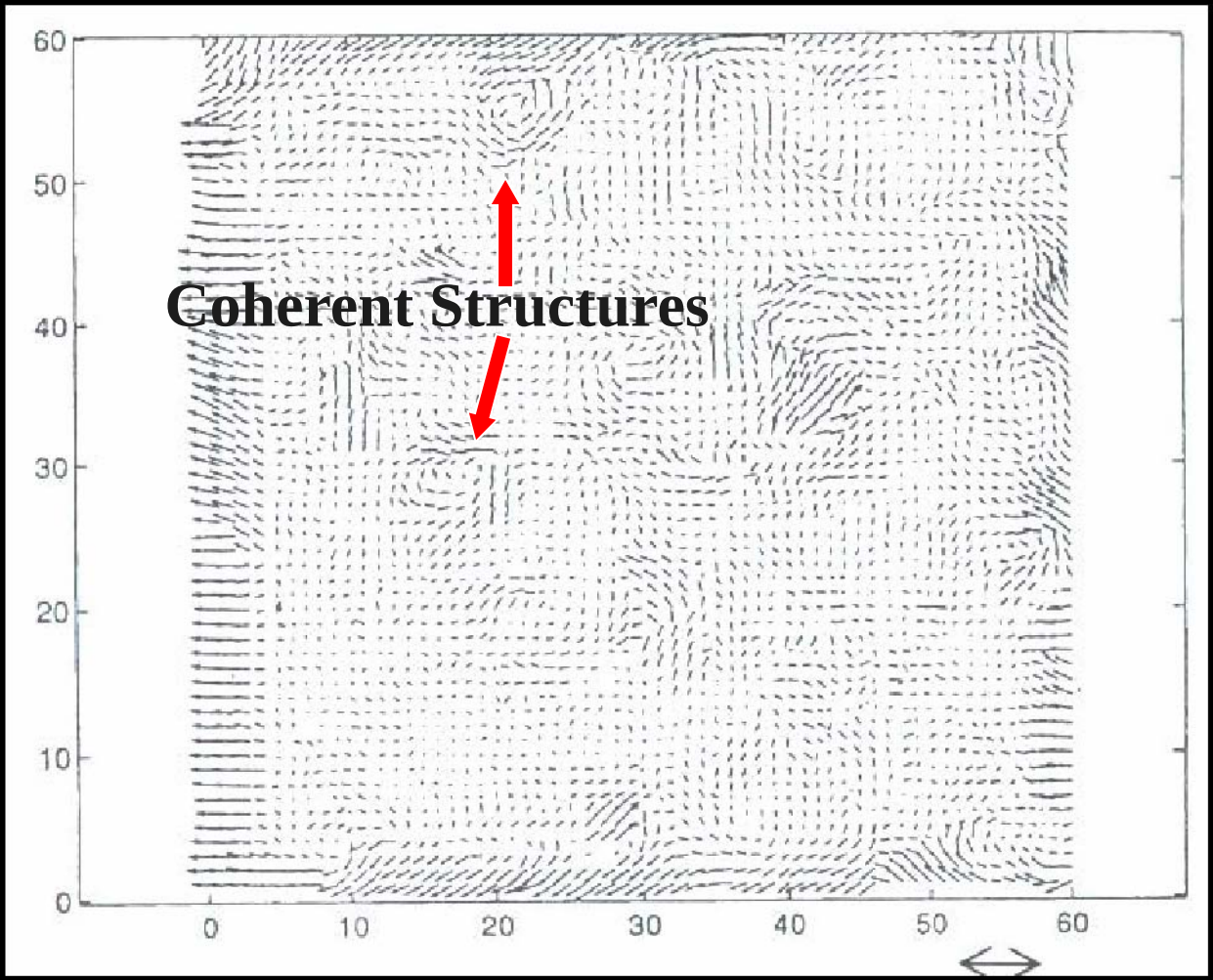
Side View

Translating Flow—Includes Mean



(Cheng et al. 1997)

Translating Flow—Subtract Mean



(Cheng et al. 1997)

Physics + Biology/Chemistry

- ***Primary Interest***:
  Reaction rates between initially distinct scalars

- ***Motivating Problems***:
  1) Wetland treatment of point-source contaminants,
  2) Biological reproductive process, broadcast spawning

- ***Focus***:
  Physical mechanisms that govern reaction between scalars

Hypothesis

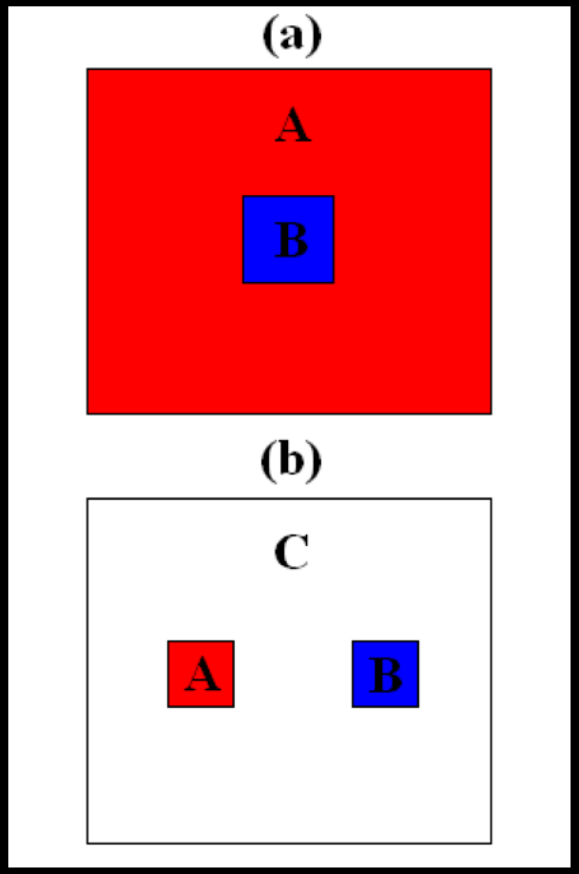
- *conventional thought: turbulence produces rapid dilution of scalars*

- *<u>we propose a contrary hypothesis</u>: while turbulence promotes dilution at longer time scales, structured velocity fields produces spatial scalar correlations and enhances reaction rates*

Two Advection-Diffusion-Reaction Classes

Class #1

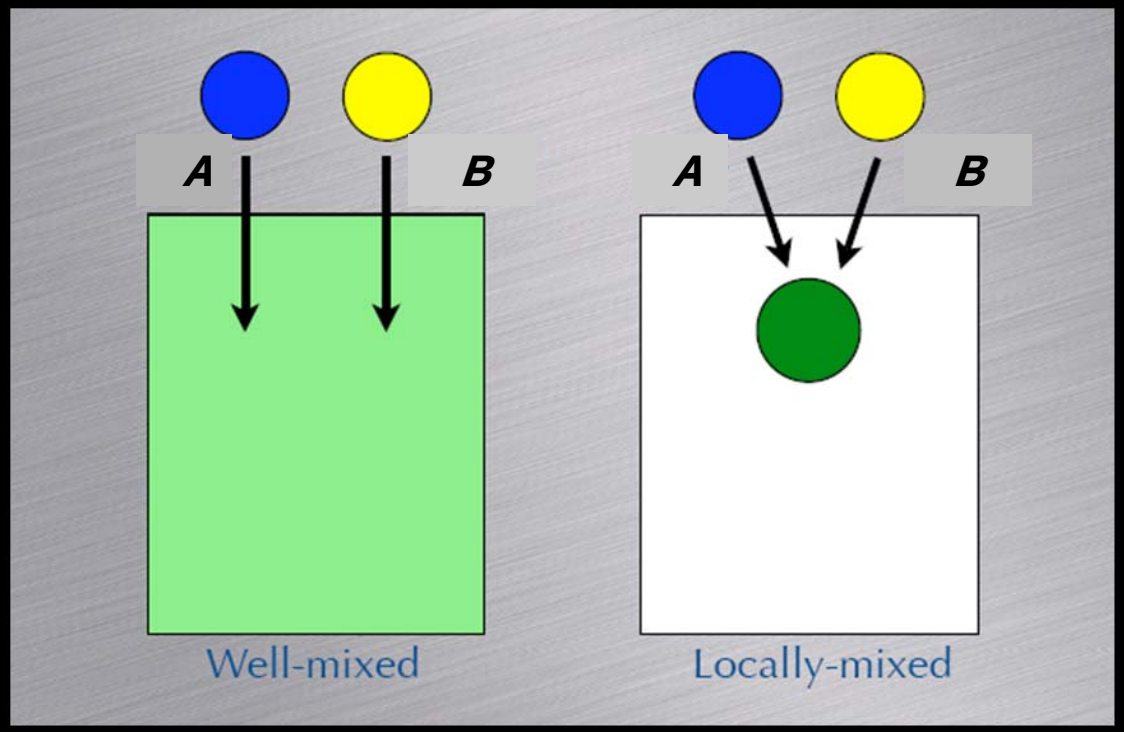
Class #2



(a) e.g., Chertkov and Lebedev 2003, (b) e.g., Metcalfe and Ottino 1994

Idealized Mixing Scenarios

Reaction Rate = kC_AC_B



Advection-Diffusion-Reaction Equations

$$\frac{dC_A}{dt} = -\vec{u} \cdot \nabla C_A + D\nabla^2 C_A - kC_A C_B$$

$$\frac{dC_B}{dt} = -\vec{u} \cdot \nabla C_B + D\nabla^2 C_B - kC_A C_B$$

Calculate Reaction Rate as: $kC_A C_B$

$$C_A = \overline{C_A} + C_A'$$

$$C_B = \overline{C_B} + C_B'$$

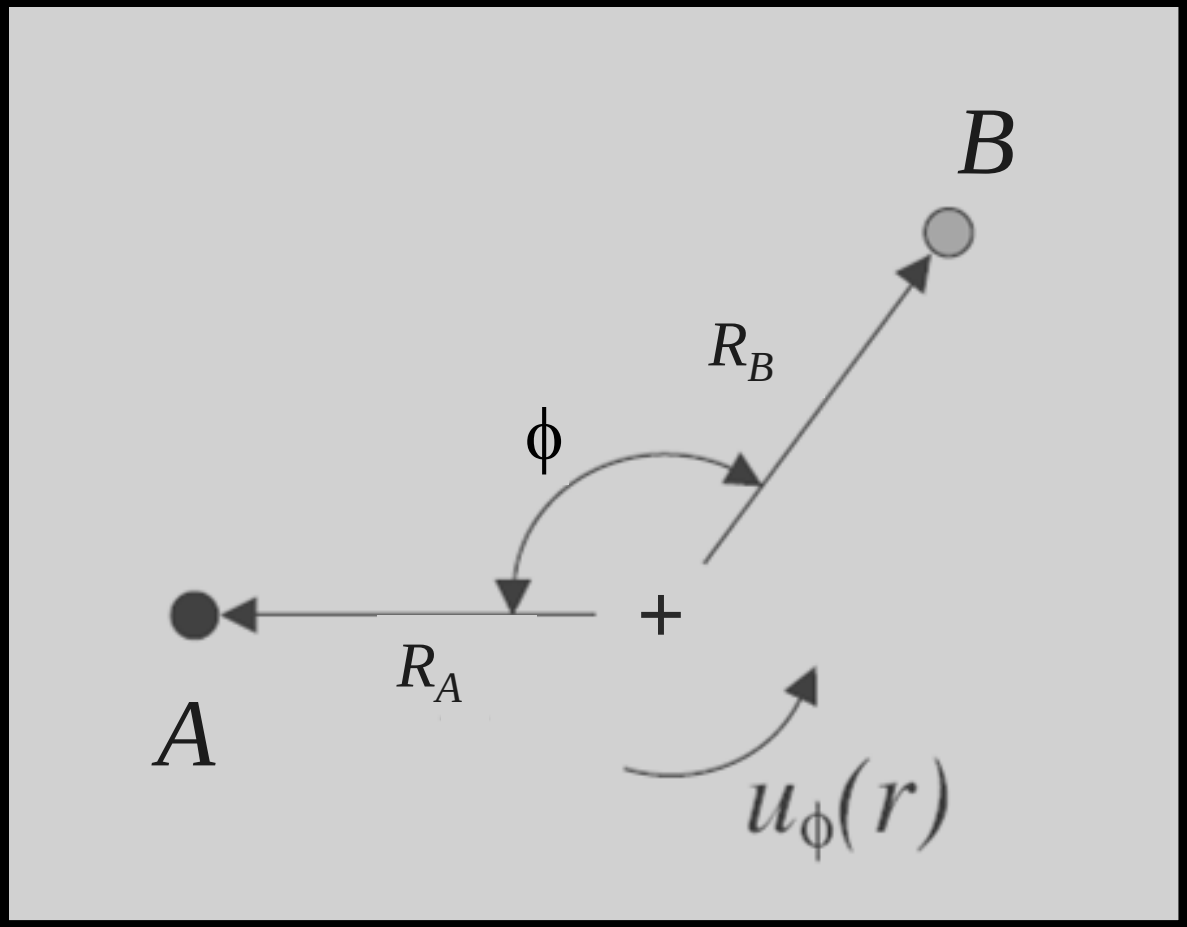
<u>Average Reaction Rate</u>: $\overline{kC_A C_B} = k\left(\overline{C_A}\,\overline{C_B} + \overline{C_A' C_B'}\right)$

What processes cause this?

Numerical Study

- *Introduce scalar sets into vortex-dominated 2-D and 3-D flows*
- *Investigate instantaneous scalar structure*
- *Use a particle tracking approach*
- *Quantify reaction rate, Θ*

Numerical Model Parameters

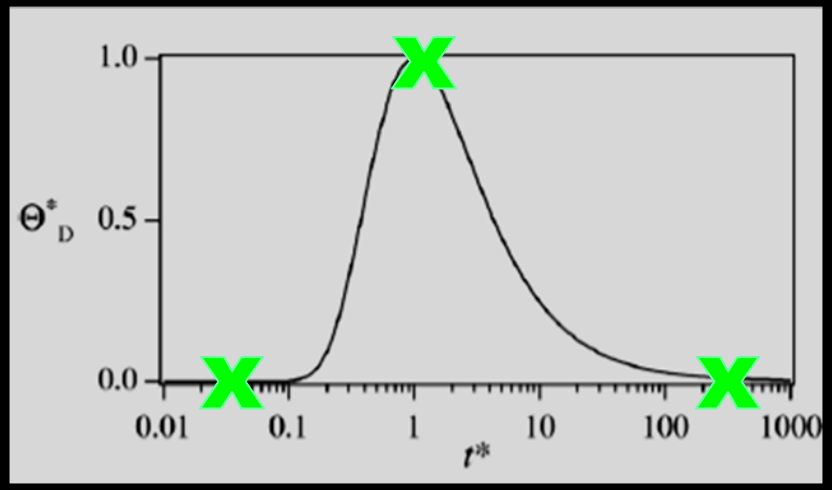


<u>ECCENTRICITIES</u>

Radial: $E = \left| R_A - R_B/(R_A + R_B) \right|$

Angular: $\phi = \phi_A - \phi_B$

Diffusion of Scalar Point Sources

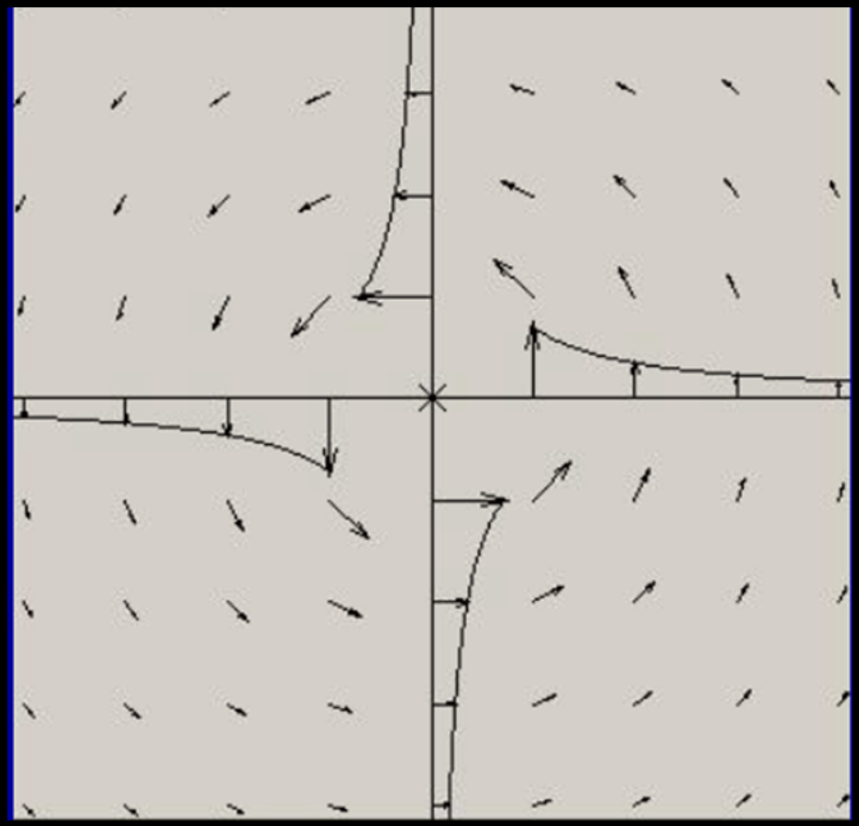


Analytical Expression for Diffusive Case:

$$\Theta_D(t) = \frac{M^2}{8\pi Dt}\exp\left[-\frac{L^2}{8Dt}\right]$$

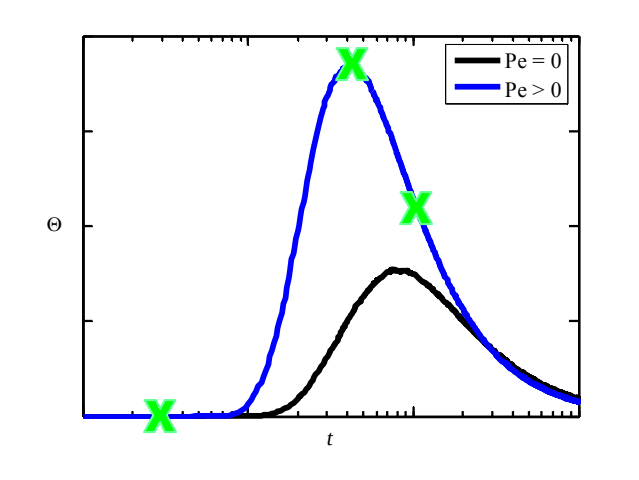
Velocity Field

Point Vortex

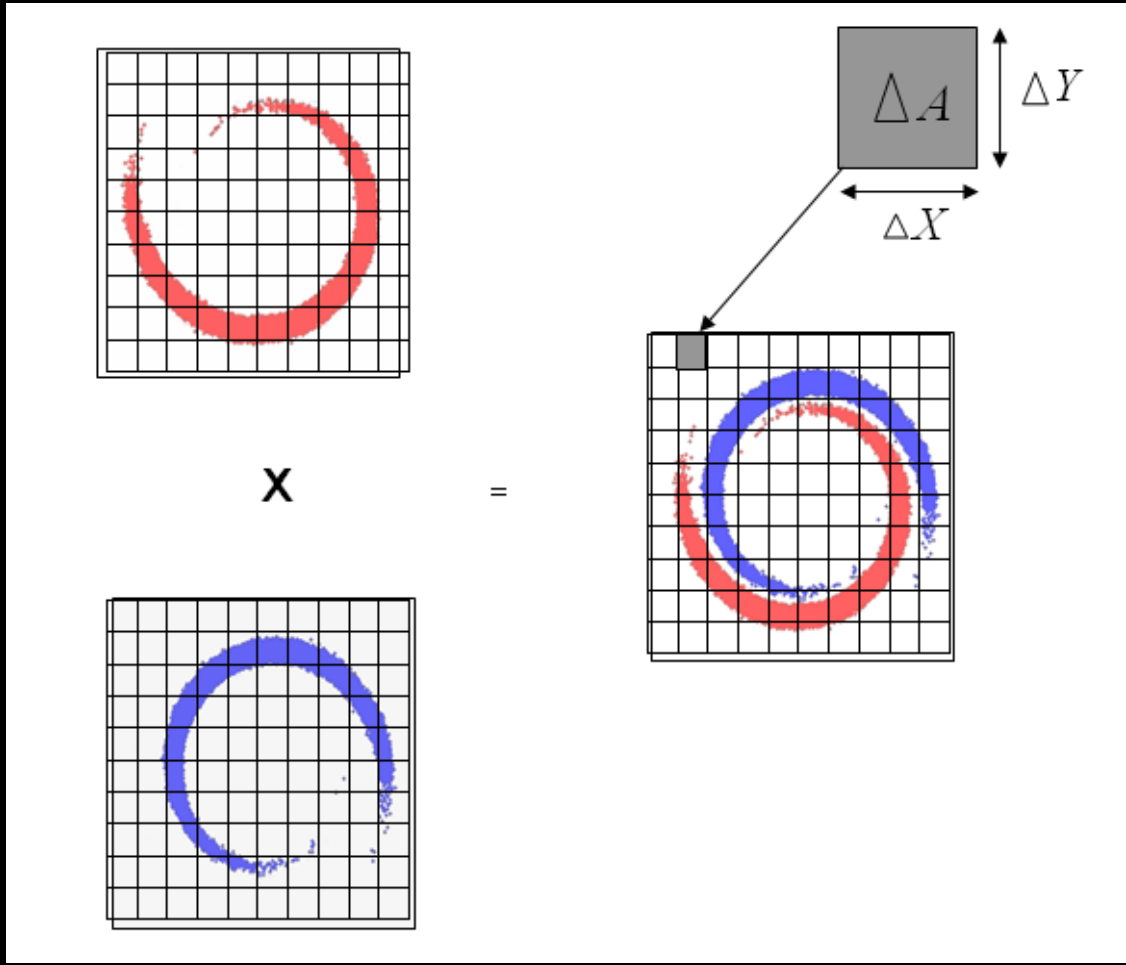


$$u_\phi(r) = \frac{\Gamma}{2\pi R}$$

Advection of Scalar Sets by a Point Vortex



Binning Procedure



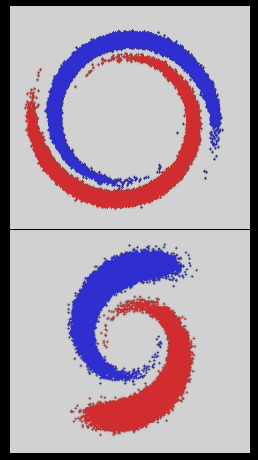
Nondimensional Variables: Pe & Da

<u>Péclet #</u>: Measure of Vortex Strength

$$\mathrm{Pe} = \frac{\Gamma}{4\pi D}\left(\frac{L}{2R}\right)^2$$

Pe ↑: Vortex spins faster (stretching ↑, spreading ↓)

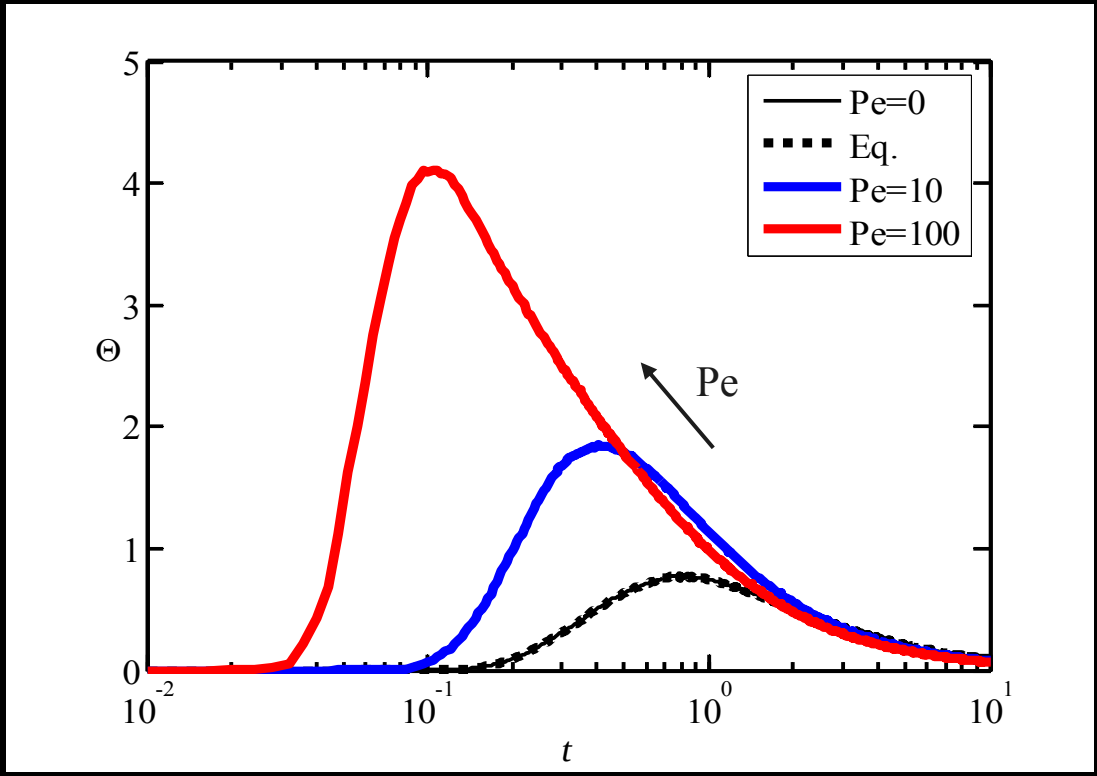
Pe ↓: Vortex spins slower (spreading ↑, stretching ↓)



<u>Damkohler #</u>: Measure of Reaction Speed

$$\mathrm{Da} = \frac{kM}{8D}$$

Effect of Pe on Θ(t)



$$\Theta = \iint kC_A C_B \, dA$$

2-D Multiple Vortex Velocity Field

- Numerical Model: Particle tracking approach
  - Bounded & Unbounded domains
  - Collection of Taylor & Point Vortices
  - Range of initial conditions (random placements) for 1) scalars, 2) vortices
- Investigate instantaneous scalar structure
- Quantify reaction rate, Θ

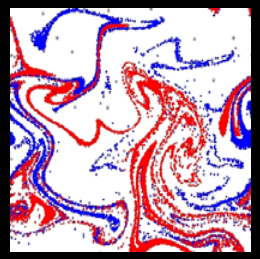
Example Velocity Field

Nondimensional Variables: Pe & Da

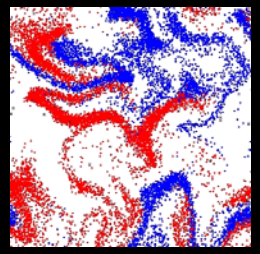
<u>Péclet #</u>: Measure of Vortex Strength

$$\mathrm{Pe} = \frac{VL}{D}$$

Pe ↑: Vortex spins faster (stretching ↑, spreading ↓)



Pe ↓: Vortex spins slower (spreading ↑, stretching ↓)

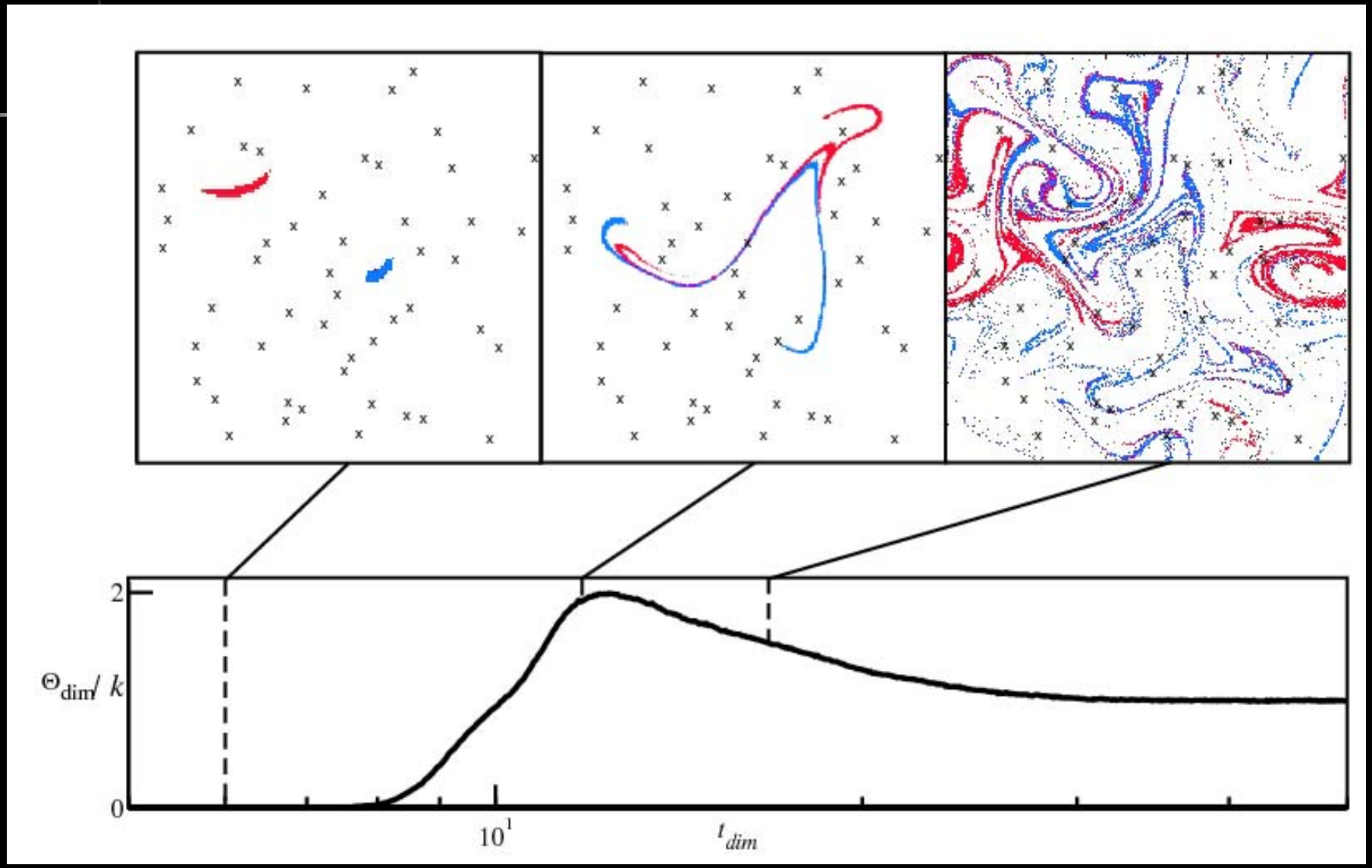


<u>Damkohler #</u>: Measure of Reaction Speed

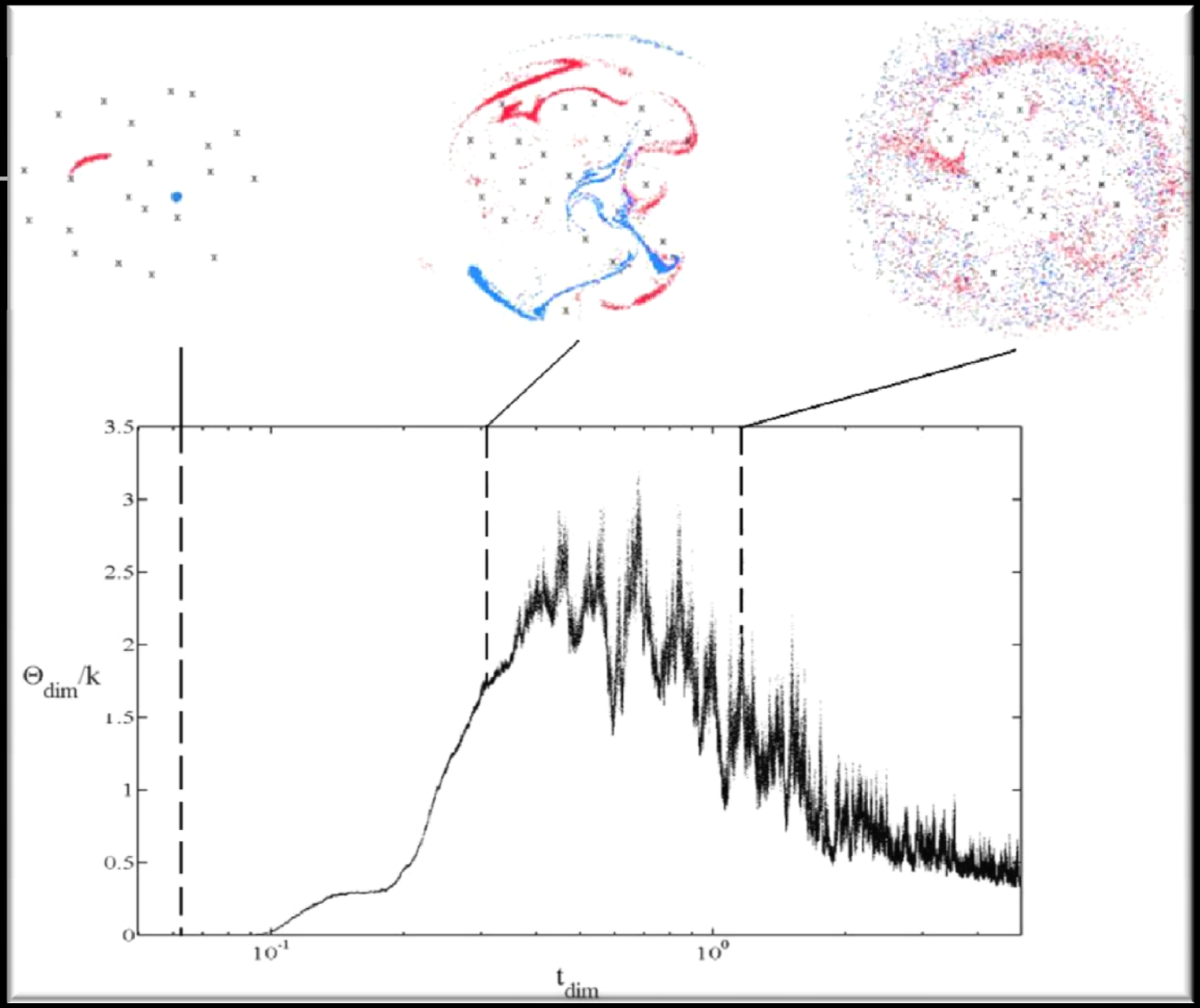
$$\mathrm{Da} = \frac{kM}{8D}$$

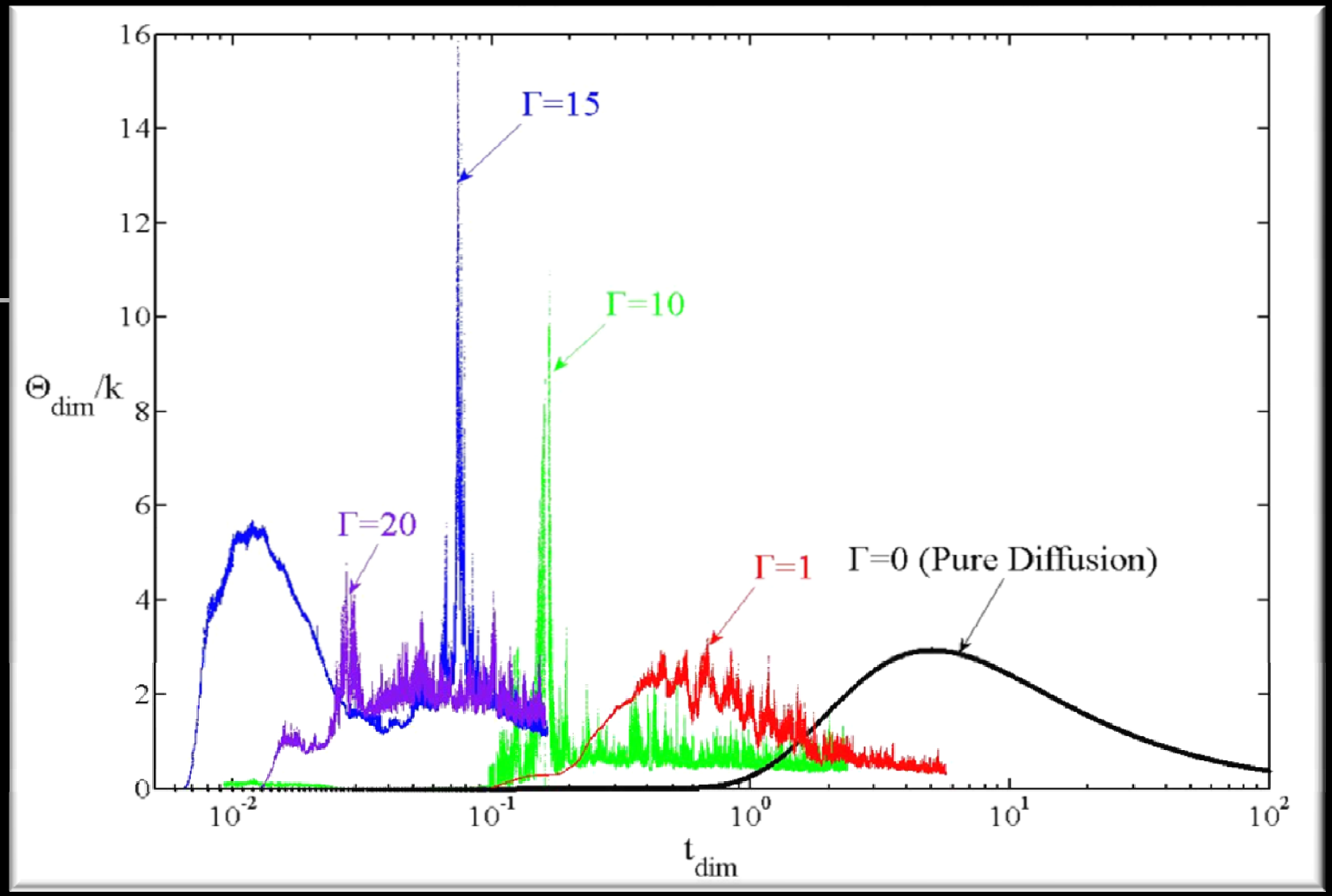
Taylor Vortex Simulation

Taylor Vortex Simulation



Point Vortex Simulation





- Fig.: Dimensional reaction rate, Θ_{dim} (normalized by reaction rate coefficient, *k*) versus dimensional time, t_{dim} for a 20 point vortex configuration. Simulations are shown for a range of vortex strengths (Γ). Note: Diffusivity, D=0.001, L=0.2 and initial scalar point source locations are $(X_A,Y_A)=(0.4,0.5)$ and $(X_B,Y_B)=(0.6,0.5)$.

2-D Multiple-Vortex Results

- Again, instantaneous processes must be considered!
- Multiple vortex velocity fields produce reaction rate enhancements beyond purely diffusive cases
- Some stirred cases do not produce significant enhancement beyond the purely diffusive case—but the smallest reaction rate *always* occurs for the case when the scalars are unstirred
- Best to model the stirring of scalars within an unbounded domain with same-sign vortices

Applications

- Wetland Treatment

- Broadcast Spawning Efficiency

Why Study Wetlands?

- Constructed wetlands are low-impact wastewater treatment that still maintains high efficiency
- They are based on natural process—require little construction , upkeep costs compared to traditional treatment plants
- Can control contaminant treatment (reactions) by increasing vegetation configuration and flow rates

Study Background

- Goal:

  Determine how stirring and mixing processes influence contaminant reactions through vegetation

- Tools:

  -Large Eddy Simulations (LES)

  -Particle Tracking Model

- Quantities of Interest:

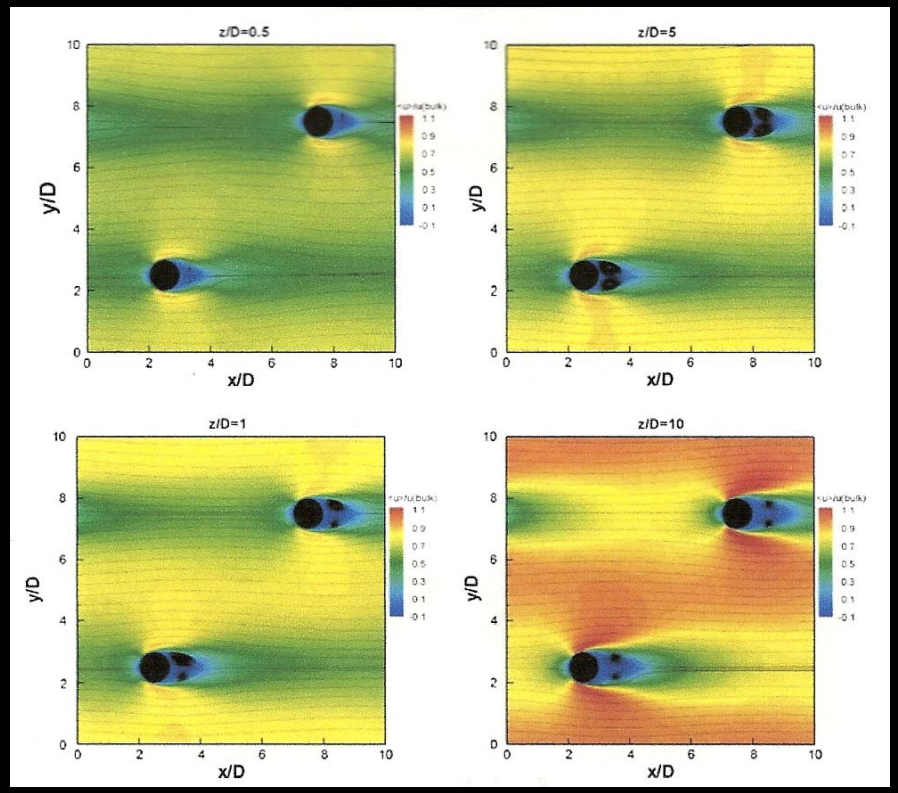
  -Hydrodynamics (velocity field, stem drag,…)

  -Reaction Rates between Contaminates/Stems

  -Contaminant Residence Times

Large Eddy Simulation (LES)

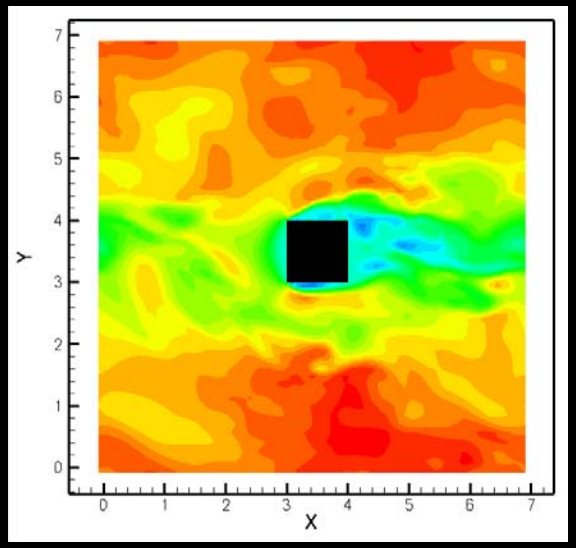
- Generates a 3D velocity field through a matrix of cylinders
- Represents idealized submerged vegetation of wetlands in a non-uniform grid
- Calibrated using field studies

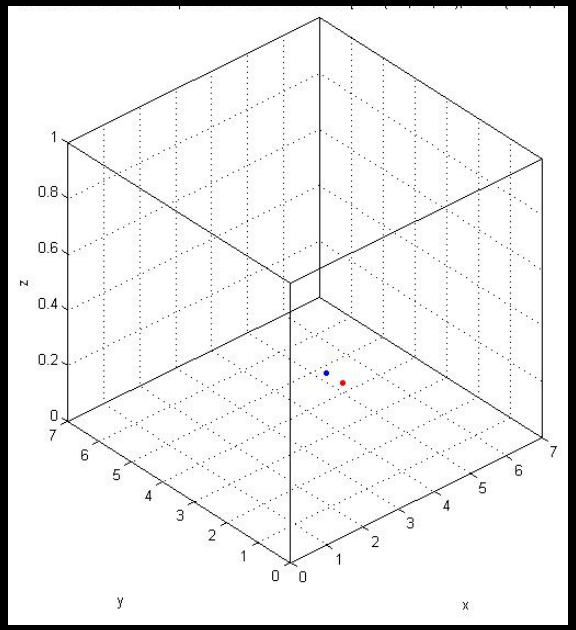


(Stoesser et al. 2009)

Combined LES & Particle-Tracking Models

- LES model provides 3D velocity fields for flow around a vegetative stem (domain: 7x7x1)
- Particles positions are recorded in time as they evolve within the domain due to the 3D velocity field
- Reaction rates between particles are calculated for each time step





Wetland Treatment Strategies

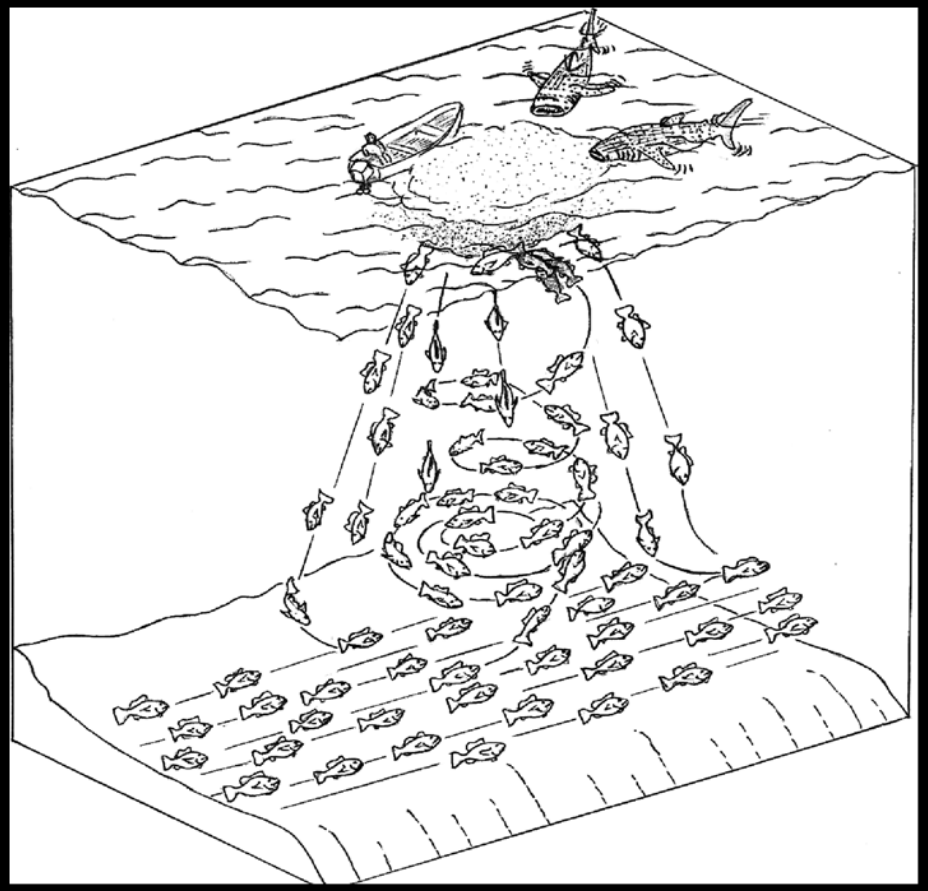
- Model simulations reveal physical stirring and mixing flow mechanisms that enhance or inhibit reactions between reactive particles
- *Preliminary* model results indicate importance of considering instantaneous physical and chemical processes when studying the most effective treatment options
- With more accurate prediction tools, utilities will be able to optimize the design of future wetlands or provide operational guidelines for existing wetlands

Broadcast Spawning Basics

- reproductive strategy used by various benthic invertebrates (e.g. sea urchins, anemones, corals) and several fish species
- male and female adults simultaneously release sperm and egg into the surrounding flow
- strategy relies on <u>turbulent stirring</u>, <u>molecular diffusion</u>, and sperm taxis to bring sperm and egg together (so fertilization reaction can take place)
- coral, in particular, have experienced impeded regeneration as their diverse ecosystems decline worldwide

Fish Aggregation, Spawning Cloud

- Large groups of fish
  - Cubera Snapper
  - Thousands Congregate
  - Color Determines Job
- Swimming Group Generate 3D Vortex
- Role of Predation?



(Heyman et al., 2005)

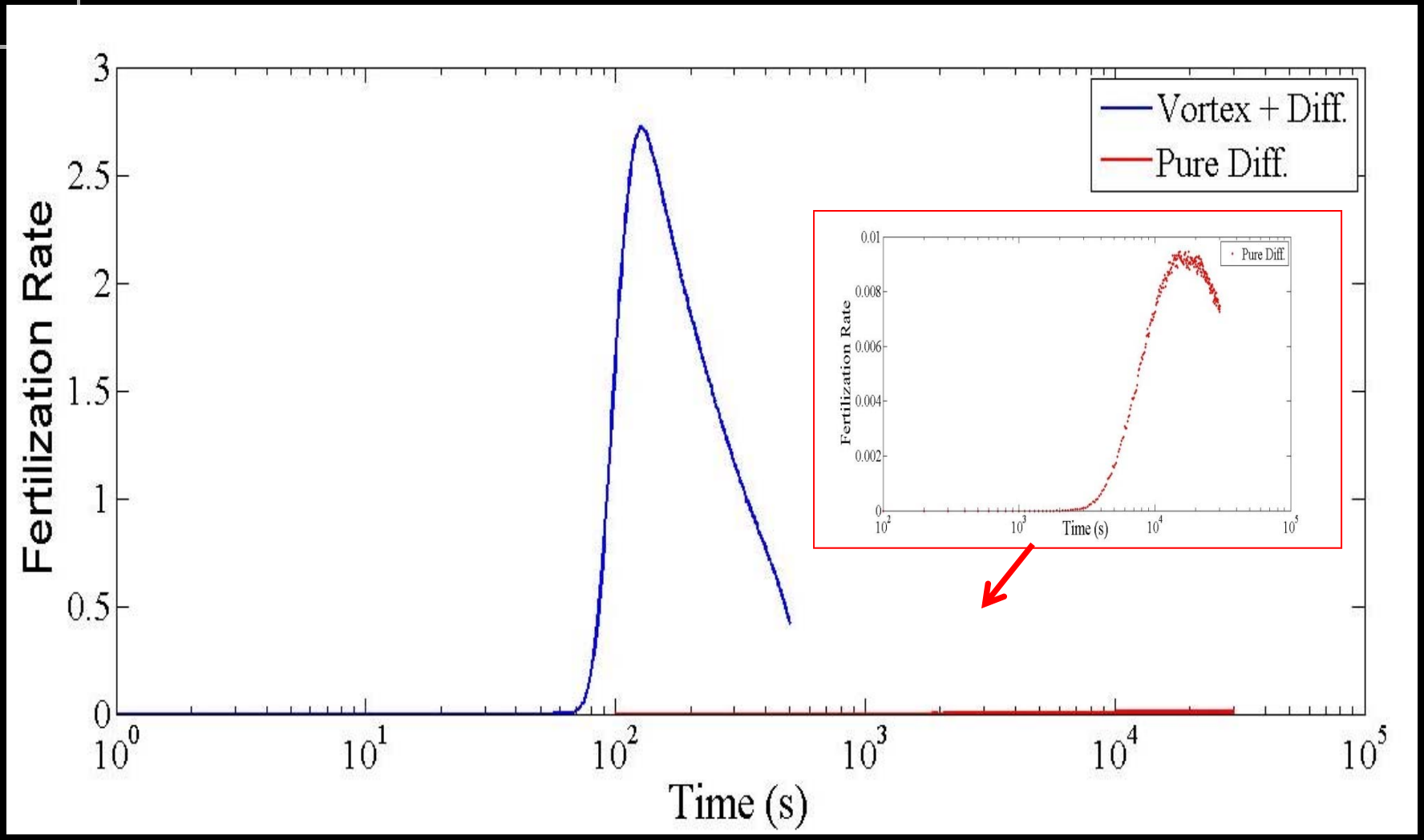
3-D Model of Egg/Sperm – Pure Diffusion ONLY

2-D Burgers Vortex Velocity Field

(slice through 3D field)

Advection & Diffusion of Egg/Sperm

Fertilization Rates Comparison:
Pure Diffusion vs. Vortex +Diffusion



Spawning Efficiency Results

- Vortex motion significantly increases spawning efficiency beyond that calculated for pure diffusion cases
- This is preliminary work, we will look at several variations on:
  - Initial gamete locations
  - Vortex parameters (i.e. strength, suction)
  - Initial gamete masses

Research Implications

- *New class of advective-diffusive-reactive problems*
- *Study results could influence the future of spawning success in broadcast spawners*
- *Chemical mixing and reaction rates in turbulent flows play a crucial role in many fields (pharmaceuticals, chemical engineering, etc.)*
- *The advection and diffusion of reactants in such fields rely on understanding the fundamental findings of this study*

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Thank You

Any Questions?

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