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Session 03B00

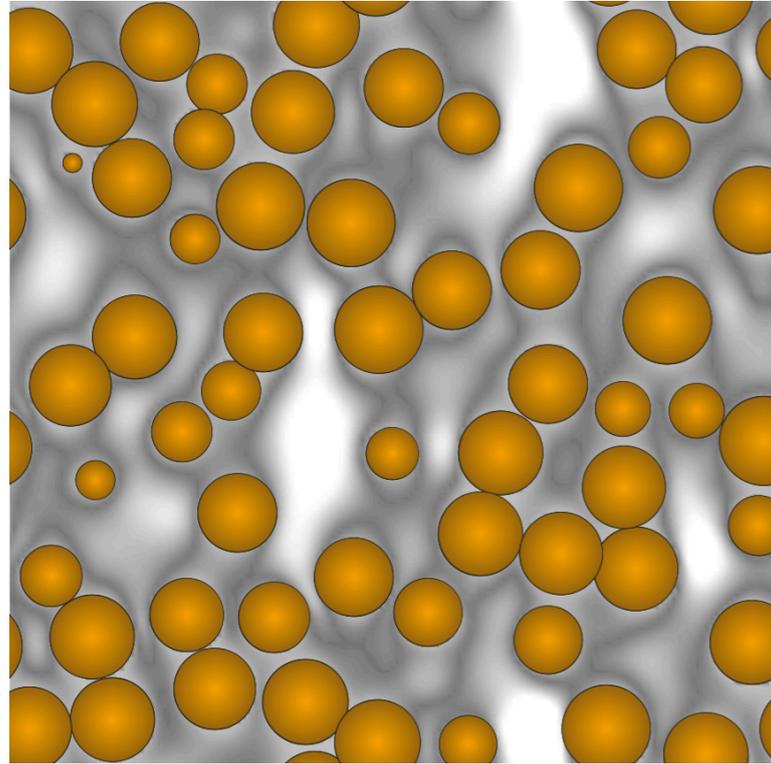
Industrial Application of Computational and Numerical
Approaches to Particle Flow II

AICHE Annual Conference
Pittsburgh, PA October 31, 2012

Simulation of Gas-Particle Flows Across Length Scales



MICRO-SCALE
~ 50 μ m-mm

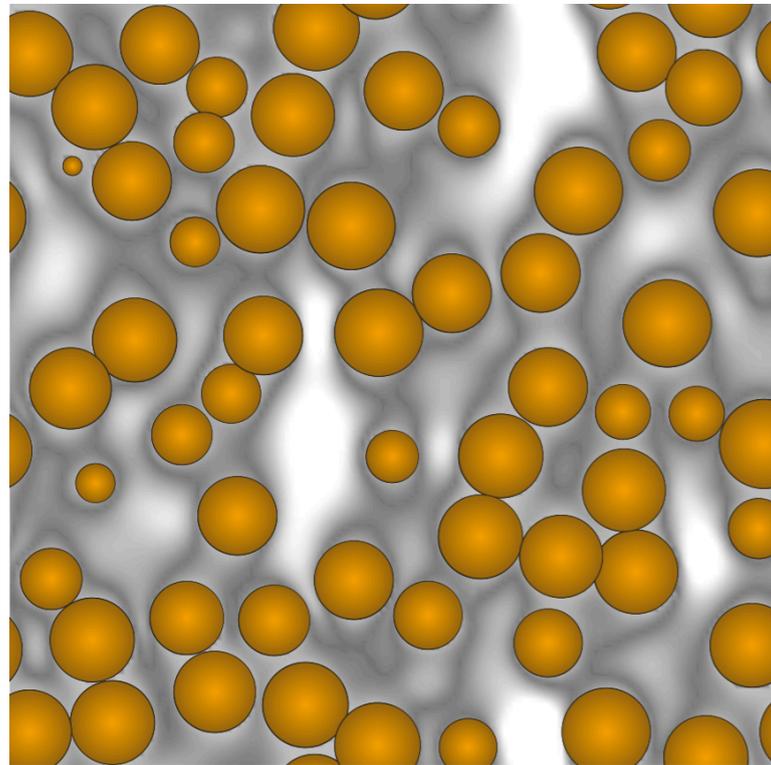


Newton's equations of motion for each particle, Navier-Stokes equations for the fluid flow in the interstices.

Simulation of Gas-Particle Flows Across Length Scales

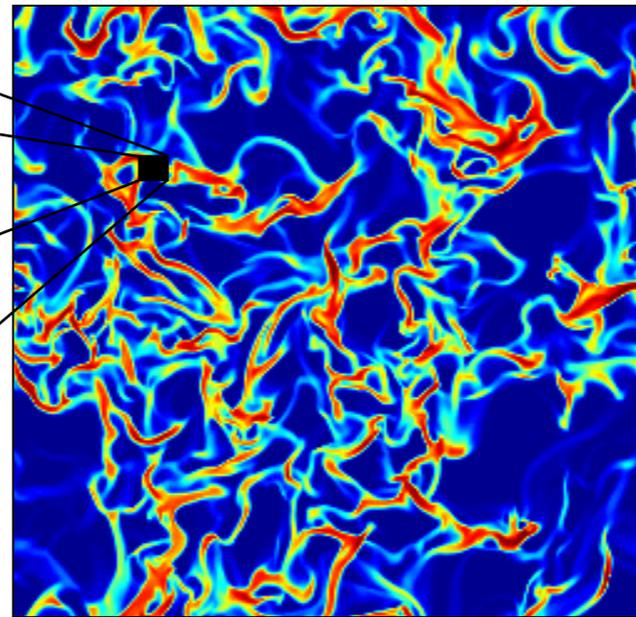


MICRO-SCALE
~ 50 μ m-mm



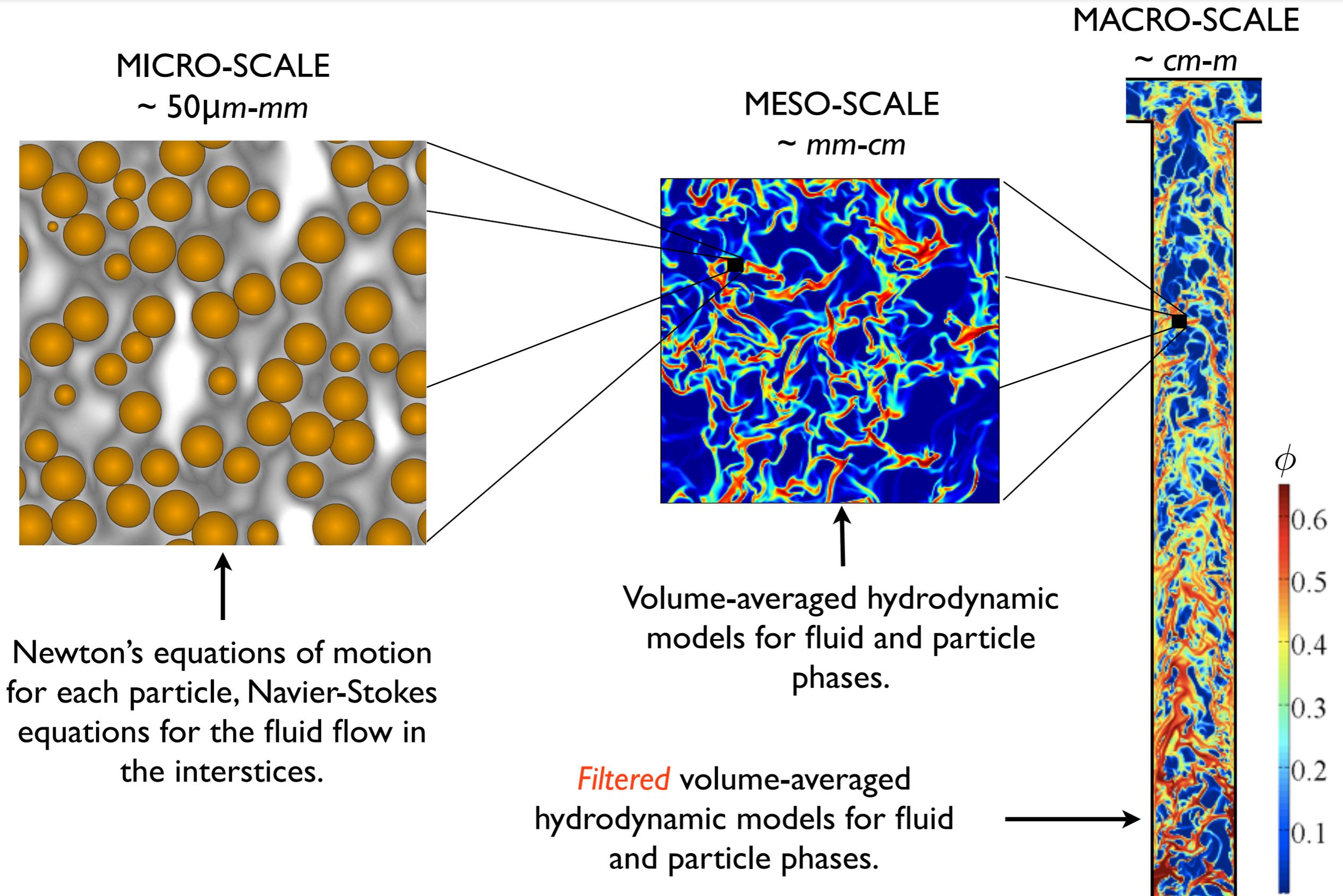
↑
Newton's equations of motion for each particle, Navier-Stokes equations for the fluid flow in the interstices.

MESO-SCALE
~ mm-cm



↑
Volume-averaged hydrodynamic models for fluid and particle phases.

Simulation of Gas-Particle Flows Across Length Scales



Development of Filtered Two-Fluid Models



- Hydrodynamics (*Igci et al, 2011*)
 - Filtered drag *
 - Filtered pressure
 - Filtered viscosity

*Li & Kwauk, 1994; Parmentier et. al, 2011

Development of Filtered Two-Fluid Models



- Hydrodynamics (*Igci et al, 2011*)
 - Filtered drag *
 - Filtered pressure
 - Filtered viscosity
- Reacting flows (*Holloway & Sundaresan, 2012*)
 - Filtered reaction rate

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Development of Filtered Two-Fluid Models



- Hydrodynamics (*Igci et al, 2011*)
 - Filtered drag *
 - Filtered pressure
 - Filtered viscosity
- Reacting flows (*Holloway & Sundaresan, 2012*)
 - Filtered reaction rate
- Thermal energy & interphase transport (**present work**)
 - Filtered energy dispersion
 - Filtered interphase heat transfer
 - Filtered scalar dispersion (**no interphase transport**)
 - Helium Tracer/Solid Particle Tracer

*Li & Kwauk, 1994; Parmentier et. al, 2011

Two-Fluid Model Equations



Continuity

$$\frac{\partial(\rho_s \phi_s)}{\partial t} + \nabla \cdot (\rho_s \phi_s \mathbf{v}_s) = 0$$

$$\frac{\partial(\rho_g \phi_g)}{\partial t} + \nabla \cdot (\rho_g \phi_g \mathbf{v}_g) = 0$$

Momentum

$$\frac{\partial}{\partial t}(\rho_s \phi_s \mathbf{v}_s) + \nabla \cdot (\rho_s \phi_s \mathbf{v}_s \mathbf{v}_s) = -\nabla \cdot \boldsymbol{\sigma}_s - \phi_s \nabla \cdot \boldsymbol{\sigma}_g + \mathbf{f} + \rho_s \phi_s \mathbf{g}$$

$$\frac{\partial}{\partial t}(\rho_g \phi_g \mathbf{v}_g) + \nabla \cdot (\rho_g \phi_g \mathbf{v}_g \mathbf{v}_g) = -\phi_g \nabla \cdot \boldsymbol{\sigma}_g - \mathbf{f} + \rho_g \phi_g \mathbf{g}$$

Granular kinetic theory

Wen & Yu (1966)

Thermal Energy

$$\rho_s C_{p_s} \left[\frac{\partial}{\partial t}(\phi_s T_s) + \nabla \cdot (\phi_s \mathbf{v}_s T_s) \right] = \nabla \cdot (k_s \nabla T_s) + \gamma(T_s - T_g)$$

$$\rho_g C_{p_g} \left[\frac{\partial}{\partial t}(\phi_g T_g) + \nabla \cdot (\phi_g \mathbf{v}_g T_g) \right] = \nabla \cdot (k_g \nabla T_g) - \gamma(T_s - T_g)$$

Gunn (1978)

Filtered Equations



Filter

$$\overline{\phi_s}(\mathbf{x}, t) = \int_{V_\infty} G(\mathbf{x}, \mathbf{y}) \phi_s(\mathbf{x}, t) d\mathbf{y}$$

$$\int_{V_\infty} G(\mathbf{x}, \mathbf{y})(\mathbf{x}, t) d\mathbf{y} = 1$$

Filtered Equations



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$$\int_{V_\infty} G(\mathbf{x}, \mathbf{y})(\mathbf{x}, t) d\mathbf{y} = 1$$

Favre Filter

$$\widetilde{\alpha_s}(\mathbf{x}, t) = \frac{\int_{V_\infty} G(\mathbf{x}, \mathbf{y}) \alpha_s(\mathbf{x}, t) \phi_s(\mathbf{x}, t) d\mathbf{y}}{\int_{V_\infty} G(\mathbf{x}, \mathbf{y}) \phi_s(\mathbf{x}, t) d\mathbf{y}}$$



Filtered Equations

Filter

$$\overline{\phi_s}(\mathbf{x}, t) = \int_{V_\infty} G(\mathbf{x}, \mathbf{y}) \phi_s(\mathbf{x}, t) d\mathbf{y}$$

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Filtered Solids Thermal Energy Equation

$$\rho_s C_{p_s} \left[\frac{\partial}{\partial t} (\overline{\phi_s \widetilde{T}_s}) + \nabla \cdot (\overline{\phi_s \widetilde{\mathbf{v}}_s \widetilde{T}_s}) \right] = \nabla \cdot (\overline{k_s \nabla T_s}) + \overline{\gamma(T_s - T_g)} + \rho_s C_{p_s} \nabla \cdot \left[\overline{\phi_s \widetilde{\mathbf{v}}_s \widetilde{T}_s} - \overline{\phi_s \mathbf{v}_s T_s} \right]$$



'dispersive' flux

Applying Mean Temperature Gradient

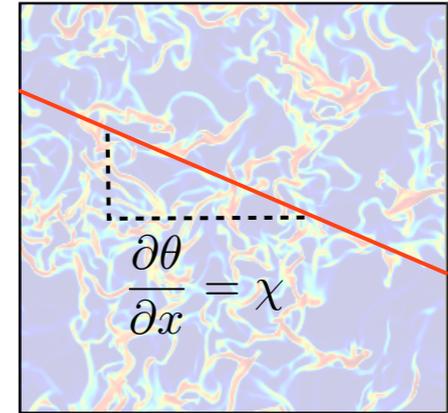


Temperature Gradient

$$T_s = T'_s + \theta(x)$$

$$T_g = T'_g + \theta(x)$$

$$\frac{\partial \theta}{\partial x} = \chi = \text{constant}$$

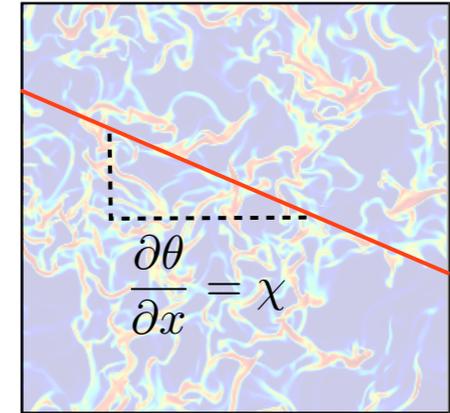


Applying Mean Temperature Gradient



Temperature Gradient

$$T_s = T'_s + \theta(x) \quad \frac{\partial \theta}{\partial x} = \chi = \text{constant}$$
$$T_g = T'_g + \theta(x)$$



Thermal Energy

$$\rho_s C_{p_s} \left[\frac{\partial}{\partial t} (\phi_s T'_s) + \nabla \cdot (\phi_s \mathbf{v}_s T'_s) \right] = \nabla \cdot (k_s \nabla T'_s) + \gamma (T'_s - T'_g) + \chi \frac{\partial k_s}{\partial x} - \rho_s C_{p_s} \phi_s v_{s_x} \chi$$
$$\rho_g C_{p_g} \left[\frac{\partial}{\partial t} (\phi_g T'_g) + \nabla \cdot (\phi_g \mathbf{v}_g T'_g) \right] = \nabla \cdot (k_g \nabla T'_g) - \gamma (T'_s - T'_g) + \chi \frac{\partial k_g}{\partial x} - \rho_g C_{p_g} \phi_g v_{g_x} \chi$$

'New' source terms

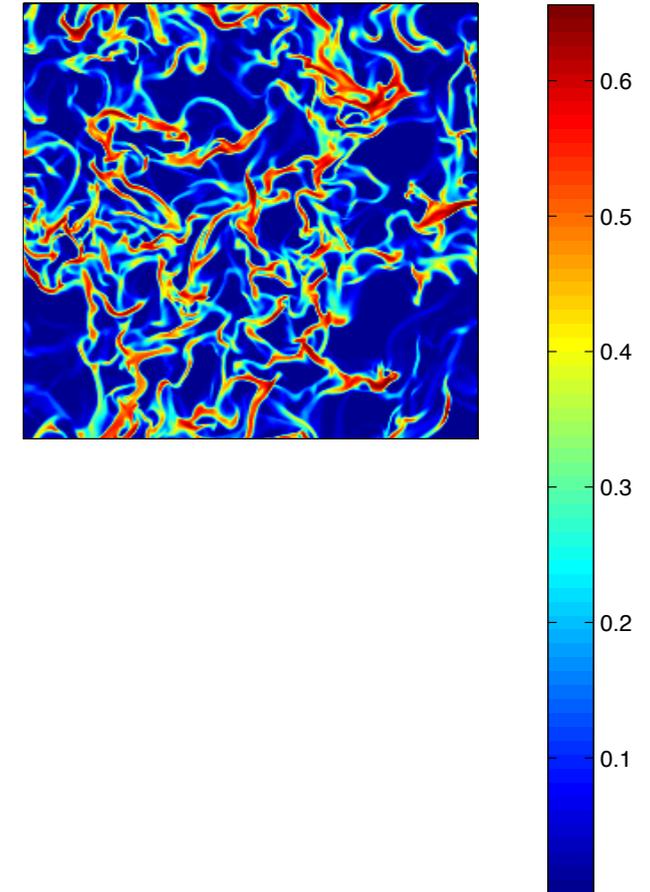
Applying Heat Sources/Sinks



Solids Heat Source

$$\dot{Q}_s \phi_s \quad \int_D \dot{Q}_s \phi_s dV = \dot{Q}_s \bar{\phi}_s V$$

ϕ_s



Applying Heat Sources/Sinks



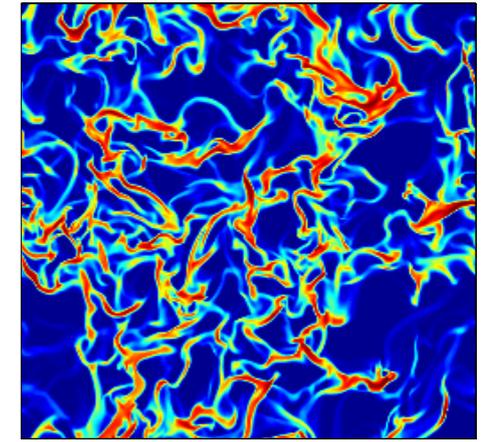
Solids Heat Source

$$\dot{Q}_s \phi_s \quad \int_D \dot{Q}_s \phi_s dV = \dot{Q}_s \bar{\phi}_s V$$

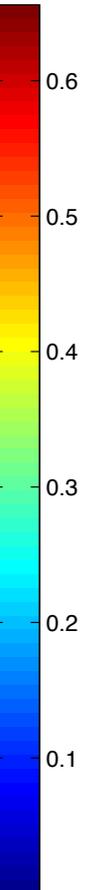
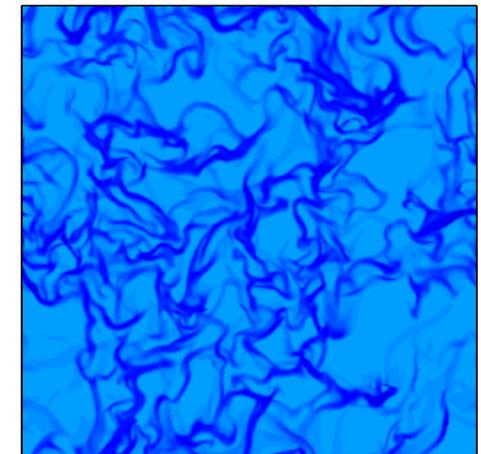
Gas Heat Sink

$$\dot{Q}_g \phi_g = \dot{Q}_s \frac{\bar{\phi}_s}{\phi_g} \phi_g \quad \int_D \dot{Q}_g \phi_g dV = \dot{Q}_s \bar{\phi}_s V$$

ϕ_s



$\frac{\bar{\phi}_s}{\phi_g} \phi_g$



Applying Heat Sources/Sinks

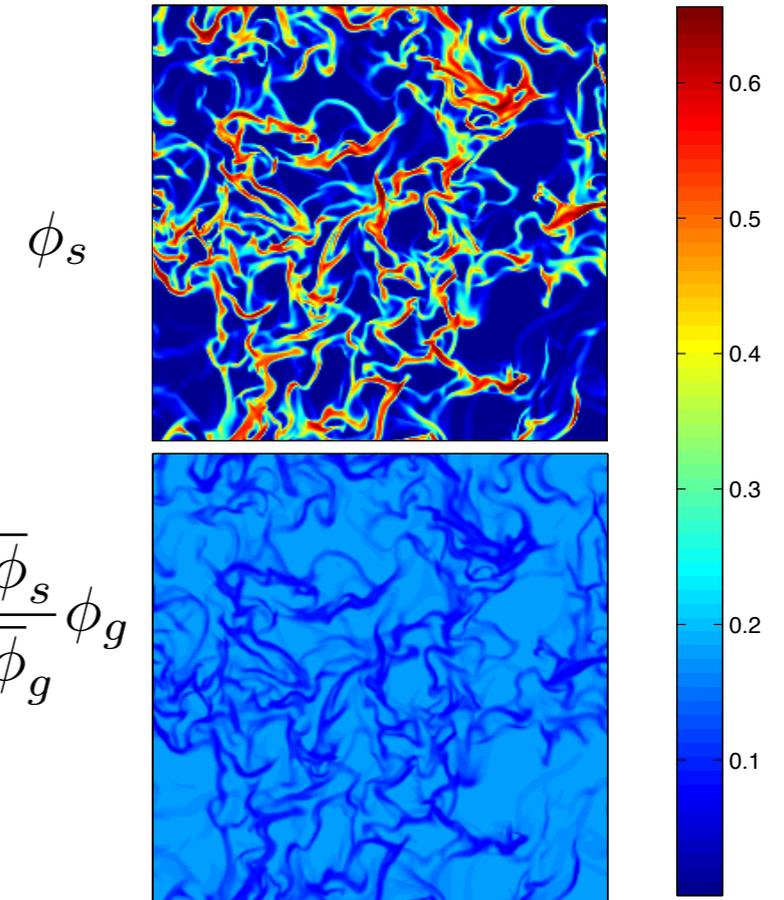


Solids Heat Source

$$\dot{Q}_s \phi_s \quad \int_D \dot{Q}_s \phi_s dV = \dot{Q}_s \bar{\phi}_s V$$

Gas Heat Sink

$$\dot{Q}_g \phi_g = \dot{Q}_s \frac{\bar{\phi}_s}{\phi_g} \phi_g \quad \int_D \dot{Q}_g \phi_g dV = \dot{Q}_s \bar{\phi}_s V$$



Thermal Energy

$$\rho_s C_{p_s} \left[\frac{\partial}{\partial t} (\phi_s T_s) + \nabla \cdot (\phi_s \mathbf{v}_s T_s) \right] = \nabla \cdot (k_s \nabla T_s) + \gamma (T_s - T_g) + \dot{Q}_s \phi_s$$

$$\rho_g C_{p_g} \left[\frac{\partial}{\partial t} (\phi_g T_g) + \nabla \cdot (\phi_g \mathbf{v}_g T_g) \right] = \nabla \cdot (k_g \nabla T_g) - \gamma (T_s - T_g) - \dot{Q}_g \phi_g$$

↑
‘New’ source/sink terms

Simulations and Filtering Procedure



2-D periodic domain with mean vertical pressure drop in gas phase set to balance weight of mixture.

Computational Domain: 32cm x 32cm

Discretization: 256 x 256 cells

Particle diameter: 75 μ m

Simulations are for FCC particles in air.
Results are suitably scaled so that they are
applicable to other systems.

Simulations and Filtering Procedure

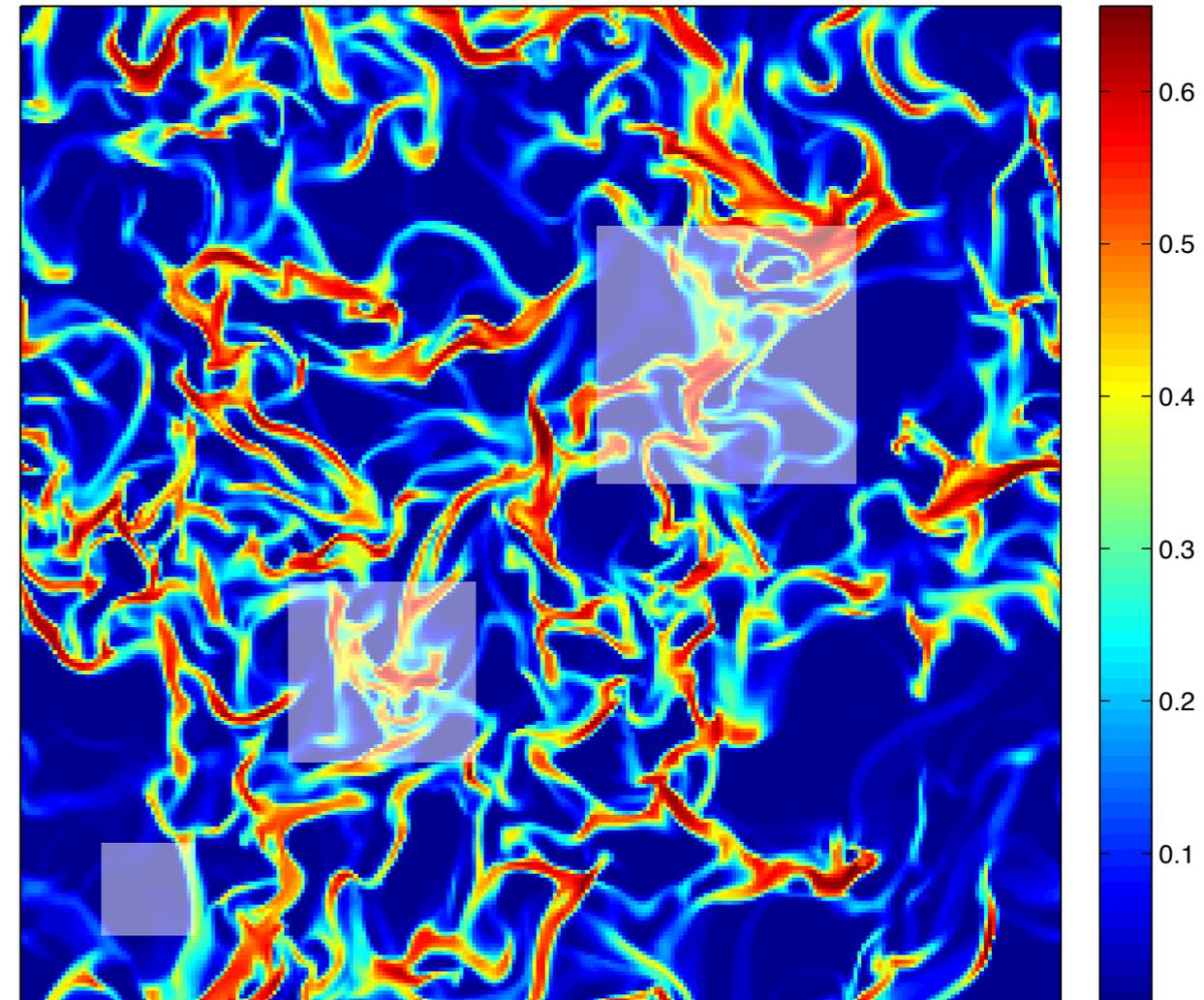


2-D periodic domain with mean vertical pressure drop in gas phase set to balance weight of mixture.

Snapshot of solids volume fraction field obtained from highly resolved simulations.



Shaded squares illustrate regions over which a filtering operation is performed.



Filtered Solids Thermal Dispersion



Filtered Solids Thermal Dispersion



$$\alpha_{sfilt} = \frac{k_{sfilt}}{\rho_s C_{p_s}} = \frac{\overline{\phi_s} \left(\widetilde{v_{s_x} T_s} - \overline{v_{s_x} T_s} \right)}{\frac{\partial \widetilde{T_s}}{\partial x}} \quad \frac{\alpha_{sfilt}}{(v_t^3/g)}$$



Filtered Solids Thermal Dispersion

$$\alpha_{s_{filt}} = \frac{k_{s_{filt}}}{\rho_s C_{p_s}} = \frac{\overline{\phi_s} \left(\overline{v_{s_x} T_s} - \overline{v_{s_x}} \overline{T_s} \right)}{\frac{\partial \overline{T_s}}{\partial x}}$$

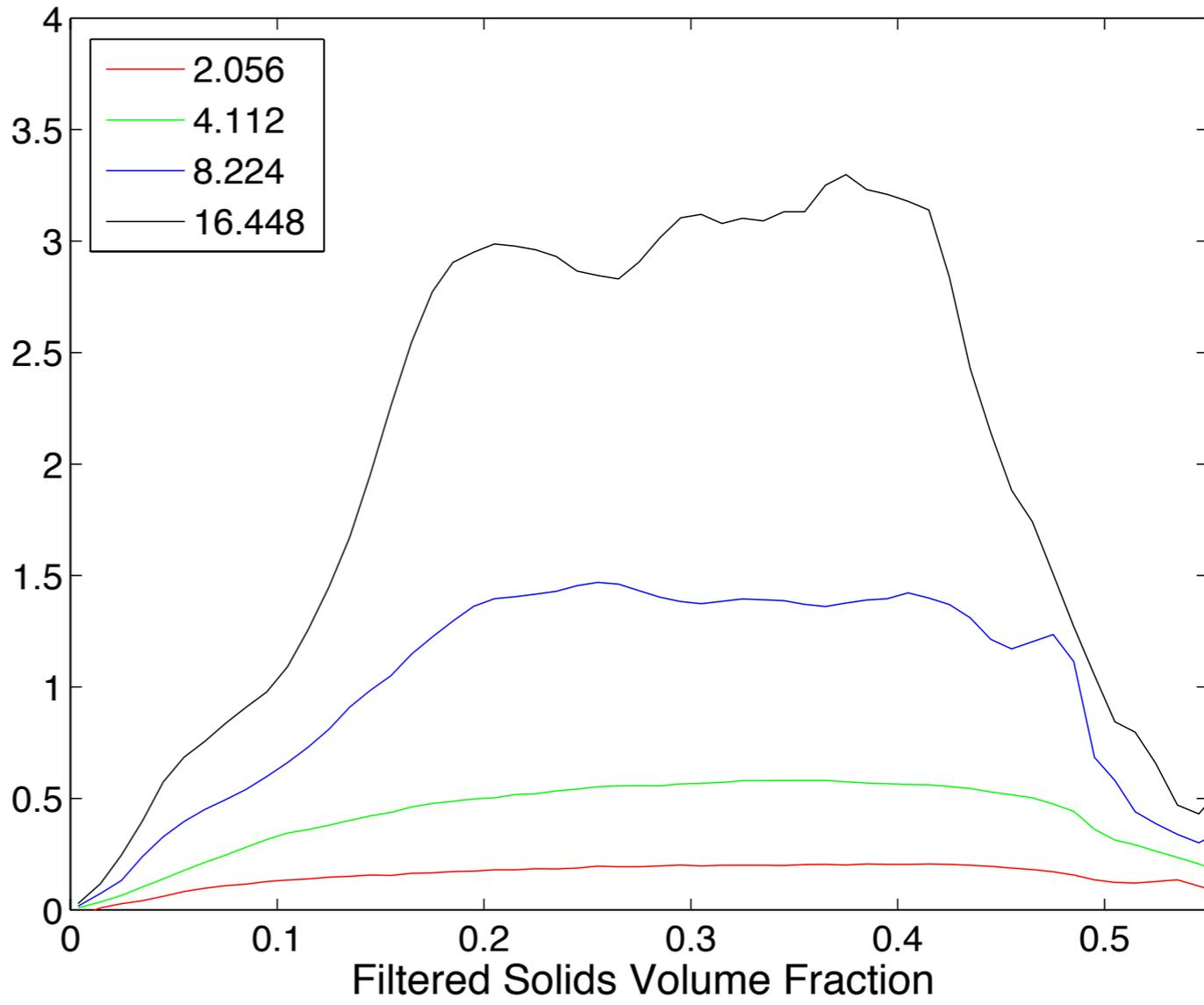
$$\frac{\alpha_{s_{filt}}}{(v_t^3/g)}$$

Curves correspond to different filter sizes.

Dimensionless filter size shown in legend $\frac{\Delta}{v_t^2/g}$

↑

$(Fr_{\Delta})^{-1}$



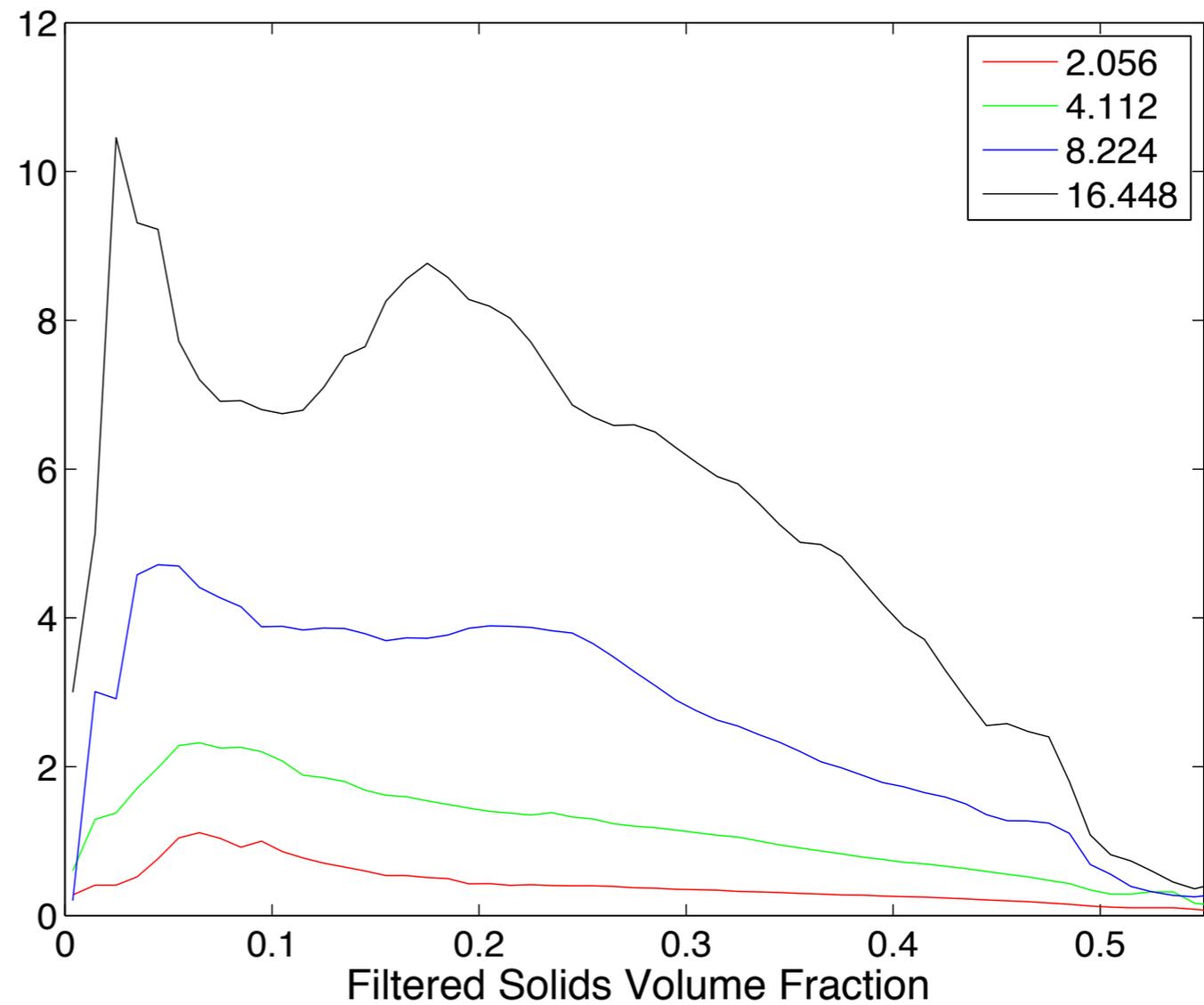
FCC particles in air

Dimensionless filter size of 2.056 corresponds to 1cm.

Filtered Gas Thermal Dispersion



$$\alpha_{g_{filt}} = \frac{k_{g_{filt}}}{\rho_g C_{p_g}} = \frac{\overline{\phi_g} \left(\widetilde{v_{gx}} \widetilde{T_g} - \widetilde{v_{gx}} \widetilde{T_g} \right)}{\frac{\partial \widetilde{T_g}}{\partial x}} \quad \frac{\alpha_{g_{filt}}}{(v_t^3/g)}$$



Filtered Gas Thermal Dispersion



$$\alpha_{g_{filt}} = \frac{k_{g_{filt}}}{\rho_g C_{p_g}} = \frac{\overline{\phi_g} \left(\widetilde{v_{gx}} \widetilde{T_g} - \widetilde{v_{gx}} T_g \right)}{\frac{\partial \widetilde{T_g}}{\partial x}}$$

$$\frac{\alpha_{g_{filt}}}{(v_t^3/g)}$$

Curves correspond to different filter sizes.

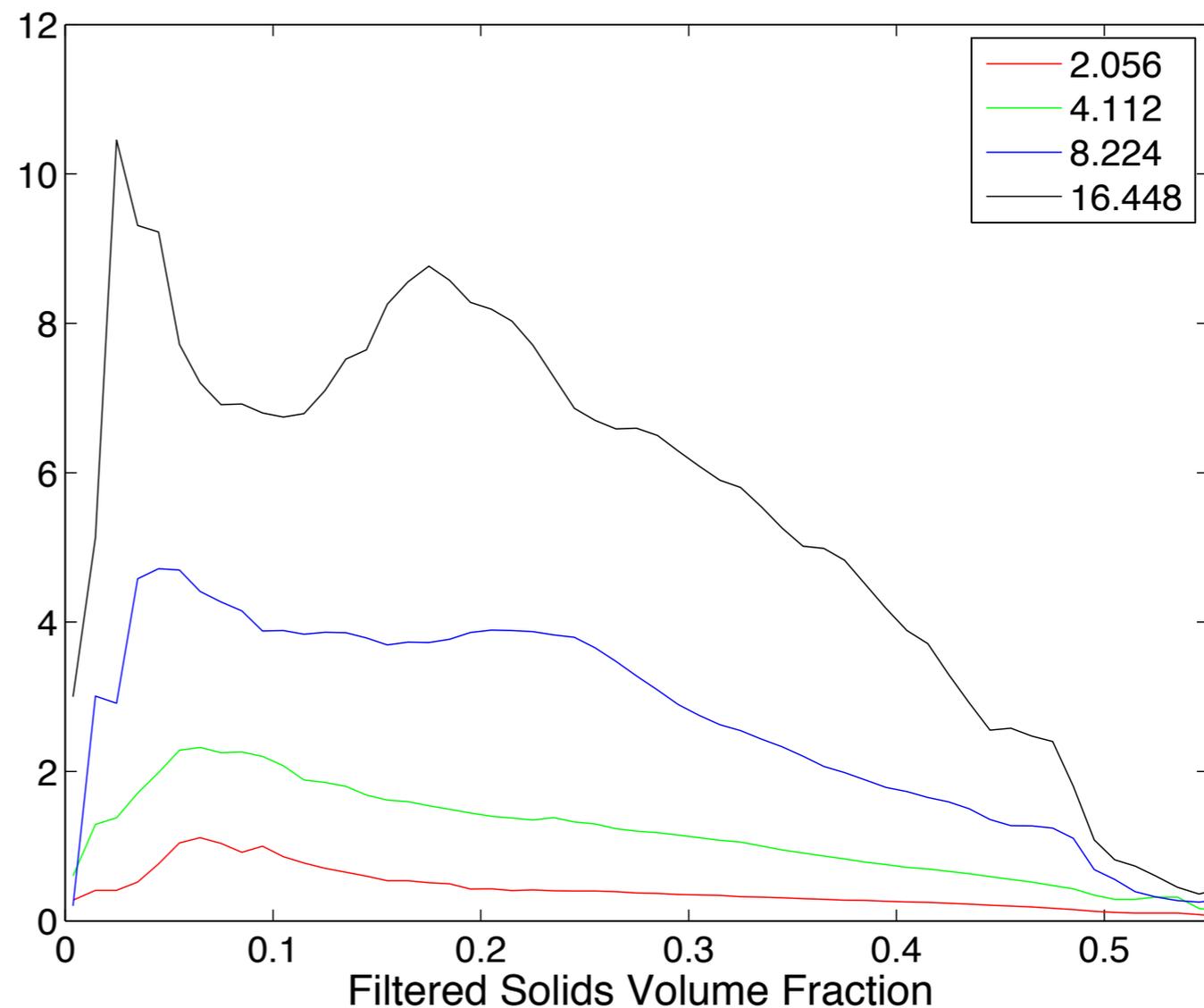
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Scaled Filtered Solids Thermal Dispersion



Scaled Filtered Solids Thermal Dispersion



$$\hat{\alpha}_{sfilt} = \frac{\alpha_{sfilt}}{(v_t^3/g)}$$

Scaled Filtered Solids Thermal Dispersion



$$\hat{\alpha}_{s_{filt}} = \frac{\alpha_{s_{filt}}}{(v_t^3/g)}$$

$$\frac{\hat{\alpha}_{s_{filt}}}{\hat{\Delta}^2 |\widetilde{S}_s|} \longleftarrow$$

Dimensionless Filtered Solids Shear Rate

$$\widetilde{S}_s = \frac{1}{2} (\nabla \tilde{v}_s + \nabla \tilde{v}_s^T) - \frac{1}{3} (\nabla \cdot \tilde{v}_s) \mathbf{I}$$

$$|\widetilde{S}_s| = \sqrt{2\widetilde{S}_s : \widetilde{S}_s}$$

Scaled Filtered Solids Thermal Dispersion

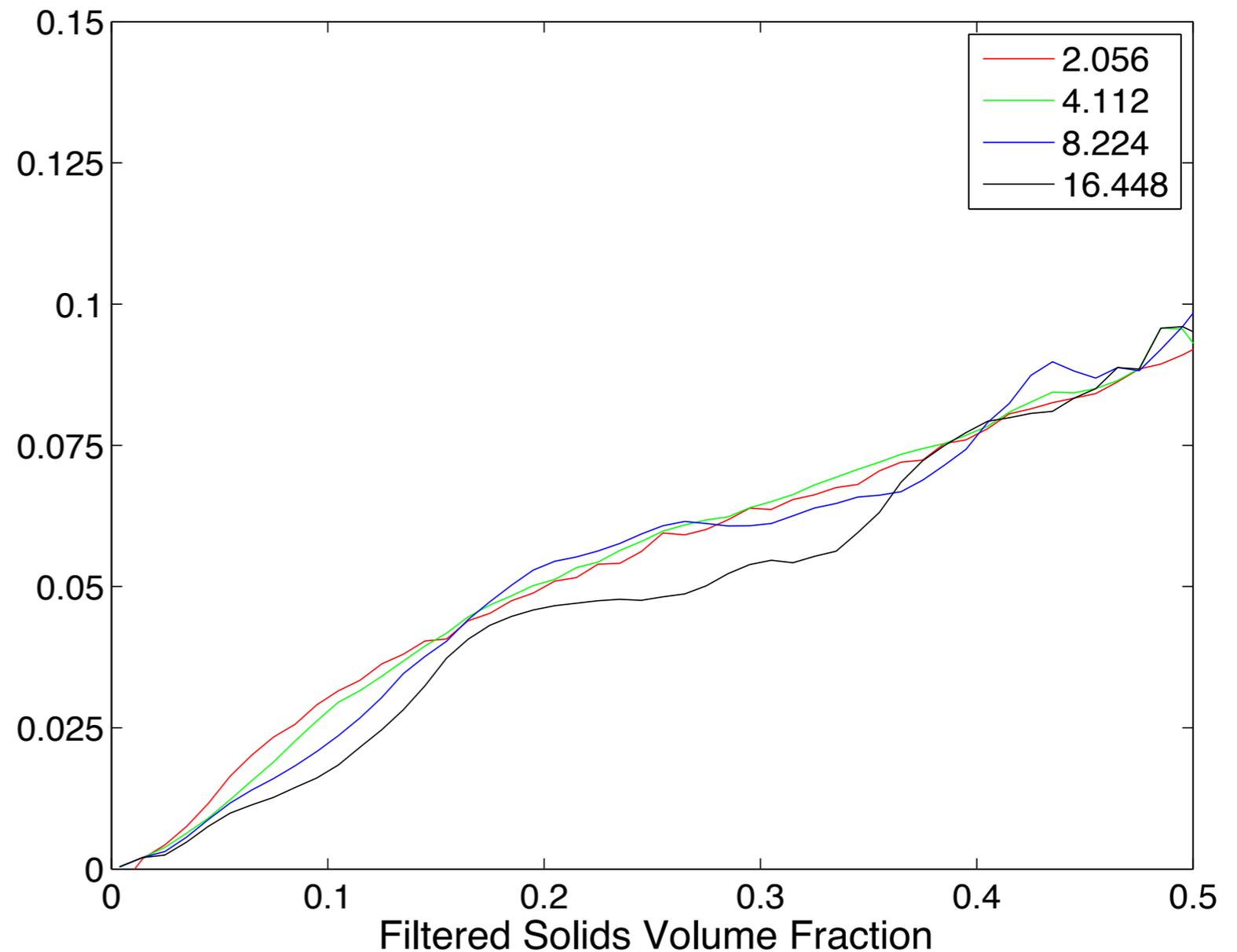


$$\hat{\alpha}_{s_{filt}} = \frac{\alpha_{s_{filt}}}{(v_t^3/g)}$$

$$\frac{\hat{\alpha}_{s_{filt}}}{\hat{\Delta}^2 |\widehat{S}_s|}$$

$$\frac{\hat{\alpha}_{s_{filt}}}{\hat{\Delta}^2 |\widehat{S}_s|} \sim 0.2 \overline{\phi_s}$$

Smagorinsky type model



Scaled Filtered Gas Thermal Dispersion



$$\hat{\alpha}_{g_{filt}} = \frac{\alpha_{g_{filt}}}{(v_t^3/g)}$$

Scaled Filtered Gas Thermal Dispersion



$$\hat{\alpha}_{g_{filt}} = \frac{\alpha_{g_{filt}}}{(v_t^3/g)}$$

$$\frac{\hat{\alpha}_{g_{filt}}}{\hat{\Delta}^2 |\widehat{S}_g|}$$

Scaled Filtered Gas Thermal Dispersion

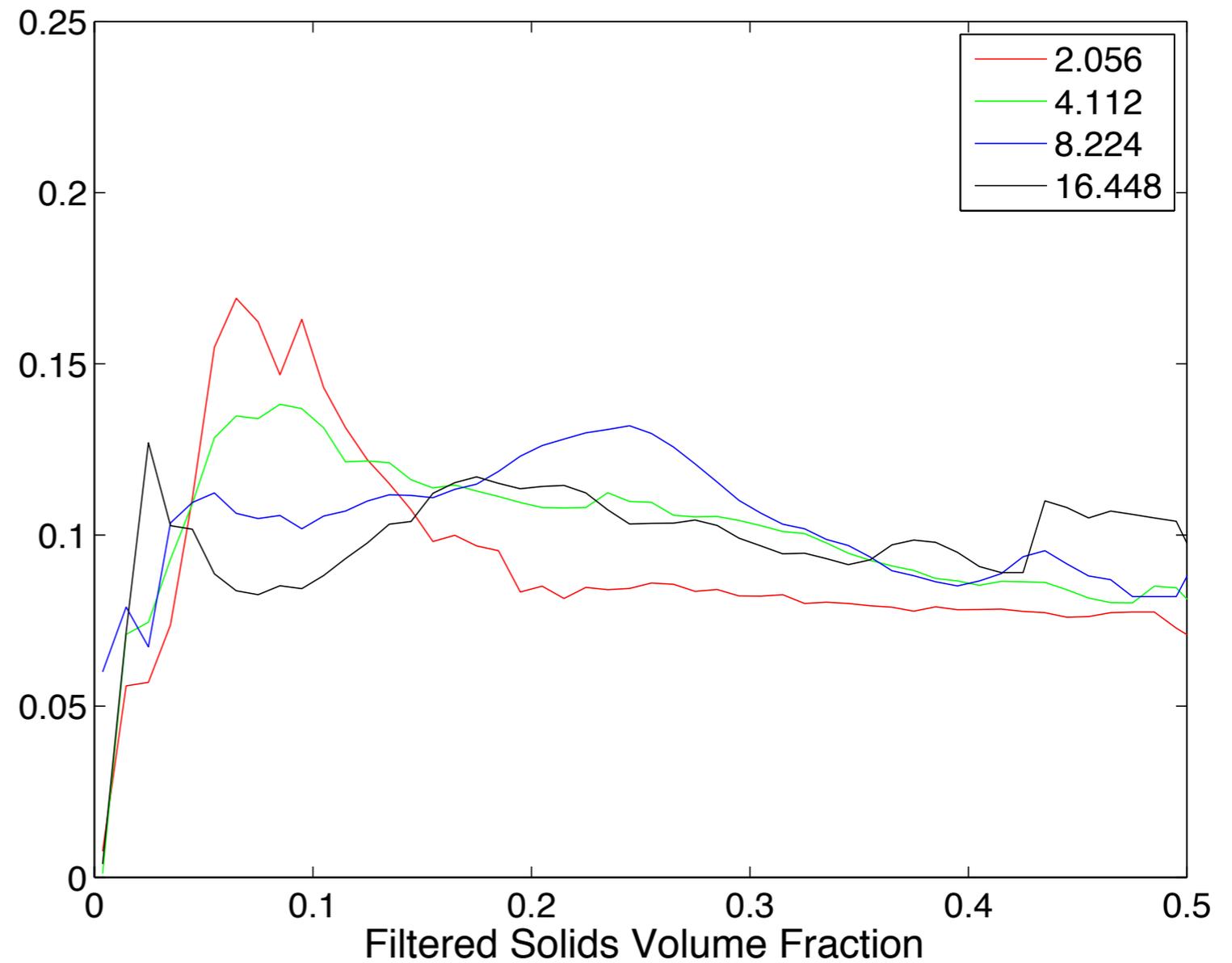


$$\hat{\alpha}_{g_{filt}} = \frac{\alpha_{g_{filt}}}{(v_t^3/g)}$$

$$\frac{\hat{\alpha}_{g_{filt}}}{\hat{\Delta}^2 |\widehat{S}_g|}$$

$$\frac{\hat{\alpha}_{g_{filt}}}{\hat{\Delta}^2 |\widehat{S}_g|} \sim 0.1(1 - e^{-60\overline{\phi_s}})$$

Smagorinsky type model



Connection to Momentum Transfer



- In single phase turbulent flows, heat transfer often modeled through a **turbulent Prandtl number**.

Connection to Momentum Transfer



- In single phase turbulent flows, heat transfer often modeled through a **turbulent Prandtl number**.
- For gas-solid flows we may define a filtered Prandtl number for each phase.

Connection to Momentum Transfer



- In single phase turbulent flows, heat transfer often modeled through a **turbulent Prandtl number**.
- For gas-solid flows we may define a filtered Prandtl number for each phase.
- Based on earlier studies of turbulent momentum transfer in gas-solid flows we find^{1,2}

$$\overline{Pr}_s \sim 0.5$$

$$\overline{Pr}_g \sim 1$$

Filtered Interphase Heat Transfer Coefficient



$$\frac{\gamma_{filt}}{\gamma(\overline{\phi_s}, \tilde{\mathbf{v}}_{slip})}$$

$$\gamma_{filt} = \frac{\overline{\gamma(T_s - T_g)}}{(\widetilde{T_s} - \widetilde{T_g})}$$

- Look for the form

$$\frac{\gamma_{filt}}{\gamma(\overline{\phi_s}, \tilde{\mathbf{v}}_{slip})} = f(\overline{\phi_s}, \tilde{\mathbf{v}}_{slip}, \Delta)$$

Filtered Interphase Heat Transfer Coefficient

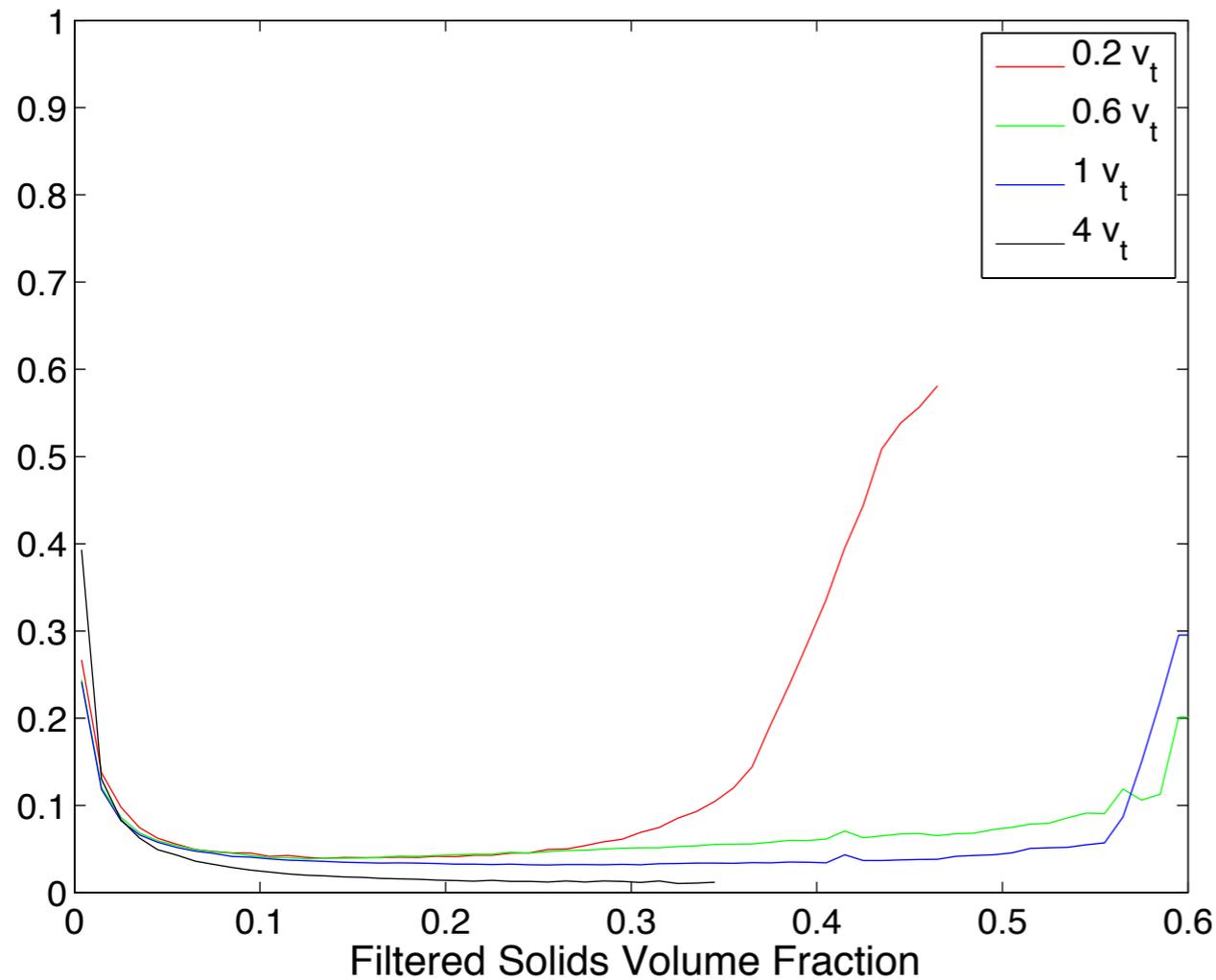


$$\frac{\gamma_{filt}}{\gamma(\overline{\phi_s}, \tilde{\mathbf{v}}_{slip})}$$

- Look for the form

$$\frac{\gamma_{filt}}{\gamma(\overline{\phi_s}, \tilde{\mathbf{v}}_{slip})} = f(\overline{\phi_s}, \tilde{\mathbf{v}}_{slip}, \Delta)$$

- Reduction in heat transfer coefficient ~ 2-3 orders of magnitude.



Dimensionless filter size of 2.056 (1cm).

Filtered Interphase Heat Transfer Coefficient

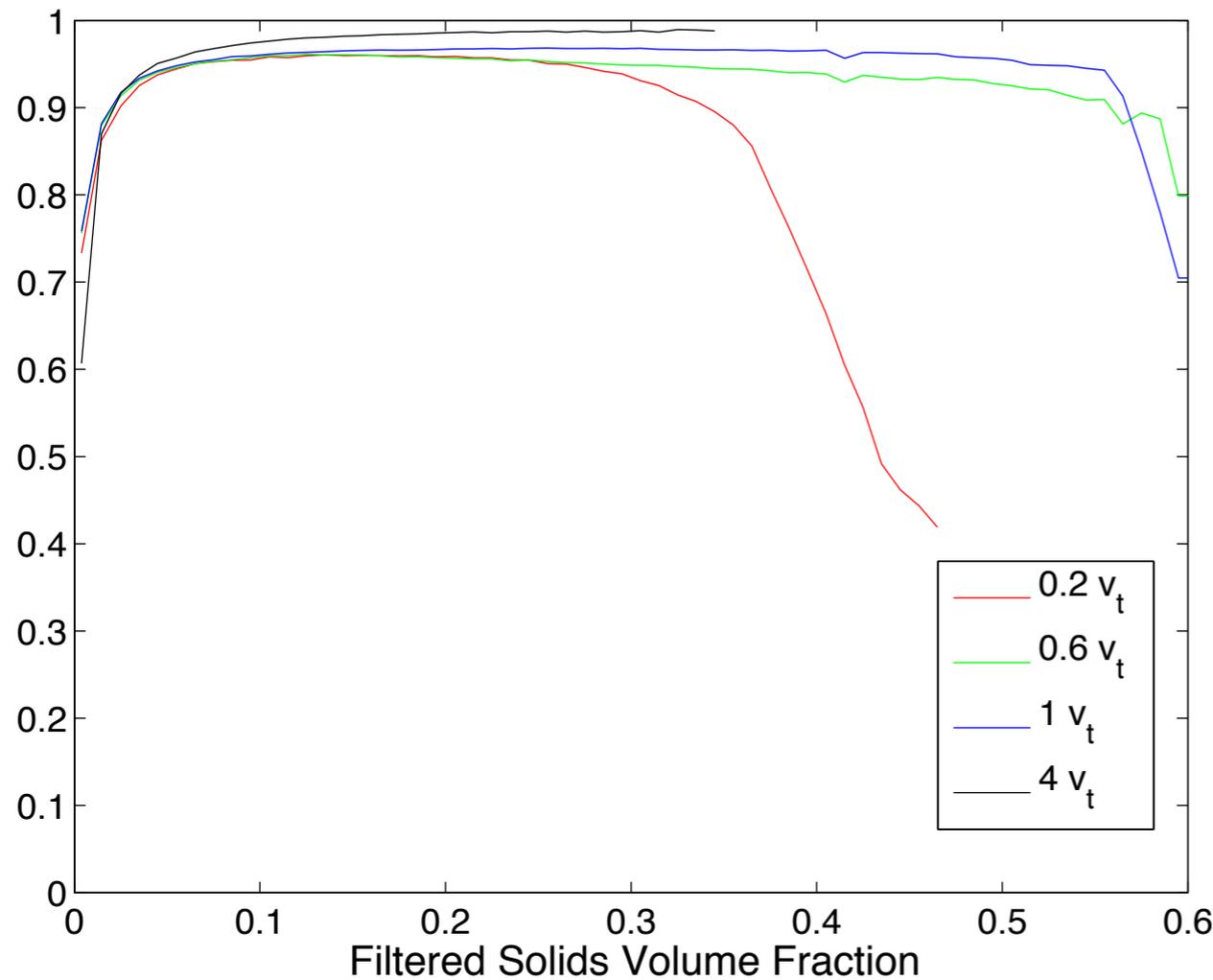


$$1 - \frac{\gamma_{filt}}{\gamma(\overline{\phi_s}, \tilde{\mathbf{v}}_{slip})}$$

- Look for the form

$$\frac{\gamma_{filt}}{\gamma(\overline{\phi_s}, \tilde{\mathbf{v}}_{slip})} = f(\overline{\phi_s}, \tilde{\mathbf{v}}_{slip}, \Delta)$$

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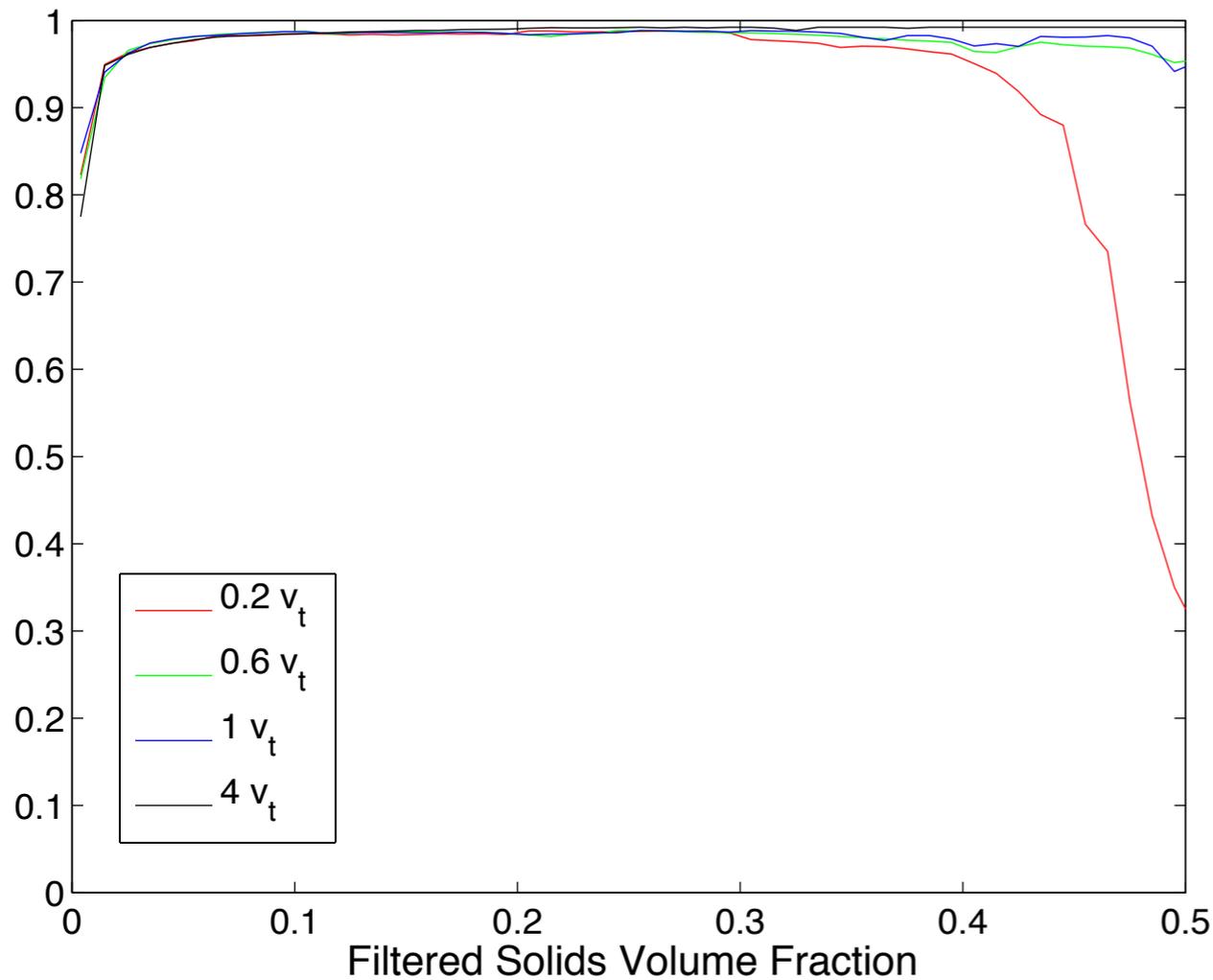


Dimensionless filter size of 2.056 (1cm).

Filtered Interphase Heat Transfer Coefficient



$$1 - \frac{\gamma_{filt}}{\gamma(\overline{\phi_s}, \tilde{\mathbf{v}}_{slip})}$$



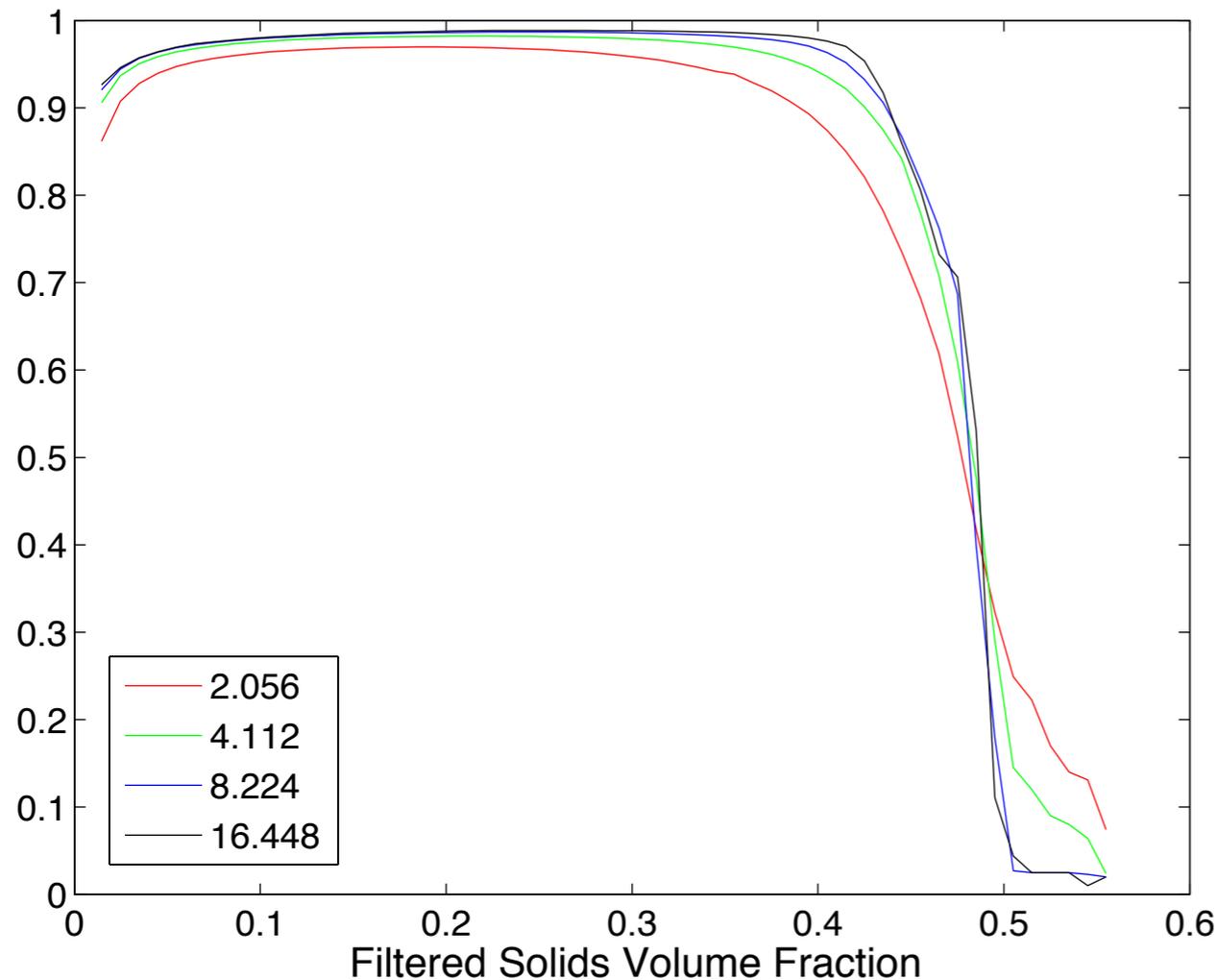
Dimensionless filter size of 8.224 (4cm).

- Look for the form
$$\frac{\gamma_{filt}}{\gamma(\overline{\phi_s}, \tilde{\mathbf{v}}_{slip})} = f(\overline{\phi_s}, \tilde{\mathbf{v}}_{slip}, \Delta)$$
- Reduction in heat transfer coefficient ~ 2-3 orders of magnitude.
- Weak function of filter size/slip velocity at larger slip velocities.
- Most realizations with low slip velocities occur in regions of high solids concentration.
- Behavior similar to filtered interphase drag coefficient, but the effect is more pronounced.

Filtered Interphase Heat Transfer Coefficient



$$1 - \frac{\gamma_{filt}}{\gamma(\overline{\phi_s}, \tilde{v}_{slip})}$$



- Look for the form

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- Reduction in heat transfer coefficient ~ 2-3 orders of magnitude.
- Weak function of filter size/slip velocity at larger slip velocities.
- Most realizations with low slip velocities occur in regions of high solids concentration.
- Behavior similar to filtered interphase drag coefficient, but the effect is more pronounced.
- In practice for large filter size we may employ

$$\frac{\gamma_{filt}}{\gamma(\overline{\phi_s}, \tilde{v}_{slip})} \sim f(\overline{\phi_s})$$



Summary

- Smagorinsky type model for filtered dispersion coefficient

$$\frac{\widehat{\alpha}_{g\,filt}}{\widehat{\Delta}^2 |\widehat{S}_g|} = h(\overline{\phi_s})$$

$$\frac{\widehat{\alpha}_{s\,filt}}{\widehat{\Delta}^2 |\widehat{S}_s|} = g(\overline{\phi_s})$$



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- Filtered Prandtl Numbers

$$\overline{Pr}_s \sim 0.5$$

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Summary

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- Filtered Prandtl Numbers $\overline{Pr}_s \sim 0.5$ $\overline{Pr}_g \sim 1$
- Filtered interphase heat transfer coefficient $\frac{\gamma_{filt}}{\gamma(\overline{\phi_s}, \tilde{\mathbf{v}}_{slip})} \sim f(\overline{\phi_s}) \ll 1$



Summary

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- Results carry over to mass transfer and tracer dispersion



Summary

- Smagorinsky type model for filtered dispersion coefficient $\frac{\widehat{\alpha}_{g\,filt}}{\widehat{\Delta}^2|\widehat{S}_g|} = h(\overline{\phi_s})$ $\frac{\widehat{\alpha}_{s\,filt}}{\widehat{\Delta}^2|\widehat{S}_s|} = g(\overline{\phi_s})$
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- Results carry over to mass transfer and tracer dispersion

Further areas for investigation

- Impact of going from 2-D to 3-D
 - Results for hydrodynamics suggest the effect is small (*Igci et. al, 2011*)

Acknowledgements



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 - ExxonMobil Research & Engineering Company

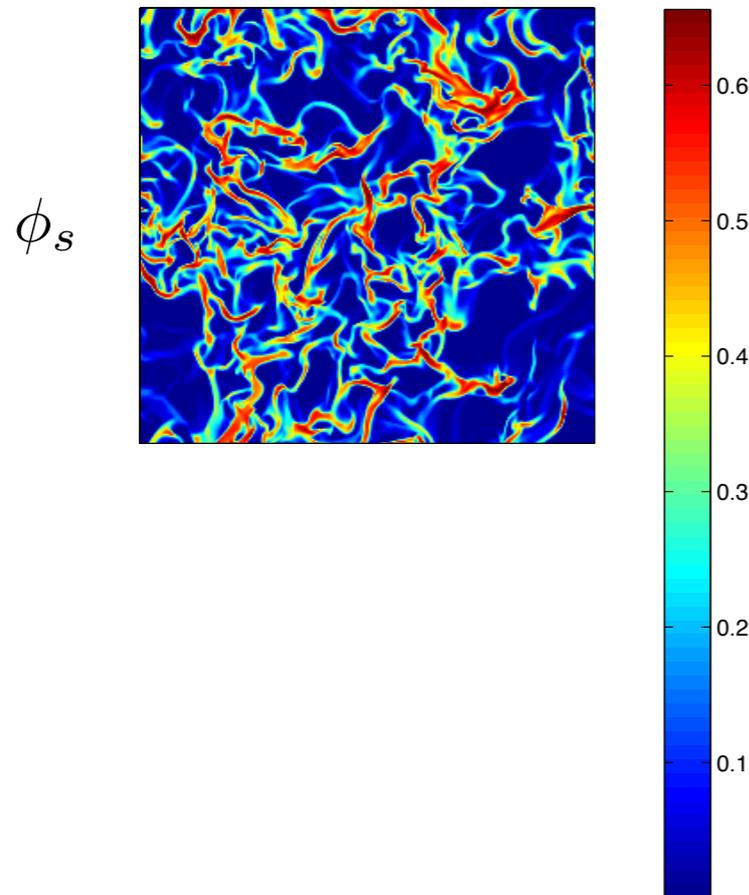
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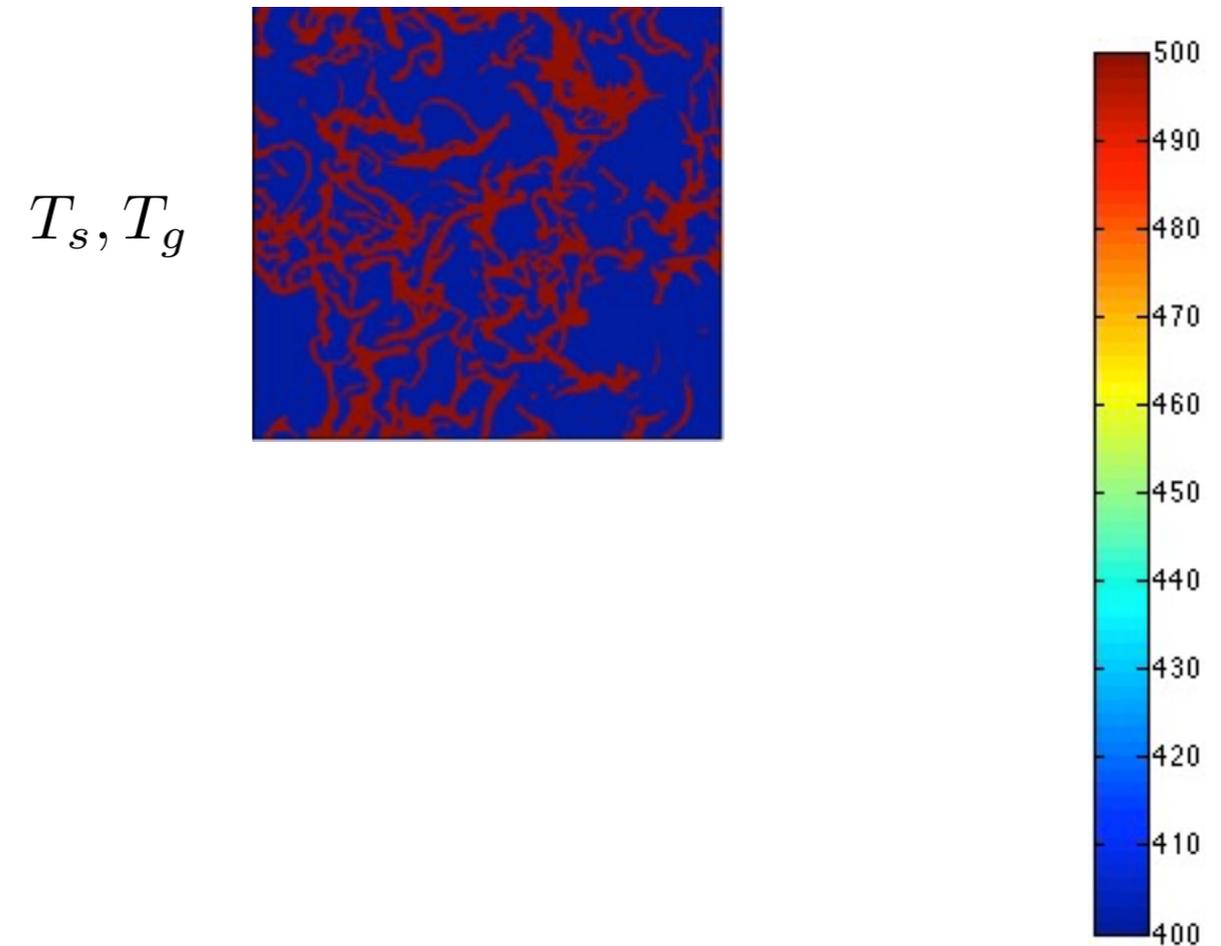
Filtered Interphase Heat Transfer Coefficient: A Preview



Solids Volume
Fraction Field



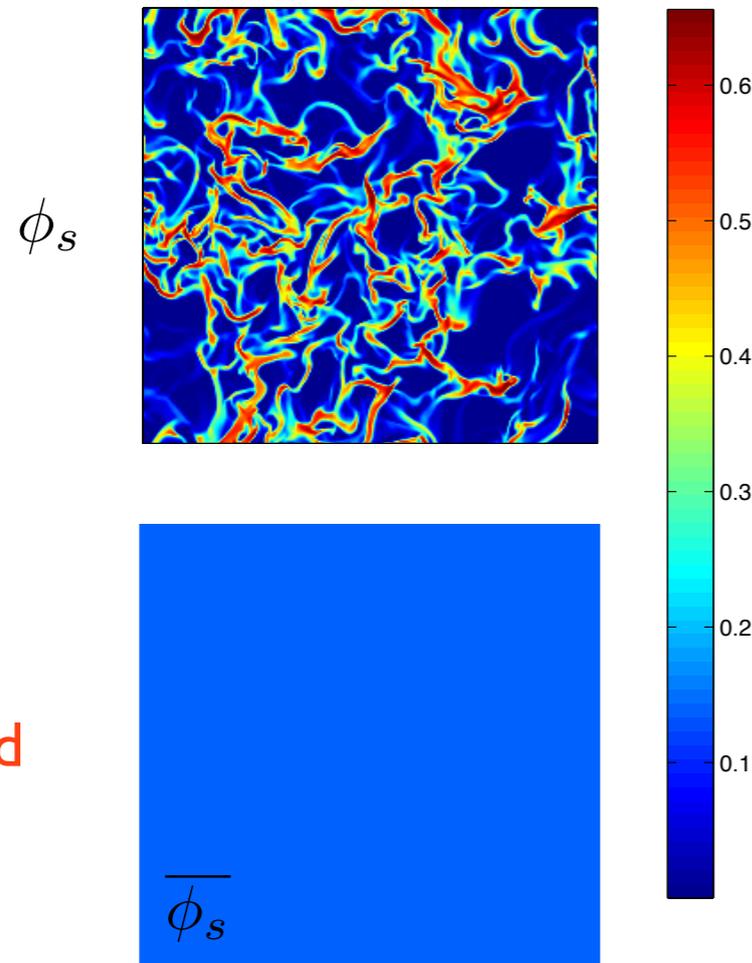
Temperature
Field



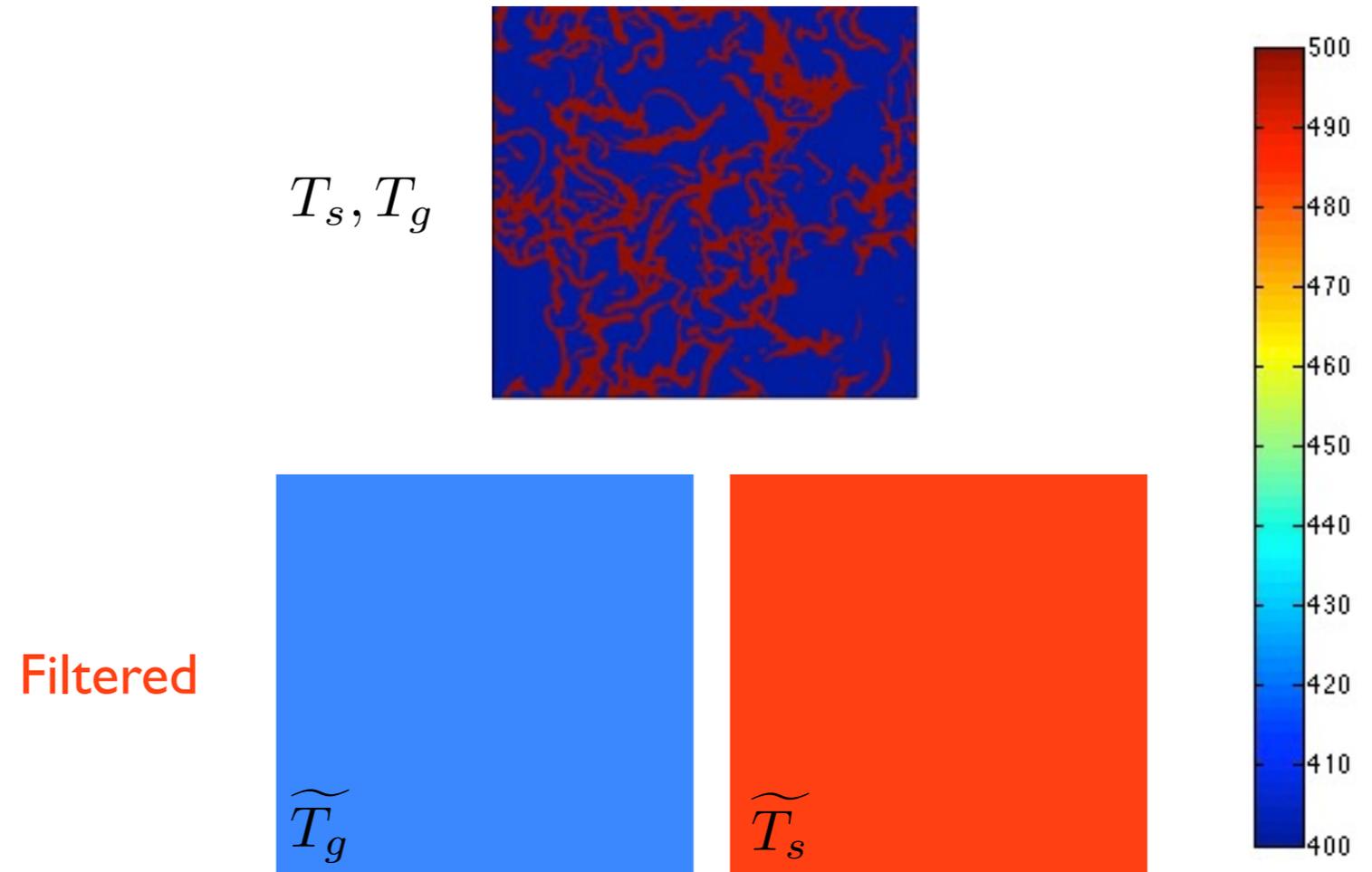
Filtered Interphase Heat Transfer Coefficient: A Preview



Solids Volume Fraction Field



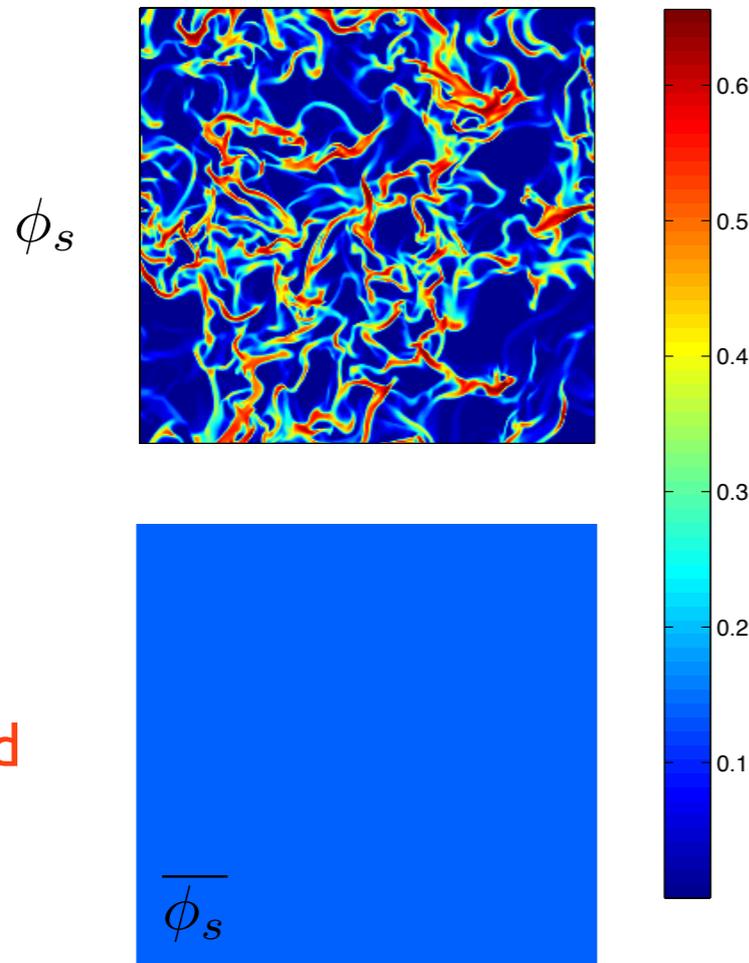
Temperature Field



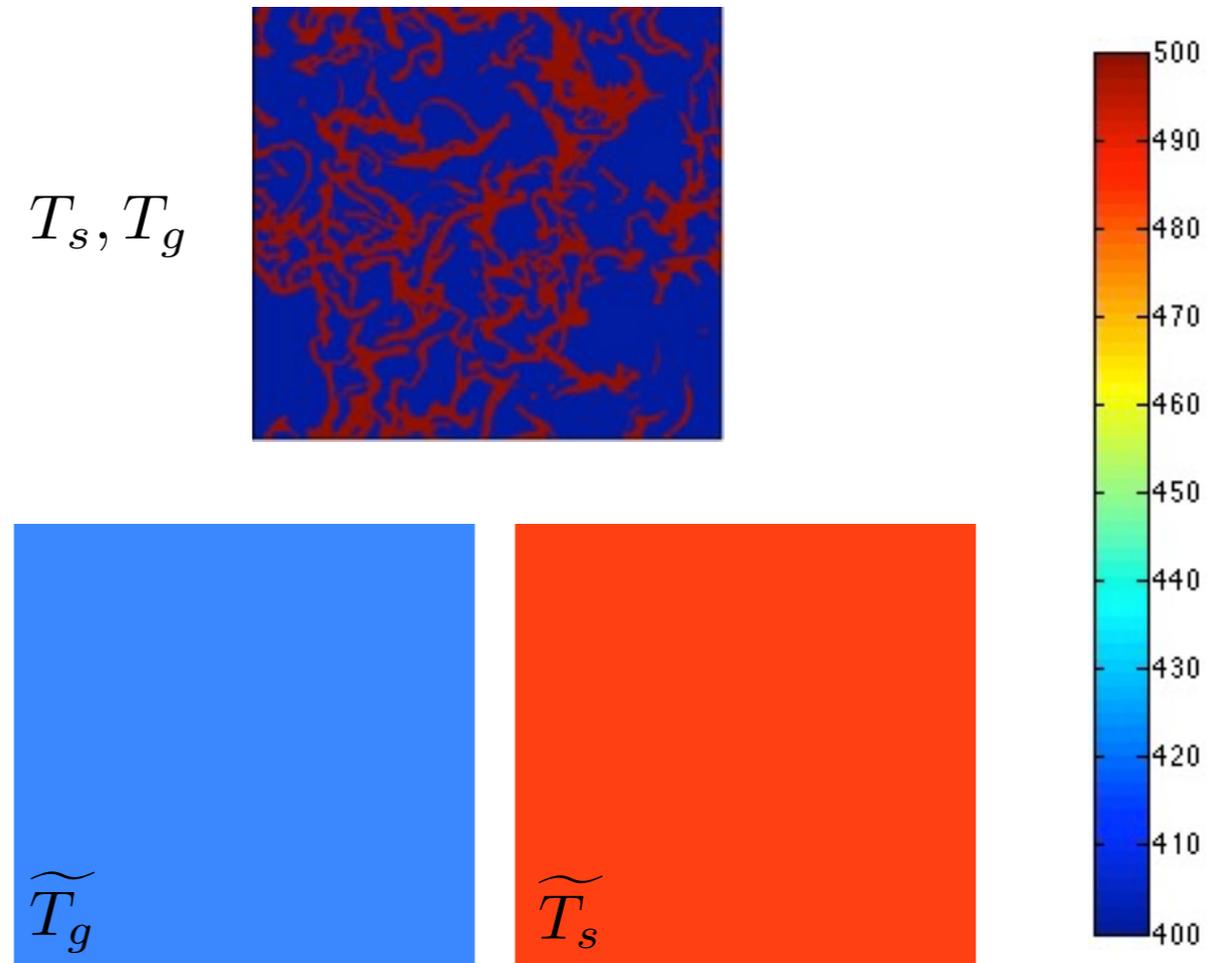
Filtered Interphase Heat Transfer Coefficient: A Preview



Solids Volume Fraction Field



Temperature Field

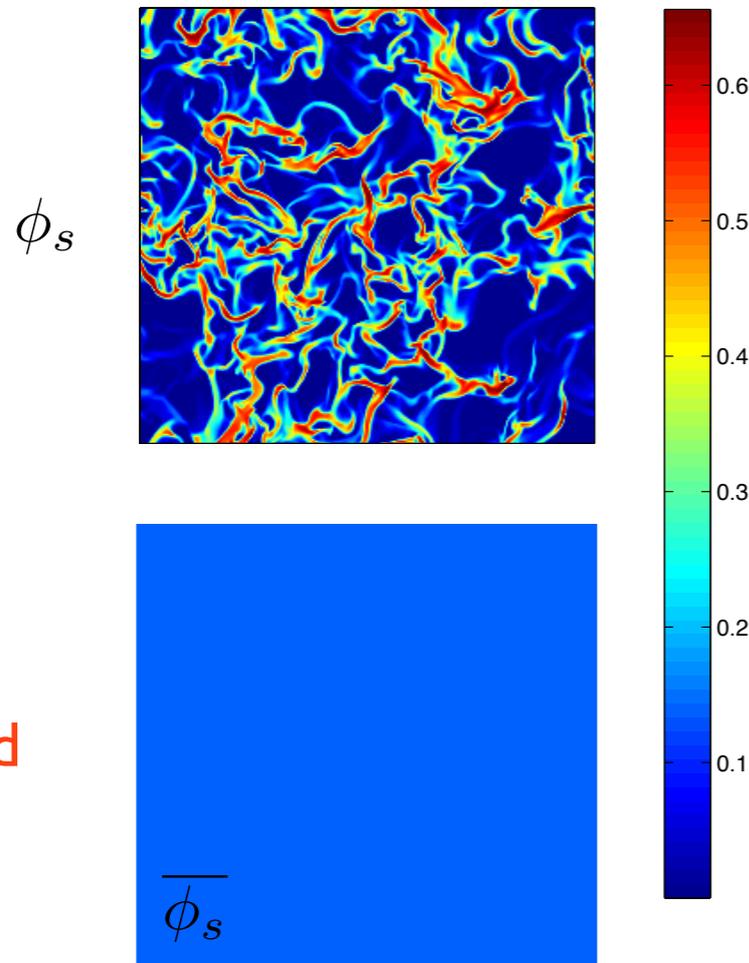


$$(\widetilde{T}_s - \widetilde{T}_g) \gg (T_s - T_g)$$

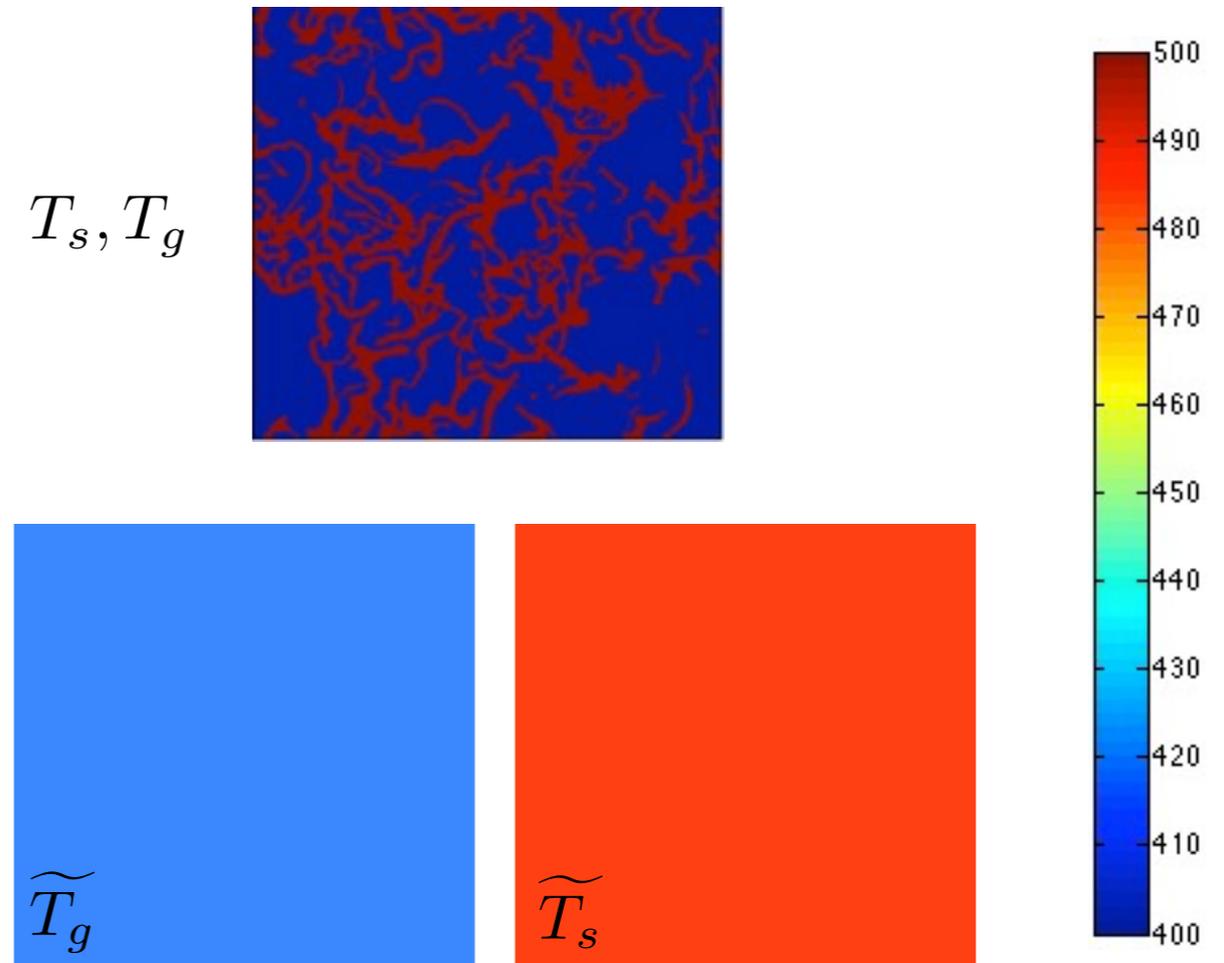
Filtered Interphase Heat Transfer Coefficient: A Preview



Solids Volume Fraction Field



Temperature Field



$$(\widetilde{T}_s - \widetilde{T}_g) \gg (T_s - T_g)$$

$$\frac{\gamma_{filt}}{\gamma(\overline{\phi_s}, \widetilde{\mathbf{v}}_{slip})} \ll 1$$

Mass Transfer & Dispersion Coefficients In the Literature

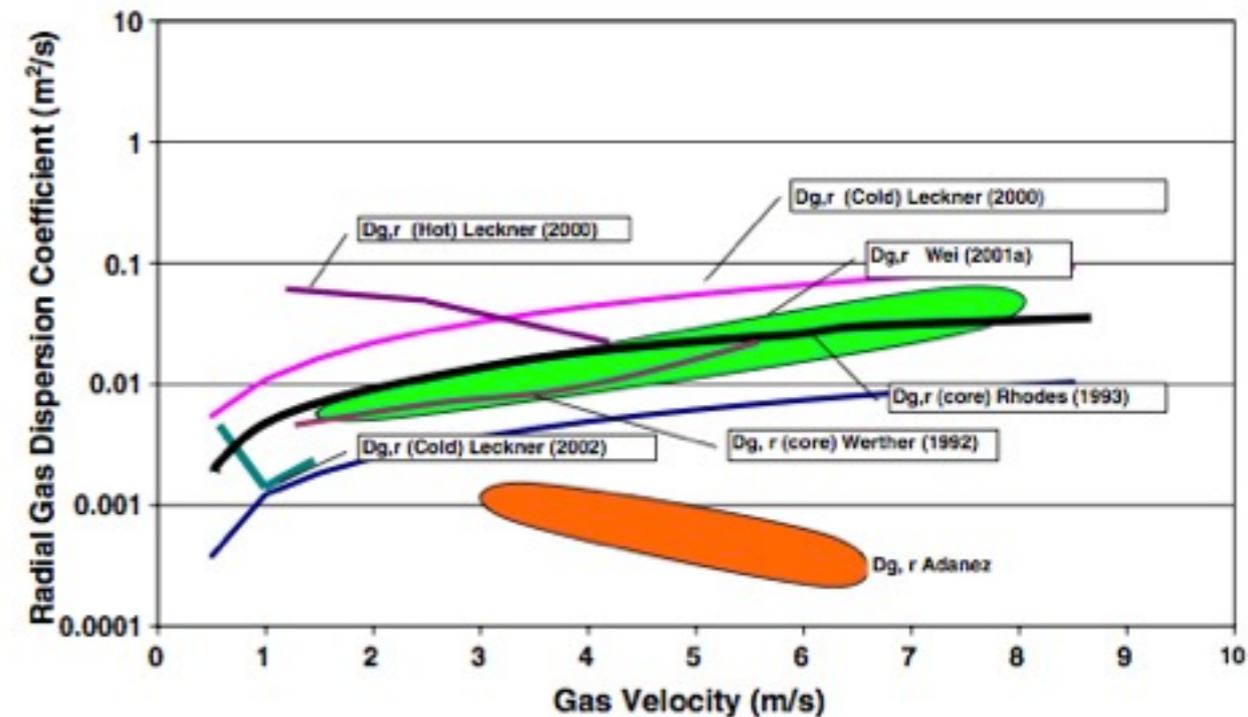
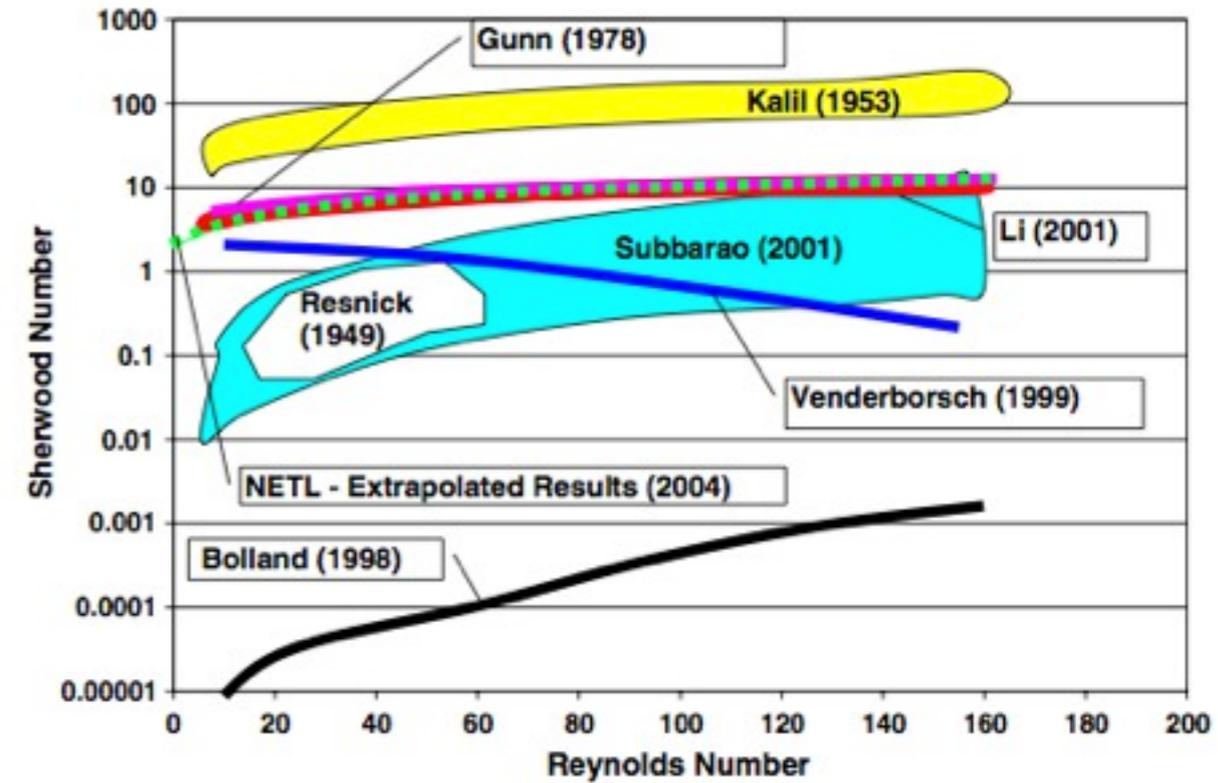


Experimental Data in the literature show considerable variation

Mass transfer coefficients differ by several orders of magnitude

Dispersion coefficients differ by several orders of magnitude

Modeling efforts suggest origins of variance related to inadequate representation of meso-scale structures (clusters/bubbles)



Interphase Heat Transfer Correlation



$$Nu = (7 - 10\phi_g + 5\phi_g^2)(1 + 0.7Re_p^{0.2}Pr^{1/3}) + (1.33 - 2.4\phi_g + 1.2\phi_g^2)Re_p^{0.7}Pr^{1/3}$$

$$\gamma = \frac{6k_g Nu}{d_p^2}$$

Filtered Transport Properties



Filtered Interphase Heat Transfer Coefficient

$$\gamma_{filt} = \frac{\overline{\gamma(T_s - T_g)}}{(\widetilde{T_s} - \widetilde{T_g})}$$

Filtered Transport Properties



Filtered Interphase Heat Transfer Coefficient

$$\gamma_{filt} = \frac{\overline{\gamma(T_s - T_g)}}{(\widetilde{T}_s - \widetilde{T}_g)}$$

Filtered Thermal Dispersion Coefficient

$$\alpha_{filt} = \frac{k_{filt}}{\rho_s C_{p_s}} = \frac{\overline{\phi_s} \left(\widetilde{\mathbf{v}_{s_x} T_s} - \mathbf{v}_{s_x} \widetilde{T}_s \right)}{\frac{\partial \widetilde{T}_s}{\partial x}}$$

Filtered Transport Properties



Filtered Interphase Heat Transfer Coefficient

$$\gamma_{filt} = \frac{\overline{\gamma(T_s - T_g)}}{\langle \widetilde{T_s - T_g} \rangle}$$

Filtered Thermal Dispersion Coefficient

$$\alpha_{filt} = \frac{k_{filt}}{\rho_s C_{p_s}} = \frac{\overline{\phi_s (\widetilde{v_{s_x} T_s} - \widetilde{v_{s_x} T_s})}}{\langle \frac{\partial \widetilde{T_s}}{\partial x} \rangle}$$

Calculated in Simulations as follows:

$$\gamma_{filt} = \frac{\langle \overline{\gamma(T_s - T_g)} \rangle}{\langle \widetilde{T_s - T_g} \rangle} \quad \alpha_{filt} = \frac{\langle \overline{\phi_s (\widetilde{v_{s_x} T_s} - \widetilde{v_{s_x} T_s})} \rangle}{\langle \frac{\partial \widetilde{T_s}}{\partial x} \rangle} \quad \langle \frac{\partial \widetilde{T_s}}{\partial x} \rangle = \chi$$