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Carbon Capture Simulation Initiative

A Sub-Grid Model for an Array of Immersed Cylinders in Coarse-Grid Multiphase Flow Simulations of a Carbon Capture Device

Avik Sarkar[1], Xin Sun[1], Sankaran Sundaresan[2]

Presented by **Kapil Agrawal[2]**

[1]Pacific Northwest National Laboratory, Richland, WA
[2]Chemical and Biological Engineering, Princeton University, Princeton, NJ

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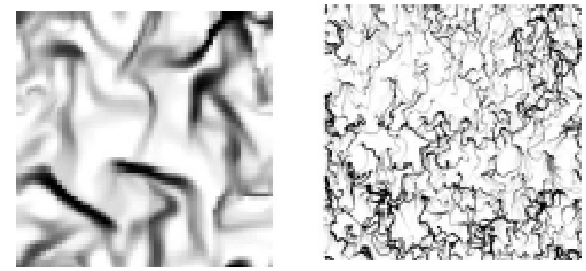
31 October 2012

U.S. DEPARTMENT OF ENERGY

Motivation

- Computationally infeasible to implement sufficiently small cells in large-scale simulations. Need to use:
  - $O(10^6)$ cells in 2D,
  - $O(10^9)$ cells in 3D.

Coarse grid　　Fine grid



Quantitatively inaccurate predictions obtained when smaller clusters are unresolved (Igci et al., 2008).

- Alternate approach is to develop “filtered” models which account for sub-grid scale structures.
  - Good progress made on two-phase gas-particle flows.
    - Igci et al., 2008;
    - Igci and Sundaresan, 2011a;
    - Igci and Sundaresan, 2011b;
    - Igci et al., 2012;
    - Parmentier et al., 2011;
    - Shi et al., 2011;
    - Hong et al., 2012.

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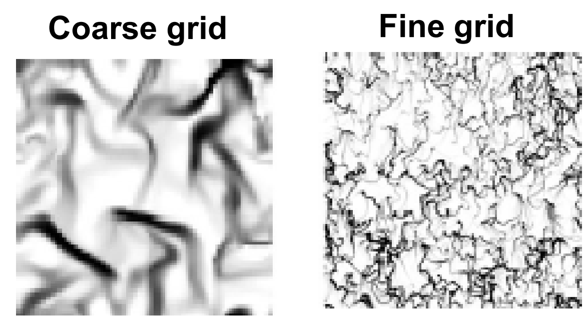

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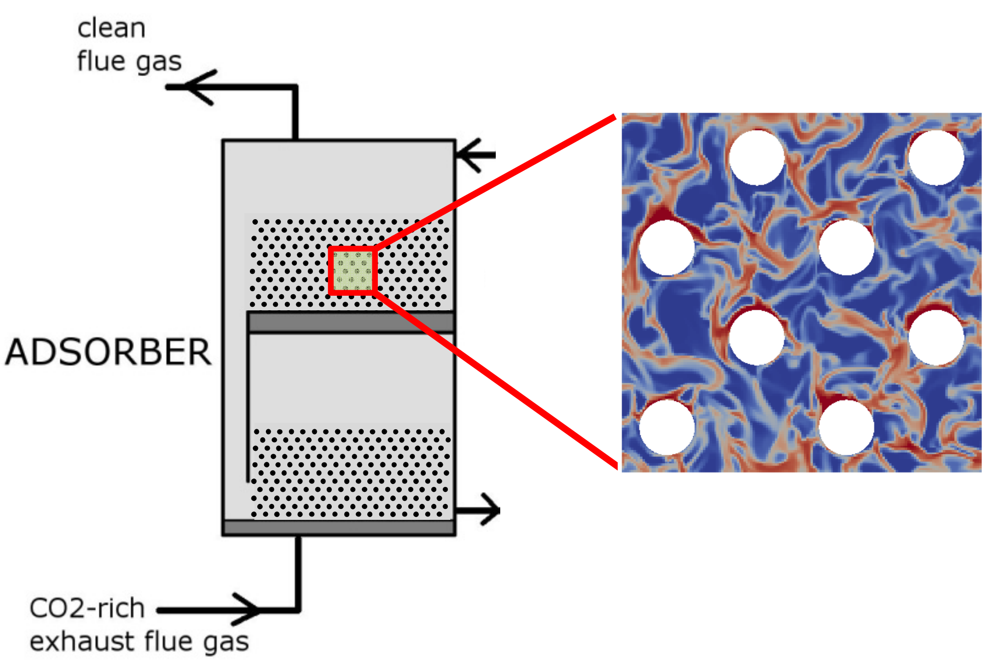
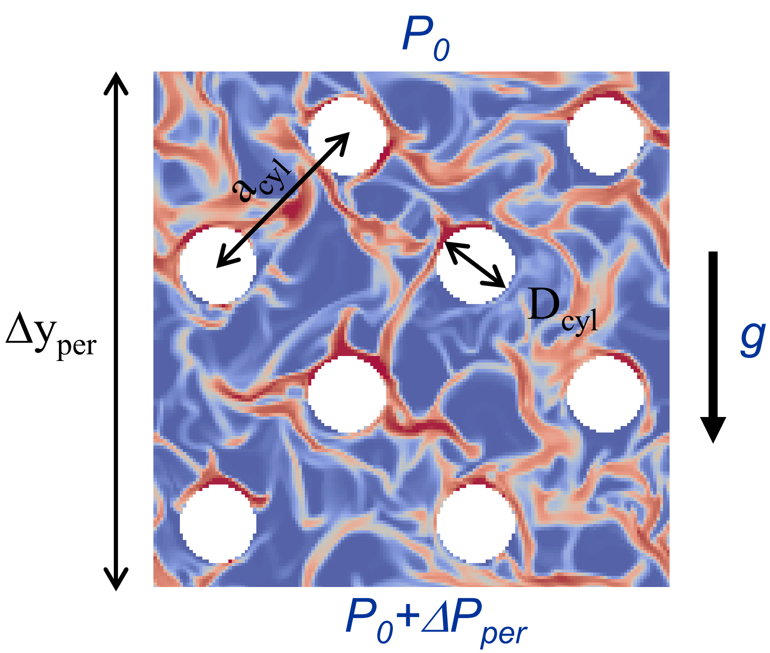
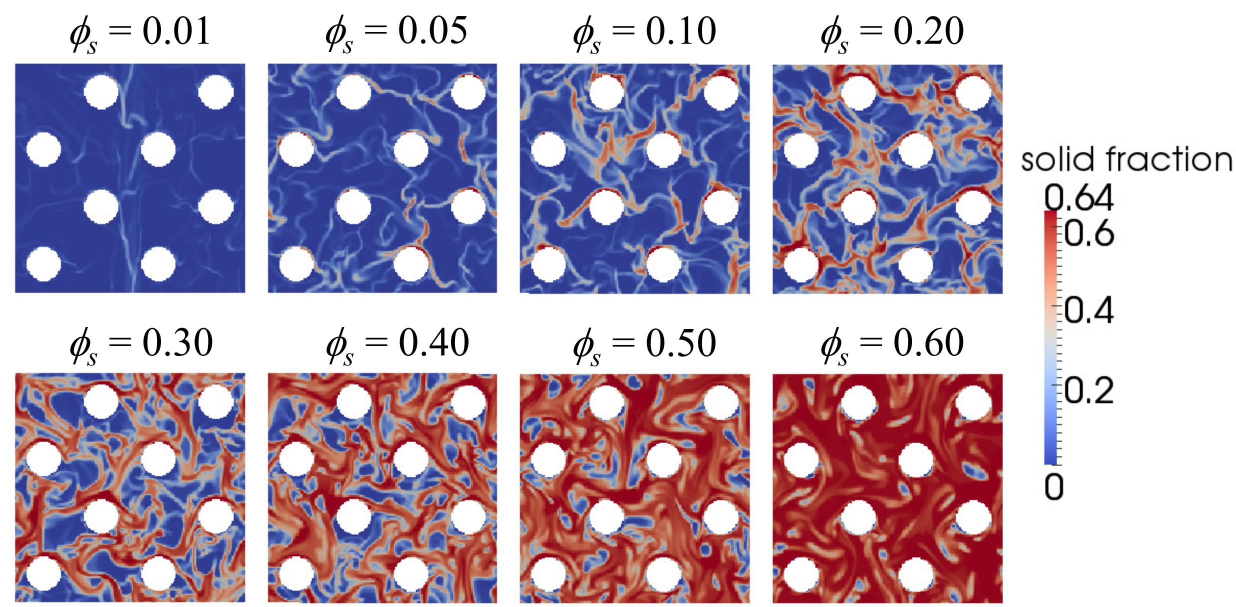


- This work focused on developing a sub-grid correction for an immersed horizontal cylinder array.
- Device of interest is a fluidized-bed “adsorber” – used to capture CO_2 from thermal power plant exhaust using amine-based particulate sorbents.
- Device length scale ~10 m, tube diameters ~1 cm.
  - Cannot resolve tubes explicitly.

Model

- A square 2D periodic domain with cylinder array.
- Models a horizontal tube bundle in a region away from the walls.
- A staggered arrangement used to prevent channeling of gas and solids between the tubes.





Velocity of gas and solids controlled by varying the vertical pressure drop ΔP_{per}.

Range of solid fractions simulated:
ϕ_s = 0.01 (dilute) to ϕ_s = 0.60 (dense).

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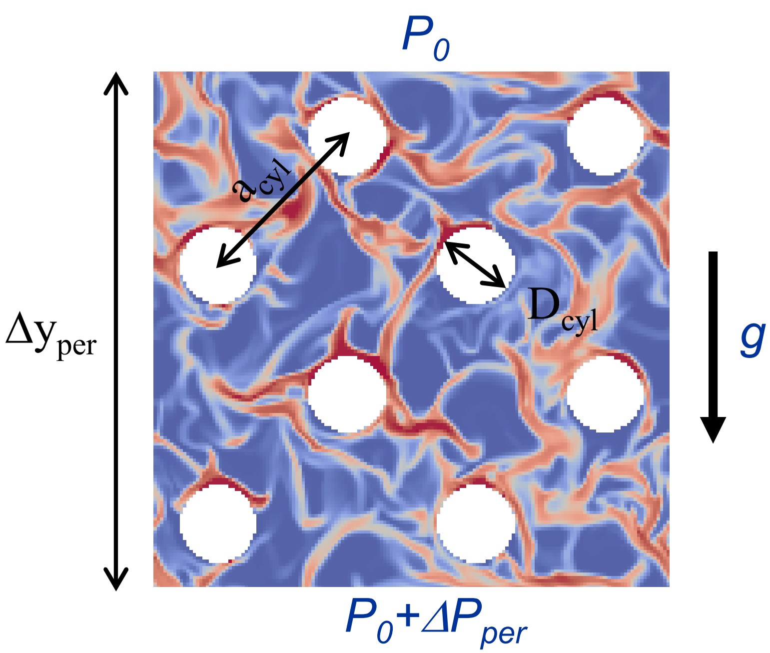

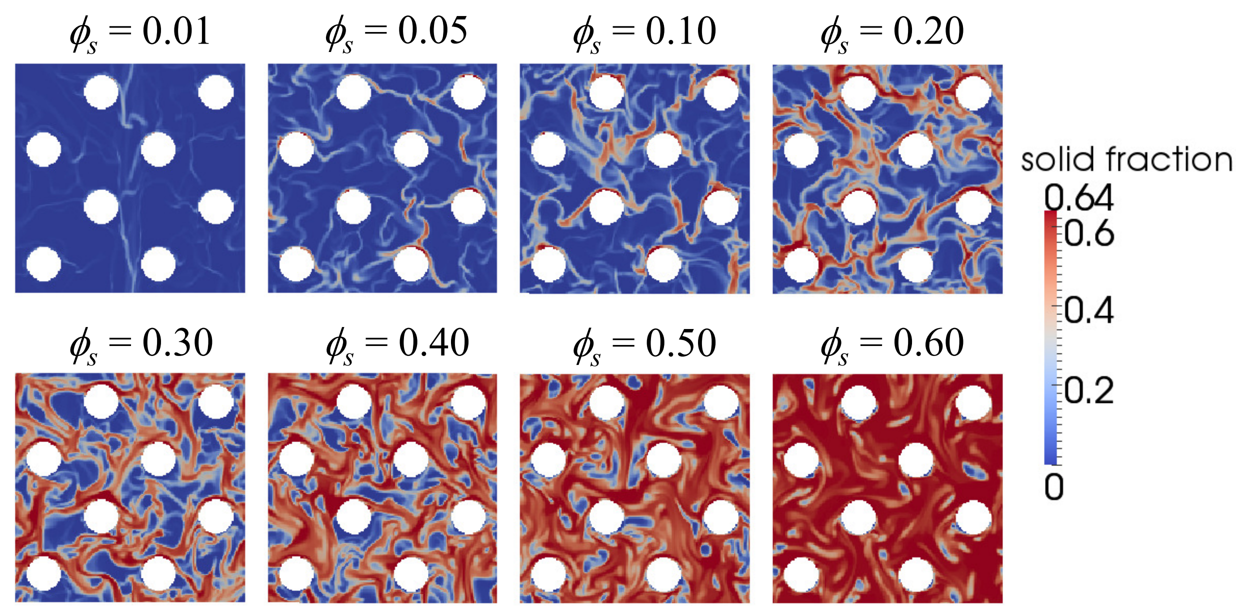

- Cylinder spacing a_{cyl} = 100 mm.
- Particle diameter d_p = 180 mm, particle density ρ_s = 441 kg/m^3.
- Gas density ρ_s = 1.14 kg/m^3 (18% CO_2, 6% steam, 76% N_2).
- Cylinder diameters investigated: D_{cyl} = 10 mm, 20 mm, 30 mm, 40 mm.

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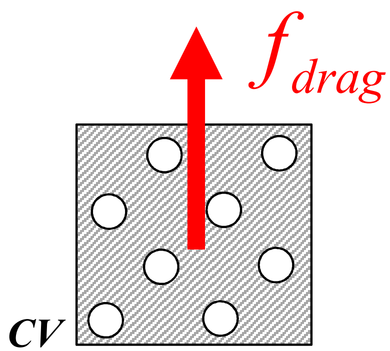
Filtering Procedure

The conservation equations are averaged over the domain to obtain the cylinder-mixture drag.

$$\frac{1}{V}\iiint_{CV}\left[\frac{\partial\left(\rho_g\phi_g'\vec{v}_g'\right)}{\partial t}+\frac{\partial\left(\rho_s\phi_s'\vec{v}_s'\right)}{\partial t}\right]dV=\underbrace{-\frac{1}{V}\iint_{\substack{\text{cylinder}\\\text{surfaces}}}\left(\boldsymbol{\sigma}_g'+\boldsymbol{\sigma}_s'\right)\cdot\hat{n}\,dS}_{f_{drag}}-\frac{1}{V}\iint_{\substack{\text{periodic}\\\text{boundaries}}}P\,\hat{n}\,dS+\frac{1}{V}\iiint_{CV}\left[\left(\rho_g\phi_g'+\rho_s\phi_s'\right)\vec{g}\right]dV$$

ϕ_g', $\vec{v}_g'$, $\boldsymbol{\sigma}_g'$, ϕ_s', $\vec{v}_s'$, $\boldsymbol{\sigma}_s'$ represent unfiltered cell-values obtained from the highly-resolved CFD simulations.



Filtered drag force exerted on gas-solid mixture by cylinders.

f_{drag} would appear in a corase-grid simulation.

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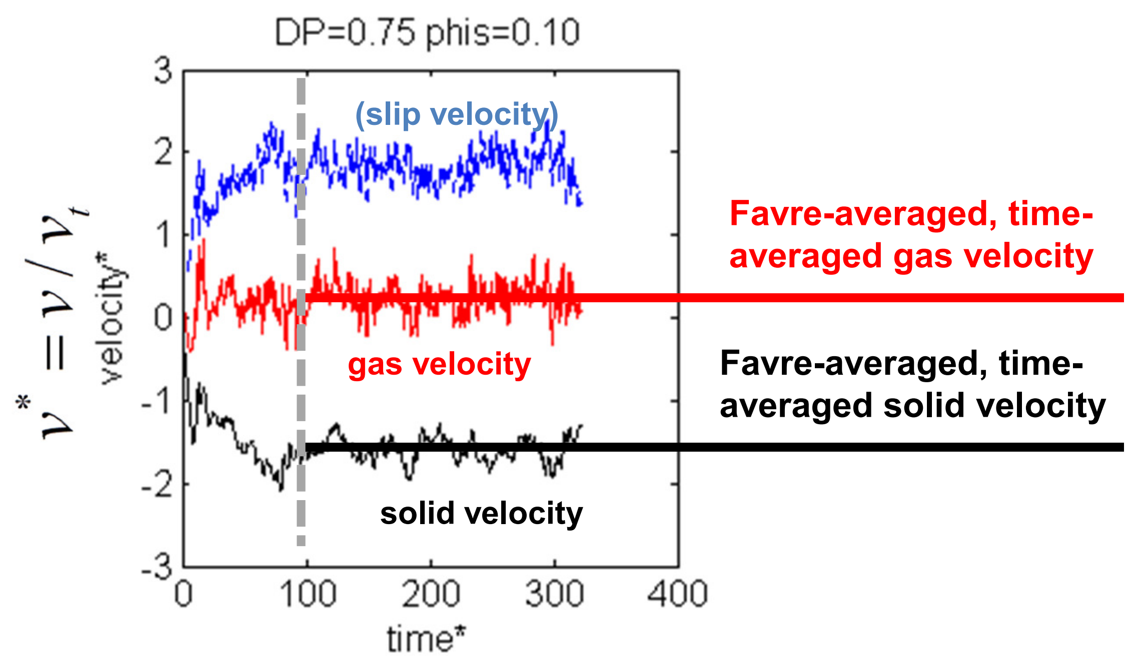
$$f_{drag}$$

Time averaging is performed to obtain statistically steady state values.



$$t^* = t\left(g / v_t\right)$$

Filtering Procedure

The conservation equations are averaged over the domain to obtain the cylinder-mixture drag.

$$\frac{1}{V}\iiint_{CV}\left[\frac{\partial\left(\rho_g\phi_g'\vec{v}_g'\right)}{\partial t}+\frac{\partial\left(\rho_s\phi_s'\vec{v}_s'\right)}{\partial t}\right]dV=\underbrace{-\frac{1}{V}\iint_{\substack{\text{cylinder}\\\text{surfaces}}}\left(\boldsymbol{\sigma}_g'+\boldsymbol{\sigma}_s'\right)\cdot\hat{n}dS}_{f_{drag}}-\frac{1}{V}\iint_{\substack{\text{periodic}\\\text{boundaries}}}P\,\hat{n}dS+\frac{1}{V}\iiint_{CV}\left[\left(\rho_g\phi_g'+\rho_s\phi_s'\right)\vec{g}\right]dV$$

The filtered variables are given by:

$$\phi_g=\frac{1}{V}\iiint_{CV}\phi_g'dV$$

$$\phi_s=\frac{1}{V}\iiint_{CV}\phi_s'dV$$

$$\phi_g v_g=\frac{1}{V}\iiint_{CV}\phi_g'v_g'dV$$

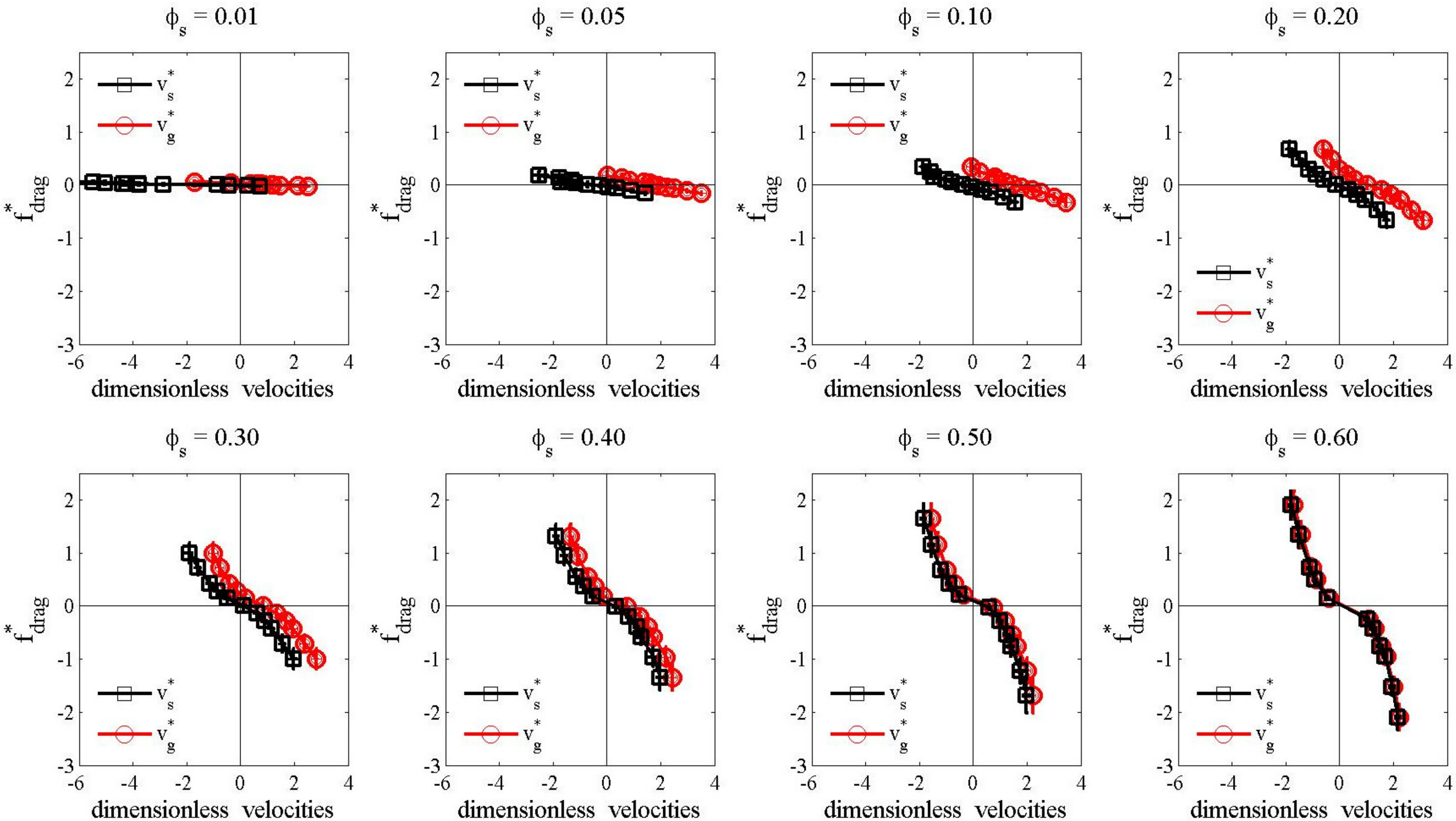
$$\phi_s v_s=\frac{1}{V}\iiint_{CV}\phi_s'v_s'dV$$

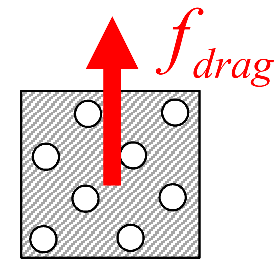
The filtered variables and Favre averaged velocities would also appear in a coarse grid simulation.

Objective: Obtain a closure for f_{drag} in terms of the filtered variables.

Filtered Drag vs. Filtered Velocities

- **Objective:** Find a closure for f^*_{drag} as a function of filtered velocities and solid fraction.
- First, plot filtered drag f^*_{drag} against filtered velocities v_s^* and v_g^*.



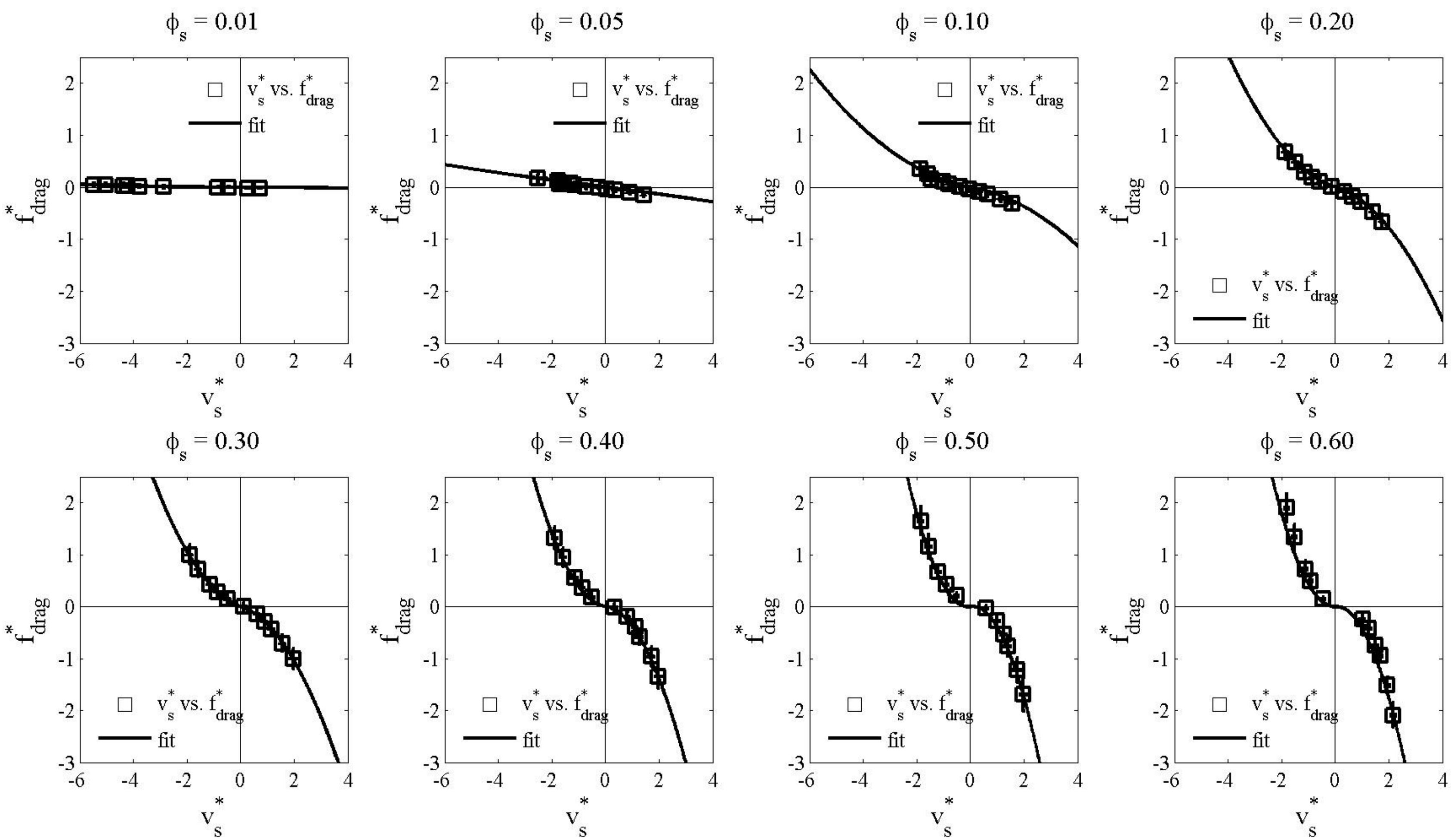


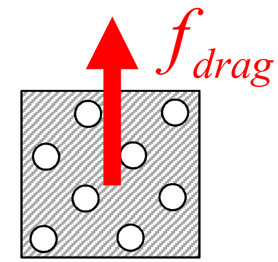
$$f^*_{drag} = \frac{f_{drag}}{\rho_s v_t^2 a_{cyl}}$$

$$v^* = \frac{v}{v_t}$$

Filtered Drag vs. Filtered Velocities

- **Objective:** Find a closure for f^*_{drag} as a function of filtered velocities and solid fraction.
- Quadratic relationship observed between filtered cylinder drag and solids velocity.



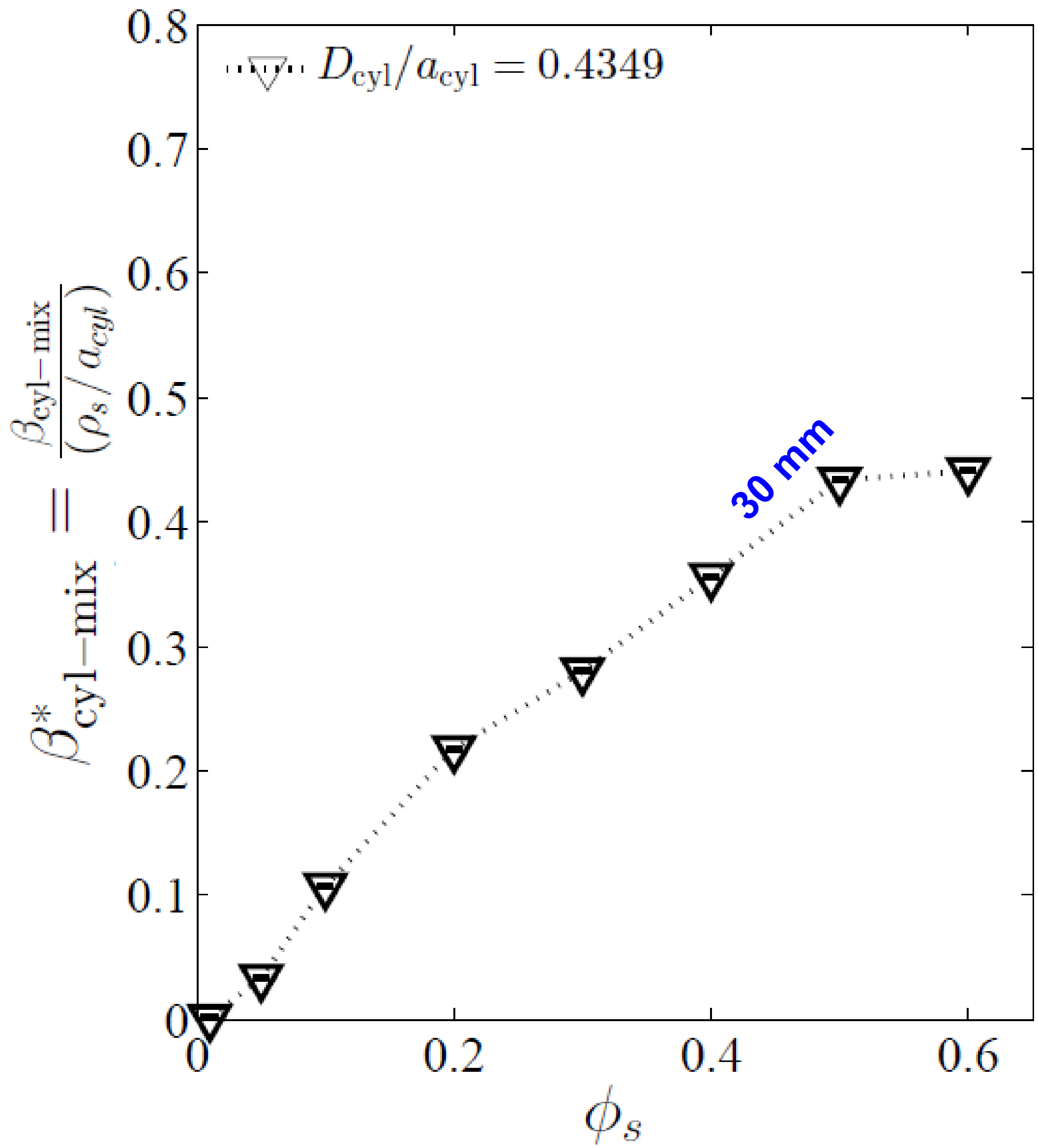


$$f^*_{drag} = \frac{f_{drag}}{\rho_s v_t^2 a_{\text{cyl}}}$$

$$v^* = \frac{v}{v_t}$$

$$f^*_{drag} = \beta^*_{\text{cyl-mix}}\left(-v^*_s \left|v^*_s\right|\right)$$

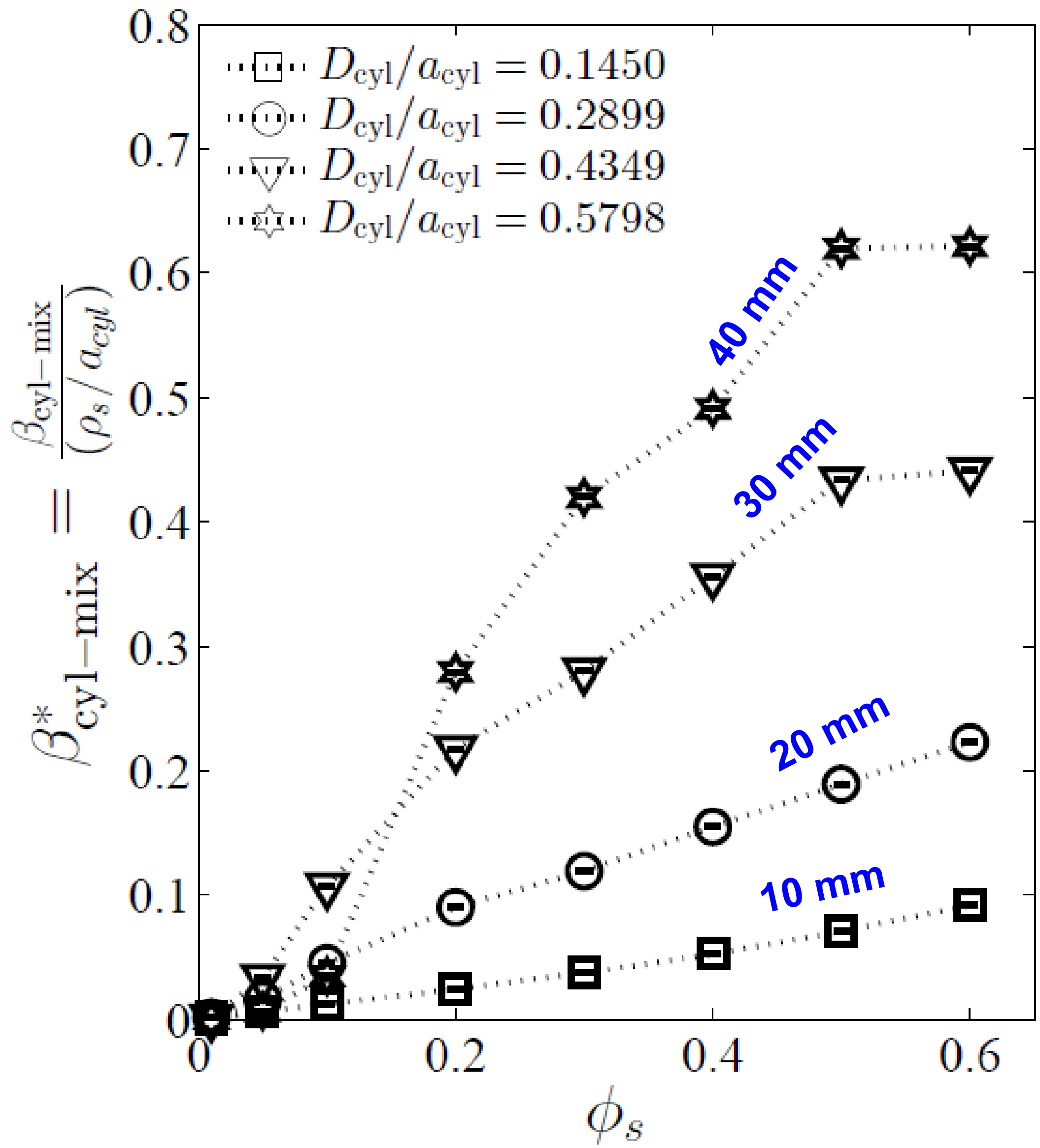
Cylinder-Suspension Sub-grid Drag Coefficient



$$f^*_{drag} = \beta^*_{cyl\text{-}mix}\left(-v^*_s\left|v^*_s\right|\right)$$

Cylinder-mixture drag coefficient $\beta^*_{cyl\text{-}mix}$ obtained from least squares fitting.

Cylinder-Suspension Sub-grid Drag Coefficient



$$f^*_{drag} = \beta^*_{cyl\text{-}mix}\left(-v^*_s\left|v^*_s\right|\right)$$

Cylinder-mixture drag coefficient $\beta^*_{cyl\text{-}mix}$ obtained from least squares fitting.

Additional simulations performed for varying cylinder diameters to determine the dependence on cylinder diameter D_{cyl}.

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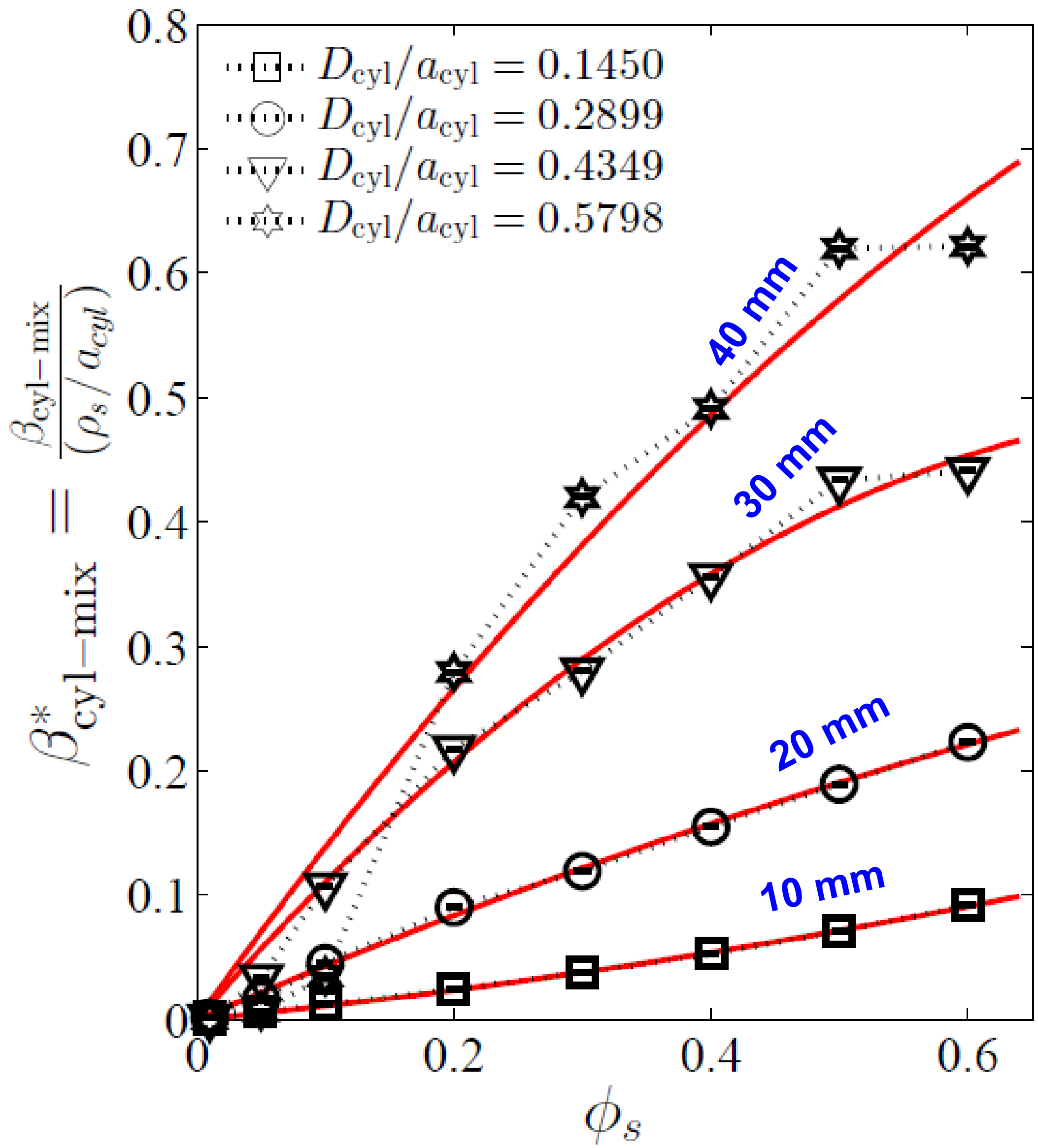

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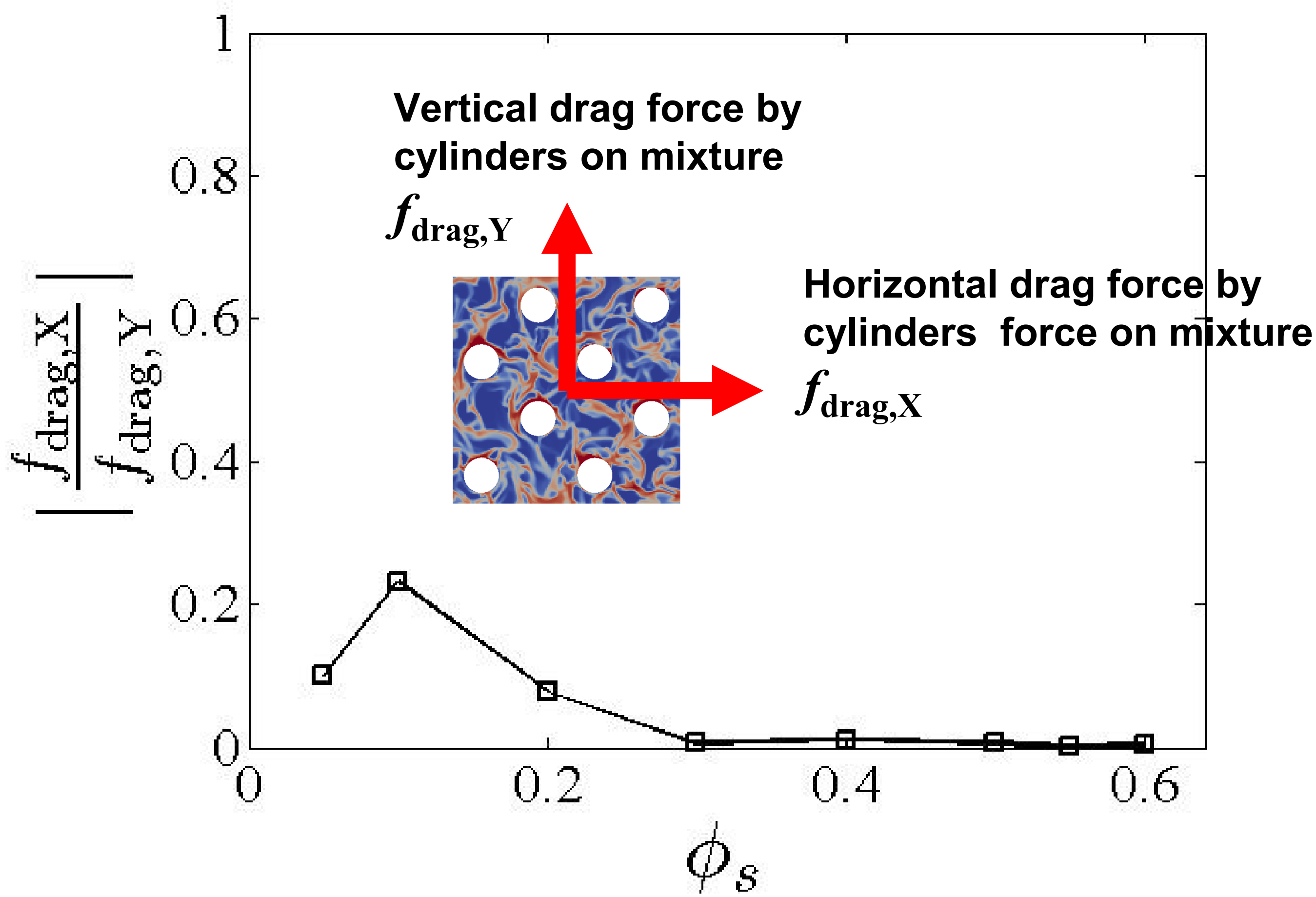
Additional simulations performed for varying cylinder diameters to determine the dependence on cylinder diameter D_{cyl}.

Quadratic polynomials used to describe the dependence on filtered solid fraction.

Horizontal Cylinder-Mixture Drag

- Additional simulations were performed with a superimposed horizontal pressure drop.
- Horizontal drag force exerted by cylinders on mixture was much smaller than vertical drag.
- The horizontal drag force may be neglected in comparison to vertical drag.



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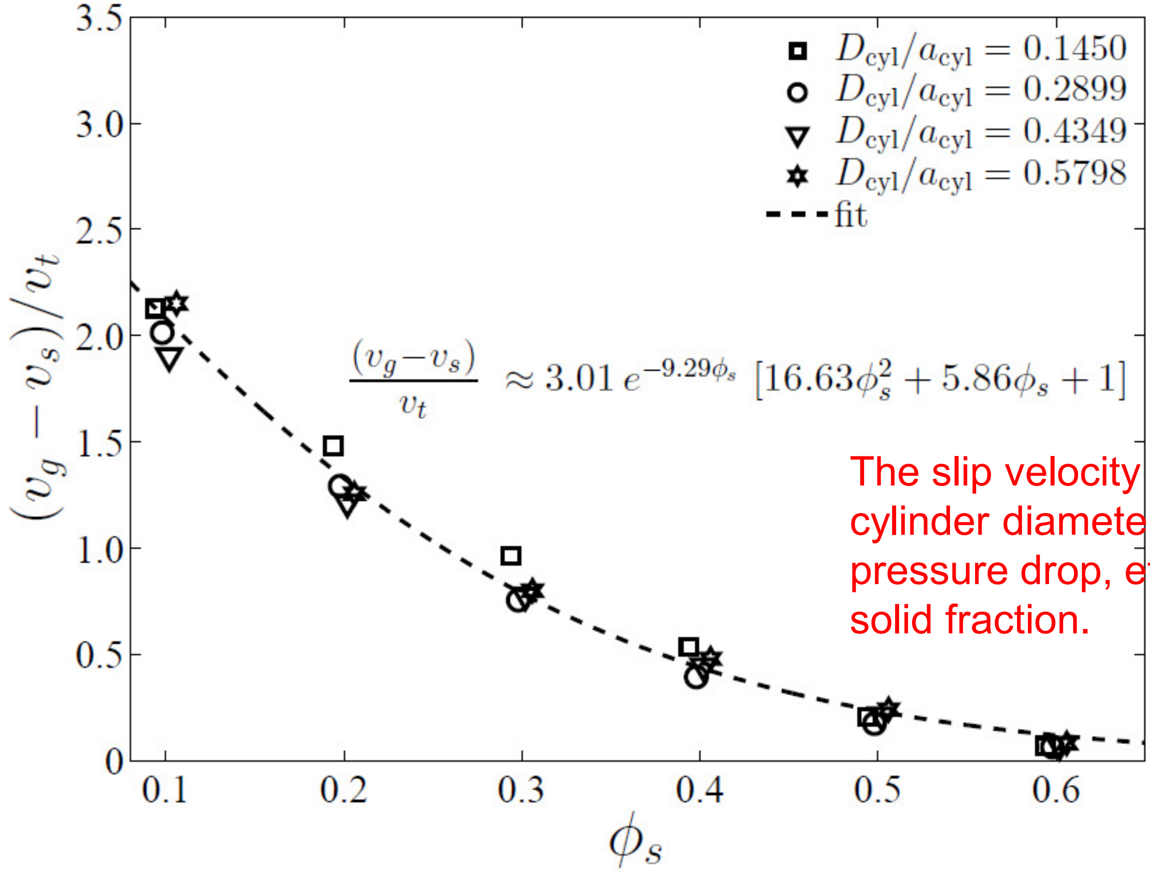
Gas-Solid Slip Velocity

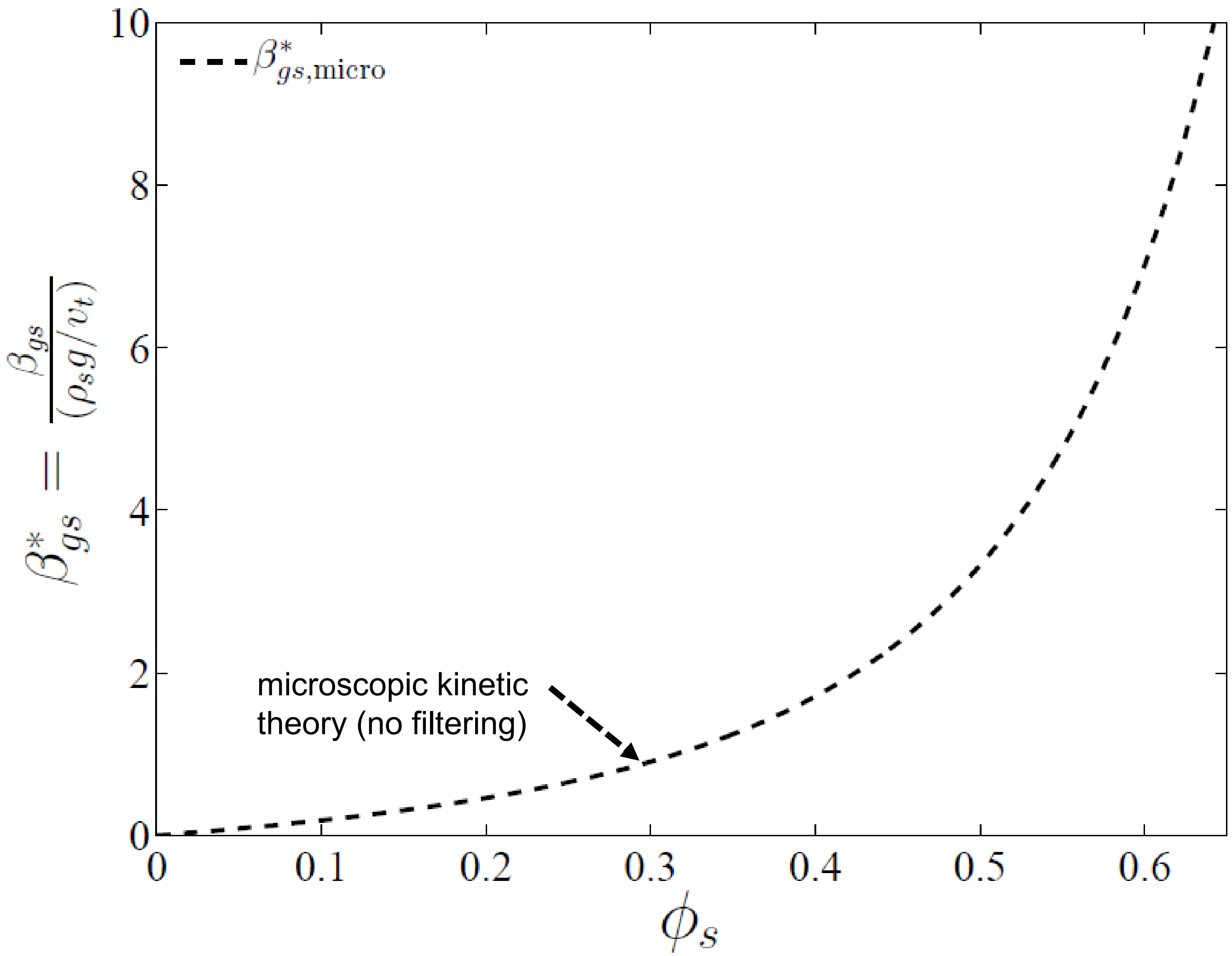
- Proposed drag model does not include contribution due to gas velocity.
- Implicitly assumes that gas and solids are locally in equilibrium.



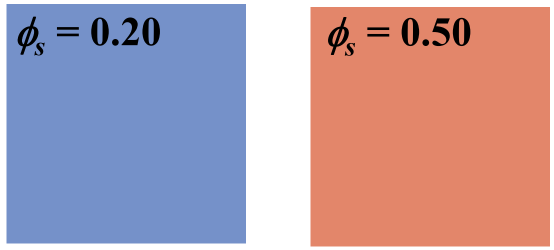
The slip velocity does not depend on cylinder diameter, gas/solid velocity, pressure drop, etc. Depends only on the solid fraction.

- Assuming local equilibrium between gas and solids is reasonable.

Influence of Cylinders on Gas-Solid Drag



Microscopic kinetic theory with no filtering, assumes perfectly homogeneous mixture.



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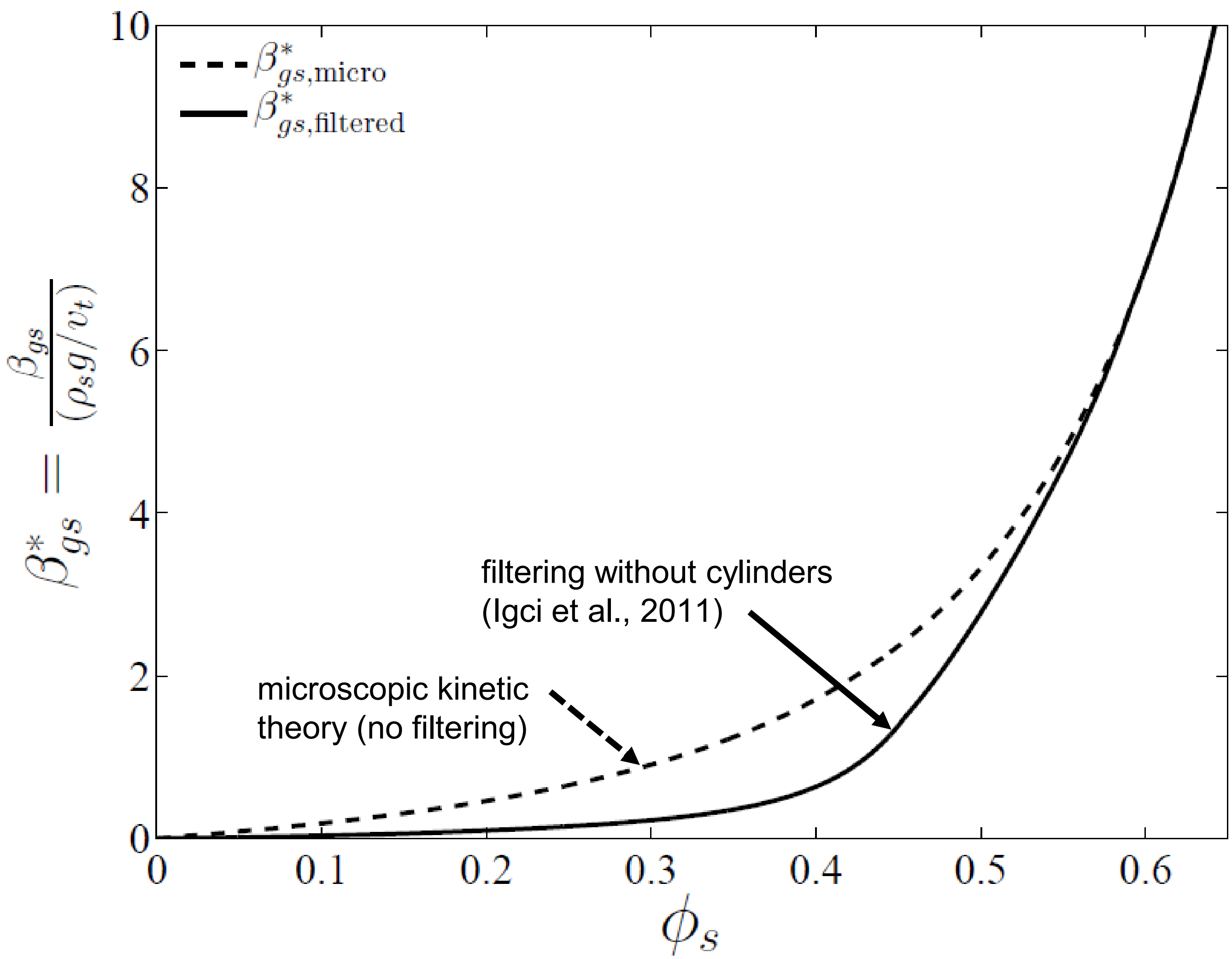

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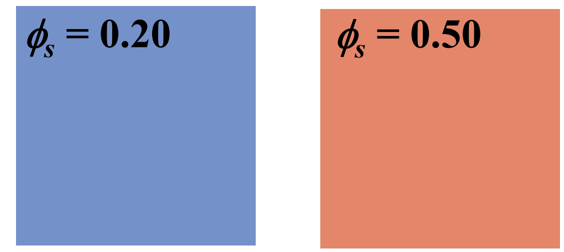
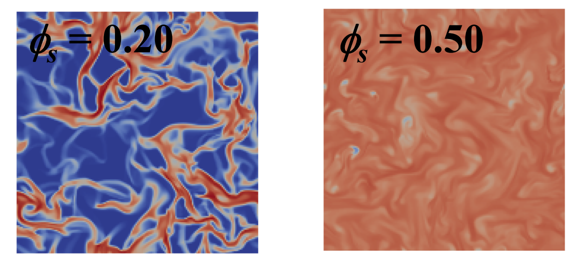


Filtering without tubes (Igci et al., 2011). Considers the correction due to sub-grid scale clusters.



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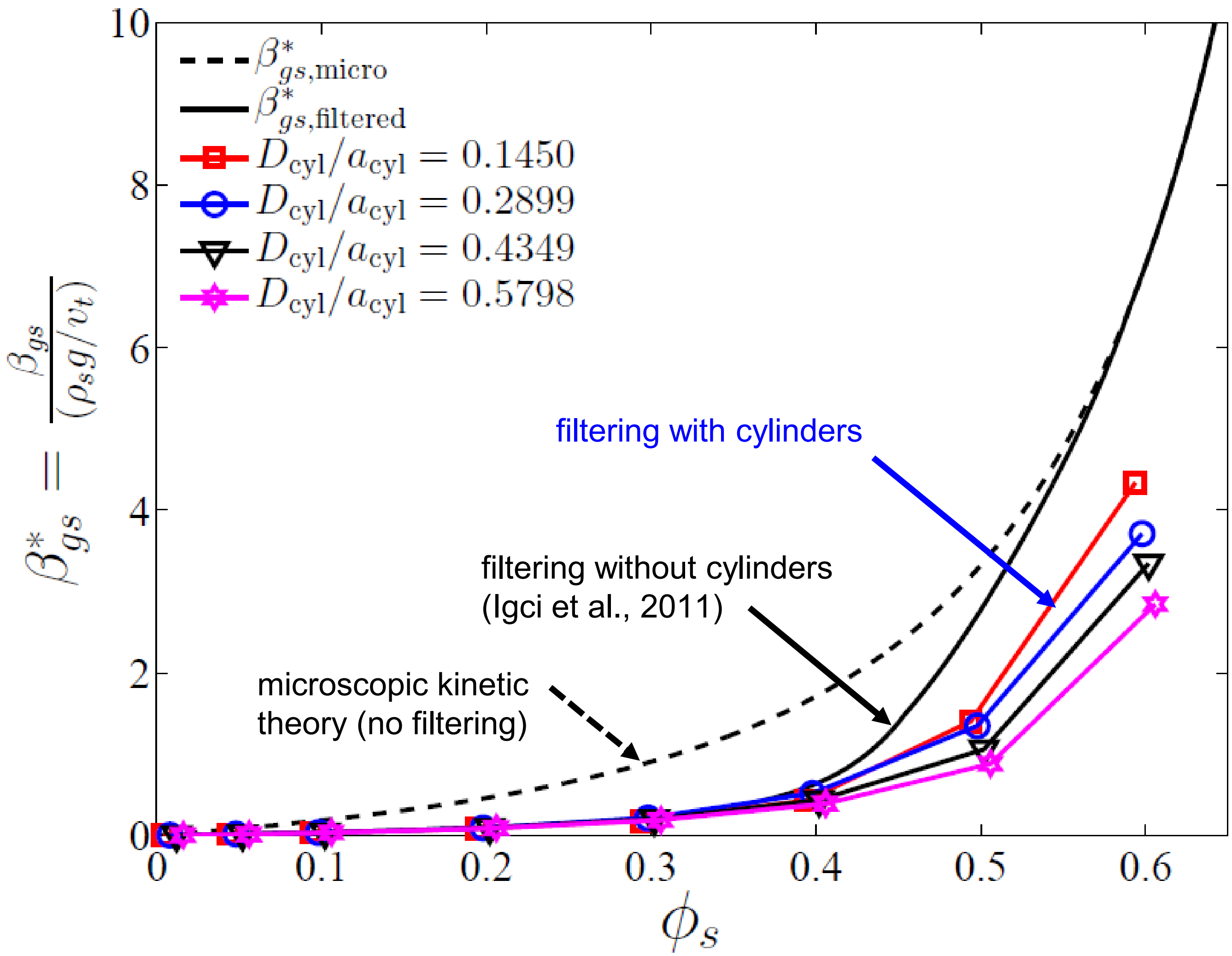

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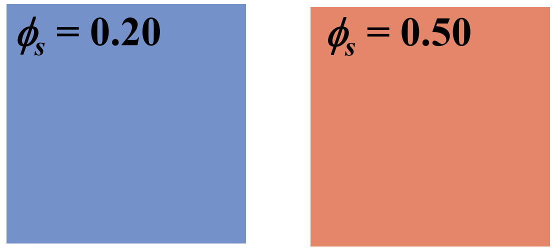

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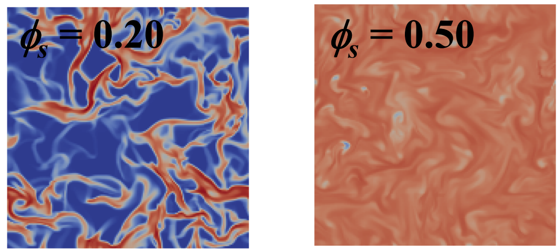
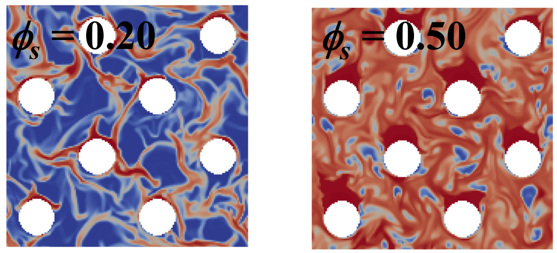


Filtered model with cylinders. Clusters seen near tubes for larger ϕ_s values.



Summary

- A sub-grid model for the vertical drag exerted by an array of cylinders developed.
  - Cylinders will appear as a uniform, stationary porous media in coarse grid simulations.
- The horizontal drag force on suspension due to cylinders is much smaller than the vertical drag.
- At larger solid fractions, presence of cylinders influences the clustering behavior, which indirectly lowers the gas-solid drag.

Future work

- Implementation and verification of the sub-grid drag model developed.
- Validation – availability of experimental data?
- Investigate other tube configurations – vertical tubes.

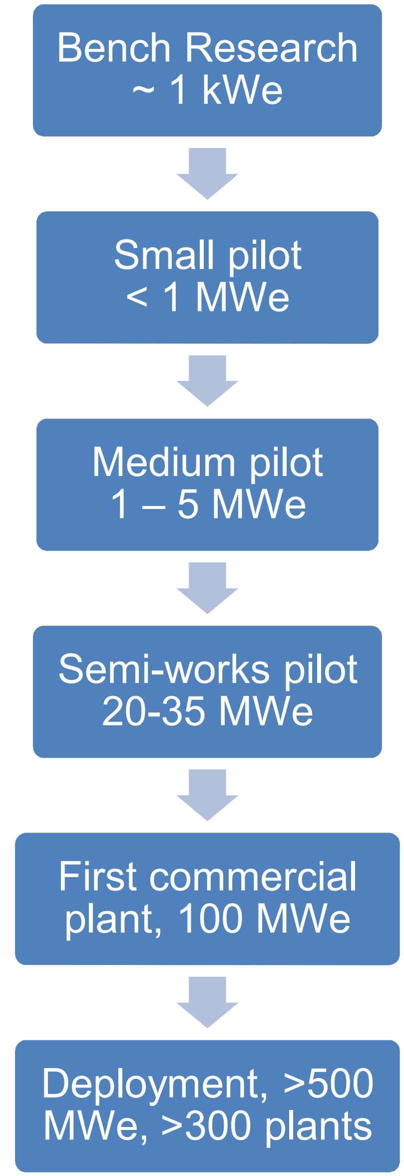
Thank You

Disclaimer

Additional Slides

Carbon Capture Challenge

- The traditional pathway from discovery to commercialization of energy technologies can be quite long, i.e., ~ 2-3 decades
- President's plan requires that barriers to the widespread, safe, and cost-effective deployment of CCS be overcome within 10 years
- To help realize the President's objectives, new approaches are needed for taking carbon capture concepts from lab to power plant, <u>quickly</u>, and at low cost and risk
- CCSI will accelerate the development of carbon capture technology, from discovery through deployment, with the help of science-based simulations



Basic Data & Models Team
Lead: Joel D. Kress, LANL
David Mebane, ORISE/NETL
Berend Smit, UCB/LBNL
Maciej Haranczyk, LBNL
Kuldeep Jariwala, LBNL
Forrest Abouelnasr, UCB/LBNL
Li-Chiang Lin, UCB/LBNL
Joe Swisher, UCB/LBNL

Particle & Devices Scale Team
Lead: Xin Sun, PNNL
Co-Lead: S. Sundaresan, Princeton U.
Sébastien Dartevelle, LANL
David DeCroix, LANL
David Huckaby, NETL
Tad Janik, PNNL
Chris Montgomery, URS/NETL
Wenxiao Pan, PNNL
Emily Ryan, Boston University
Avik Sarkar, PNNL
Dongmyung Suh, PNNL
Zhijie Xu, PNNL
Wesley Xu, PNNL

Plant Operations & Control Team
Lead: Stephen E. Zitney, NETL
Co-Lead: Prof. D. Bhattacharyya, WVU/NETL
Eric A. Liese, NETL
Srinivasa Modekurti, WVU/NETL
Priyadarshi Mahapatra, URS/NETL
Mike McClintock, FCS/NETL
Graham T. Provost, FCS/NETL
Prof. Richard Turton, WVU/NETL

Process Synthesis & Design Team
Lead: David C. Miller, NETL
Co-Lead: Nick Sahnidis, CMU/NETL
Larry Biegler, CMU/NETL
Ignacio Grossmann, CMU/NETL
Jeff Siirola, CMU/NETL
Alison Cozad, CMU/NETL
John Eslick, ORISE/NETL
Andrew Lee, ORISE/NETL
Hosoo Kim, ORISE/NETL
Murthy Konda, ORISE/NETL
Zhihong Yuan, CMU/NETL
Linlin Yang, CMU/NETL
Alex Dowling, CMU/NETL

Uncertainty Quantification Team
Lead: Charles Tong, LLNL
Co-lead: Guang Lin, PNNL
K. Sham Bhat, LANL
David Engel, PNNL
Leslie Moore, LANL
Brenda Ng, LLNL
Jeremy Ou, LLNL
Yelena Sholokhova, LLNL
Joanne Wendelberger, LANL

Software Development Support Team
Lead: Paolo Calafiura, LBNL
Co-lead: Keith Beattie, LBNL
Tim Carlson, PNNL
Val Hendrix, LBNL
Dan Johnson, PNNL
Doug Olson, LBNL
Simon Patton, LBNL
Gregory Pope, LLNL

Integration Framework Team
Lead: Deb Agarwal, LBNL
Khushbu Agarwal PNNL
Joshua Boverhof, LBNL
Tom Epperly, LLNL
John Eslick, ORISE/NETL
Dan Gunter, LBNL
Ian Gorton, PNNL
Keith Jackson, LBNL
James Leek, LLNL
Jinliang Ma, URS/NETL
Douglas Olson, LBNL
Sarah Poon, LBNL
Poorva Sharma, PNNL
Yidong Lang, CMU/NETL

Risk Analysis & Decision Making Team
Lead: Bruce Letellier, LANL
Co-Lead: Dave Engel, PNNL
Brian Edwards, LANL
Mary Ewers, LANL
Ed Jones, LLNL
Rene LeClaire, LANL

Director: Madhava Syamlal, NETL

Technical Team Lead: David Miller, NETL

Lab Leads:
David Brown , LBNL
John Grosh, LLNL
Melissa Fox , LANL
Mohammad Khaleel, PNNL

IAB Coordinator: John Shinn

Project Coordinator: Roger Cottrell

Carbon Capture Simulation Initiative

Identify promising concepts → Reduce the time for design & troubleshooting → Quantify the technical risk, to enable reaching larger scales, earlier → Stabilize the cost during commercial deployment

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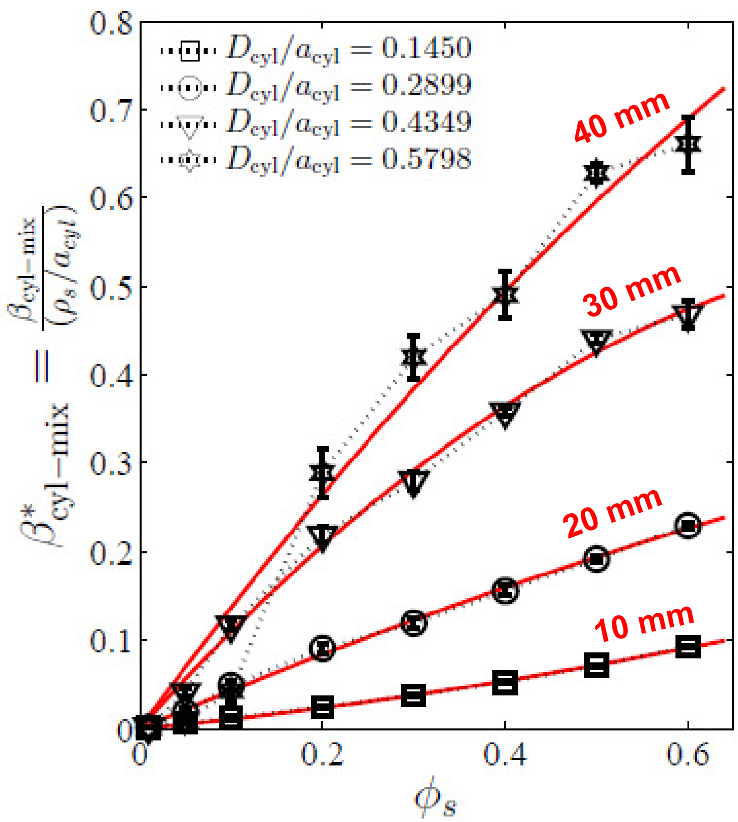
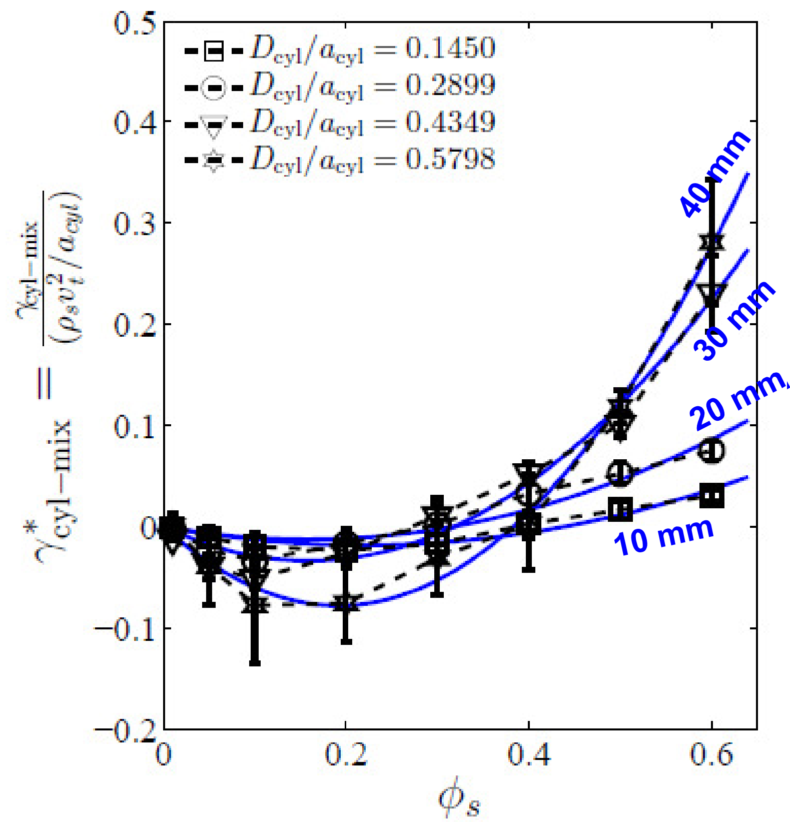
Cylinder-Suspension Sub-grid Drag Coefficients – Alternate Fit I





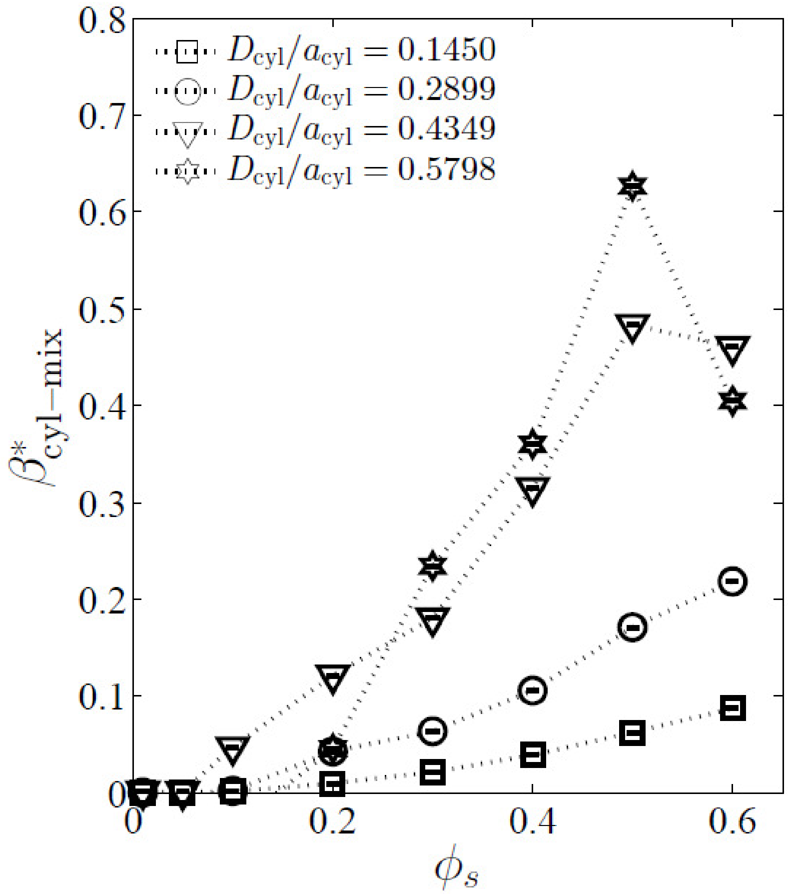
- Determine the coefficients:
  - $\beta^*_{cyl\text{-}mix}$
  - $\gamma^*_{cyl\text{-}mix}$

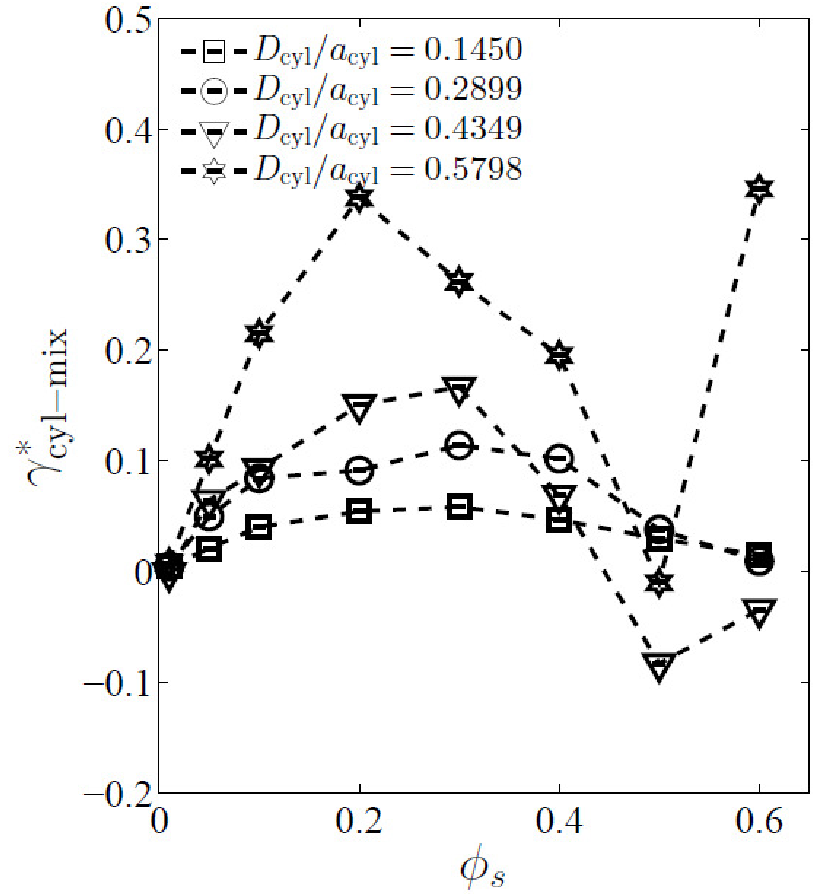
  by least squares fit as a function of the solid fraction.
- Perform additional simulations for varying cylinder diameter.
- Fit a family of curves for $\beta^*_{cyl\text{-}mix}$ and $\gamma^*_{cyl\text{-}mix}$ for varying diameter and solid fraction.

$$f^*_{drag} = \beta^*_{\text{cyl-mix}}\left(-v^*_s\left|v^*_s\right|\right) + \gamma^*_{\text{cyl-mix}}$$

D_{cyl}/a_{cyl} (D_{cyl})	$\beta^*_{\text{cyl-mix}}$	$\gamma^*_{\text{cyl-mix}}$
0.1450 (10 mm)	$0.0847\phi_s^2 + 0.1018\phi_s$	$0.3814\phi_s^2 - 0.1674\phi_s$
0.2899 (20 mm)	$-0.1081\phi_s^2 + 0.4424\phi_s$	$0.5074\phi_s^2 - 0.1607\phi_s$
0.4349 (30 mm)	$-0.6095\phi_s^2 + 1.1559\phi_s$	$1.3334\phi_s^2 - 0.4248\phi_s$
0.5789 (40 mm)	$-0.4363\phi_s^2 + 1.4110\phi_s$	$2.1284\phi_s^2 - 0.8151\phi_s$

Cylinder-Suspension Sub-grid Drag Coefficients – Alternate Fit II



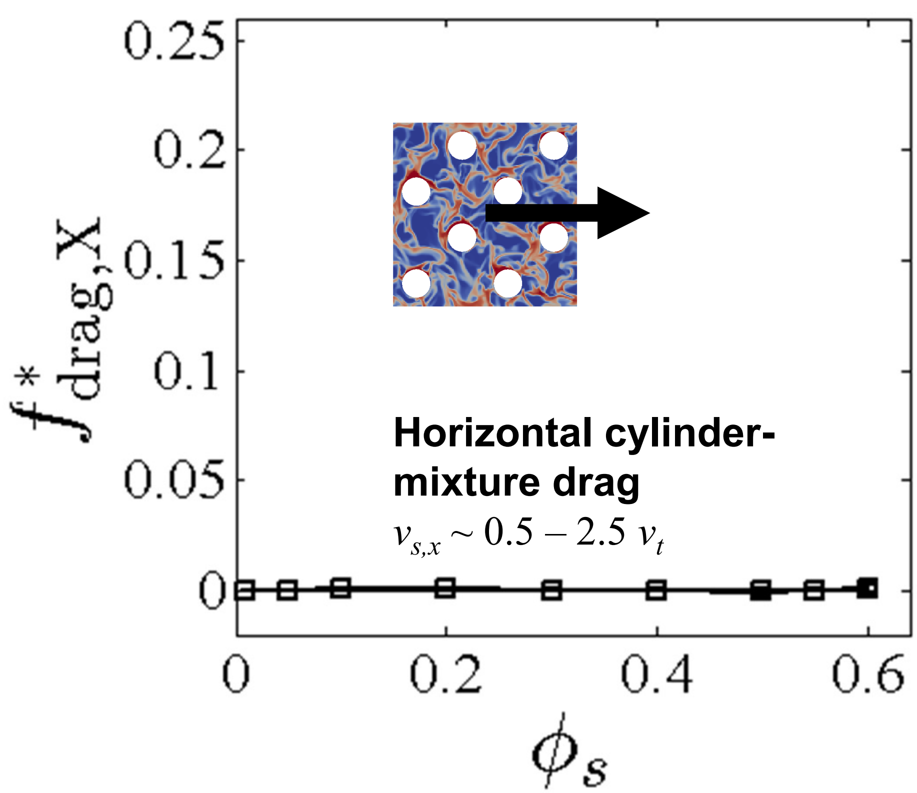


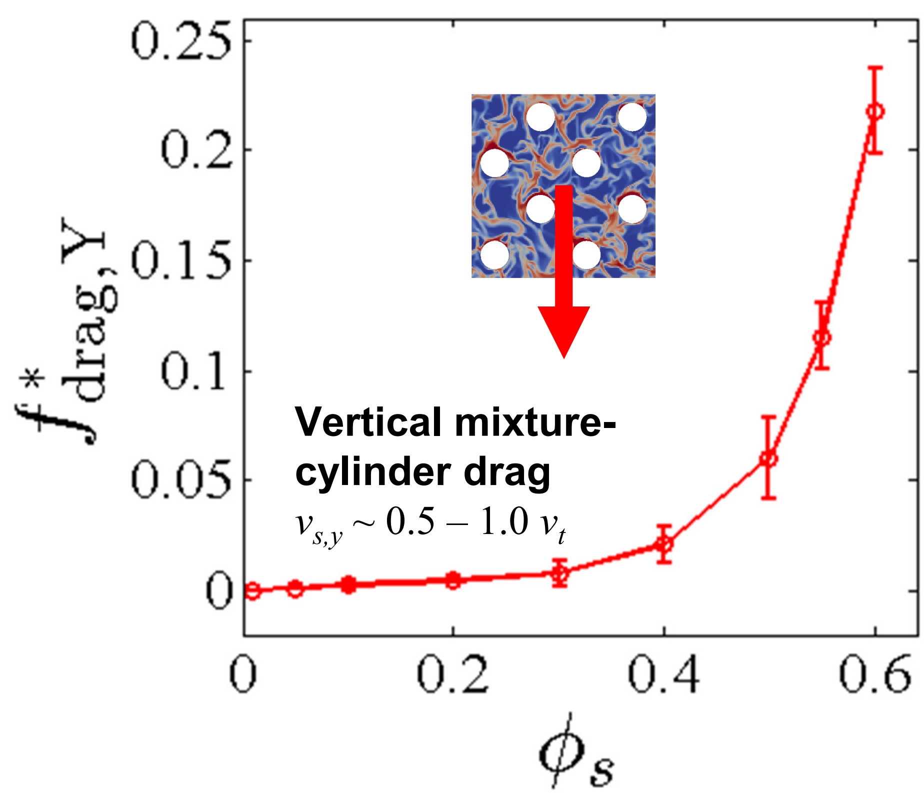
$$f^*_{drag} = \beta^*_{\text{cyl-mix}}\left(-v^*_s\left|v^*_s\right|\right) + \gamma^*_{\text{cyl-mix}}\left(-v^*_s\right)$$

Poor fit without any trends. Data suggests that there is no linear velocity dependent term, only the quadratic term.

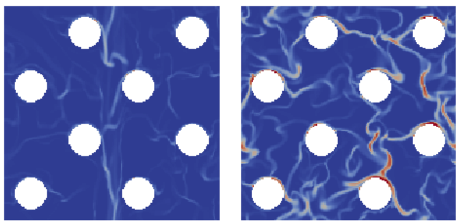
Horizontal Cylinder-Mixture Drag

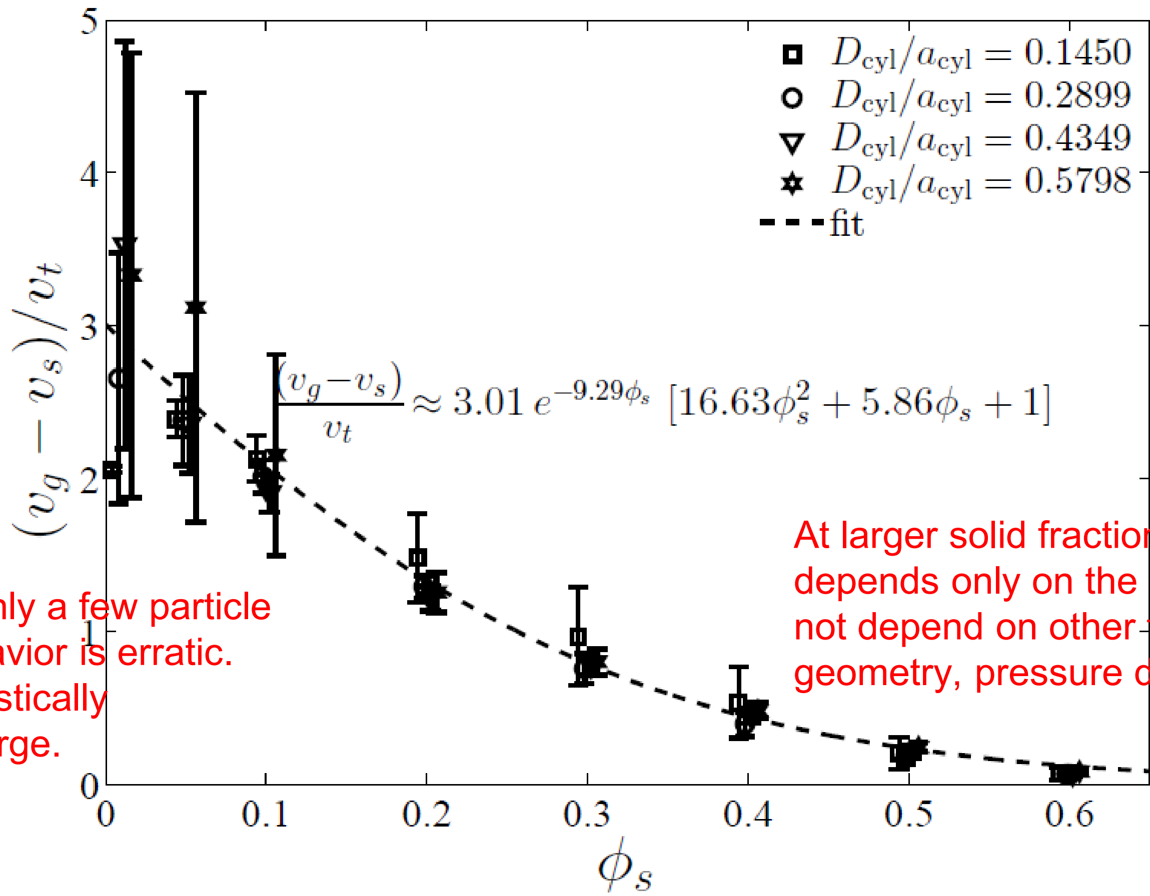
- Additional simulations were performed with a superimposed horizontal pressure drop.
- Horizontal cylinder-mixture drag measurements were much smaller than the vertical drag.
- This suggests that the horizontal drag exerted by the cylinders on mixture may be negligible in comparison to vertical drag.





Gas-Solid Slip Velocity



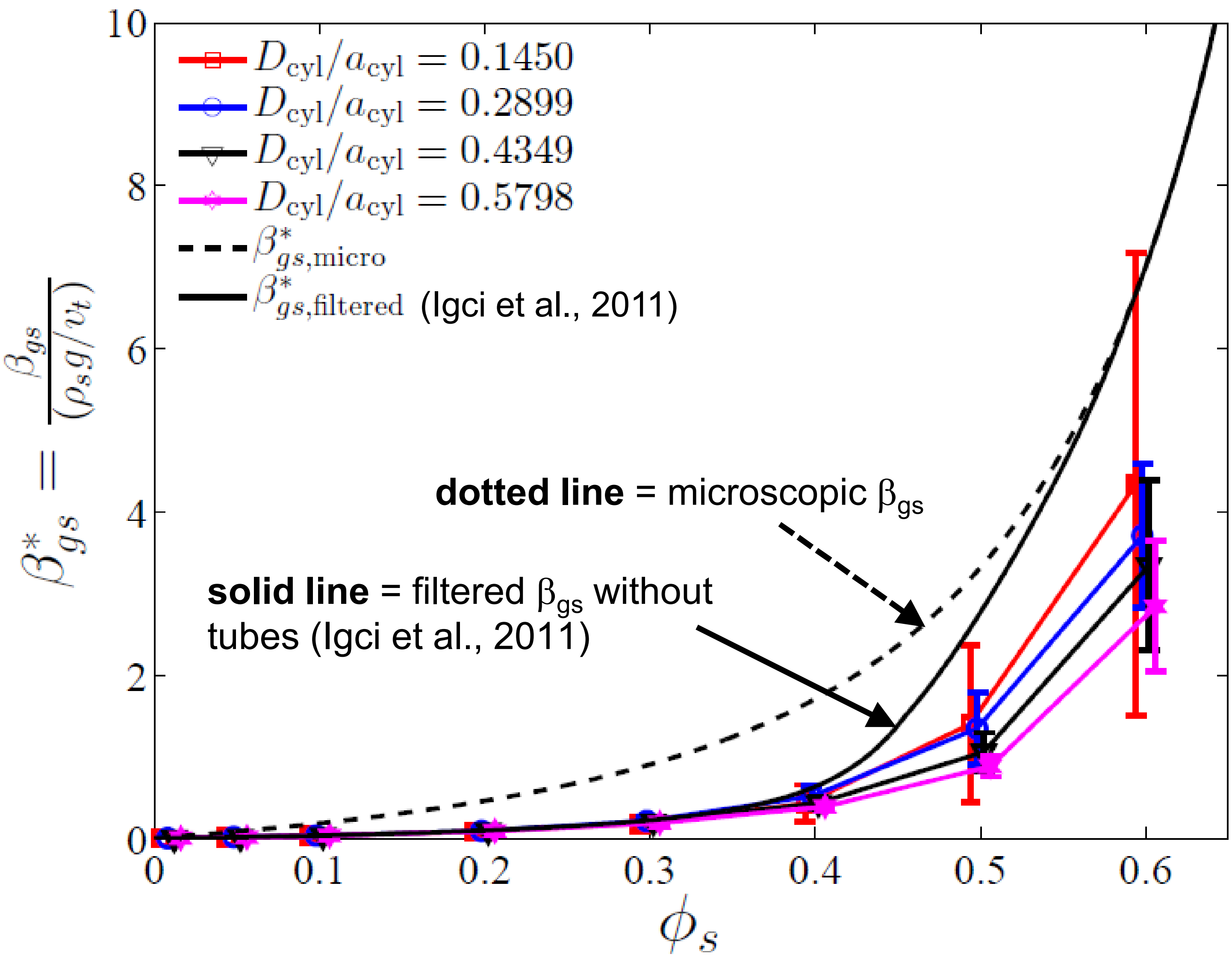


At smaller solid fractions, only a few particle clusters exist and their behavior is erratic. Measurements are not statistically meaningful and scatter is large.

At larger solid fractions, the slip velocity depends only on the solid fraction, and does not depend on other factors (cylinder geometry, pressure drop, etc.)

- For the solid fraction range of interest (ϕ_s > 0.10), slip velocity depends only on solid fraction.
- Assuming local equilibrium between gas and solids is reasonable.

Effect of Cylinders on Gas-Solid Drag



- The gas-solid drag is over-predicted when using larger cells without sub-grid correction (Igci et al., 2011).
- Fine-scale cluster formation allows gas to bypass these clusters, which lowers the gas-solid drag.
- For smaller solid fractions (ϕ_s < 0.35), addition of cylinders found to agree with predictions from Igci et al. (2011).
- For ϕ_s > 0.35, a further reduction in the drag is observed.
- Drag reduction is greater for larger cylinders.

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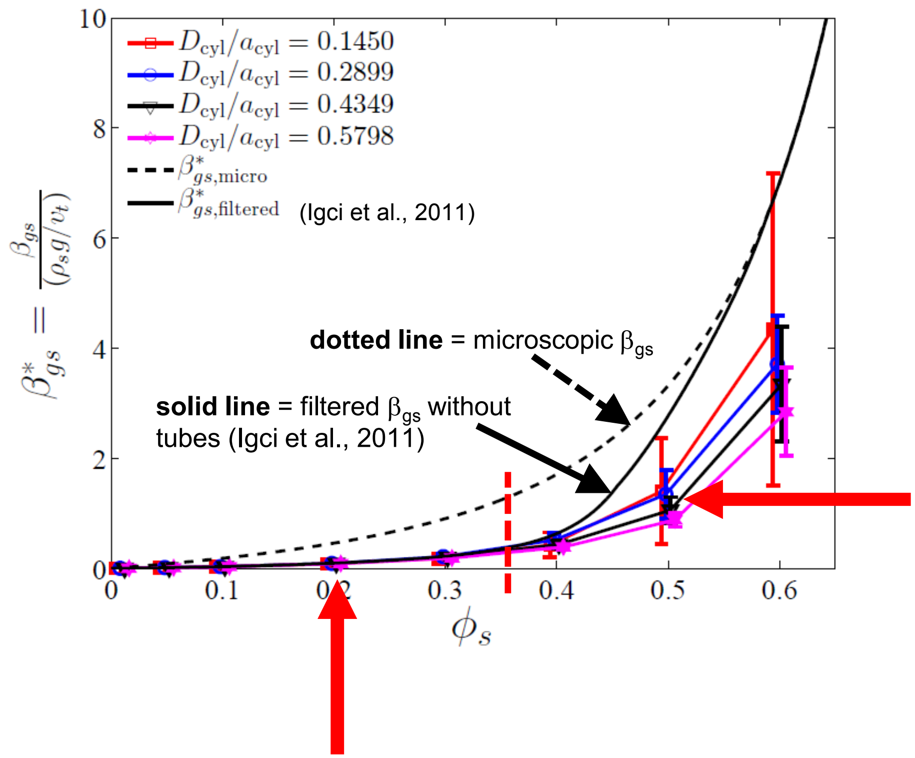
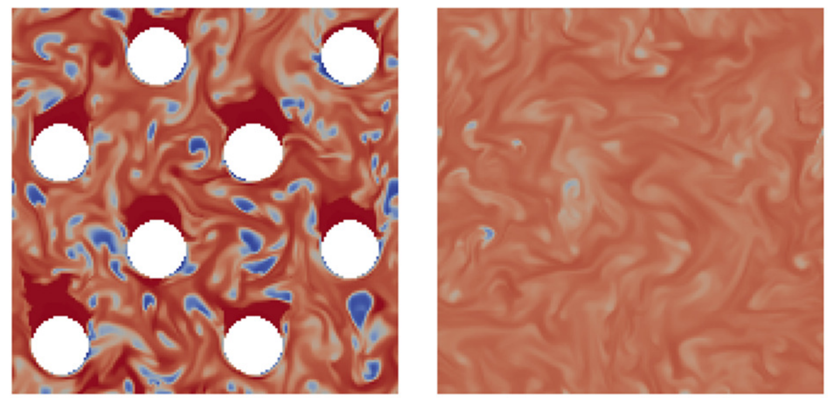
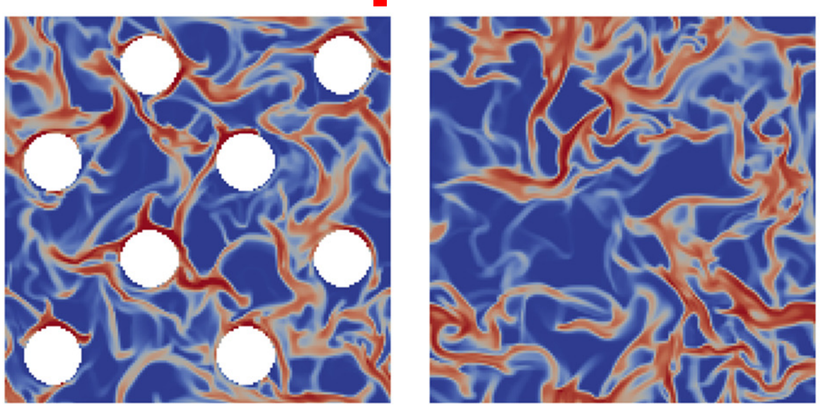
Gas-Solid Drag Reduction By Cylinders



At larger solid fractions, dense packed clusters form in the vicinity of the cylinders. Gas flow can easily bypass these dense clusters near the tubes, which results in a further reduction in gas-solid drag. (Indirect influence of cylinders on gas-solid flow.)

$\phi_s = 0.50$

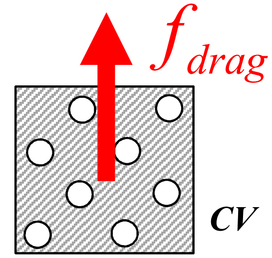




$\phi_s = 0.20$

At smaller solid fractions, the gas-solid microstructure (characteristic cluster length-scales) appears to be qualitatively unaffected by the cylinders. The gas-solid drag follow the predictions obtained for system without cylinders (Igci et al., 2011).

Filtering Procedure



The conservation equations are averaged over the domain to obtain the cylinder-mixture drag.

$$\frac{1}{V}\iiint_{CV}\left[\frac{\partial\left(\rho_g\phi_g^{'}\vec{v}_g^{'}\right)}{\partial t}+\frac{\partial\left(\rho_s\phi_s^{'}\vec{v}_s^{'}\right)}{\partial t}\right]dV=\boxed{-\frac{1}{V}\iint_{\substack{\text{cylinder}\\ \text{surfaces}}}\left(\boldsymbol{\sigma}_g^{'}+\boldsymbol{\sigma}_s^{'}\right)\cdot\hat{n}dS}-\frac{1}{V}\iint_{\substack{\text{periodic}\\ \text{boundaries}}}P\,\hat{n}dS+\frac{1}{V}\iiint_{CV}\left[\left(\rho_g\phi_g^{'}+\rho_s\phi_s^{'}\right)\vec{g}\right]dV$$

f_{drag} **cylinder-mixture drag**

$\phi_g^{'},\ \vec{v}_g^{'},\ \boldsymbol{\sigma}_g^{'},\ \phi_s^{'},\ \vec{v}_s^{'},\ \boldsymbol{\sigma}_s^{'}$ represent unfiltered cell-values obtained from the highly-resolved simulations.

The filtered quantities are given by:

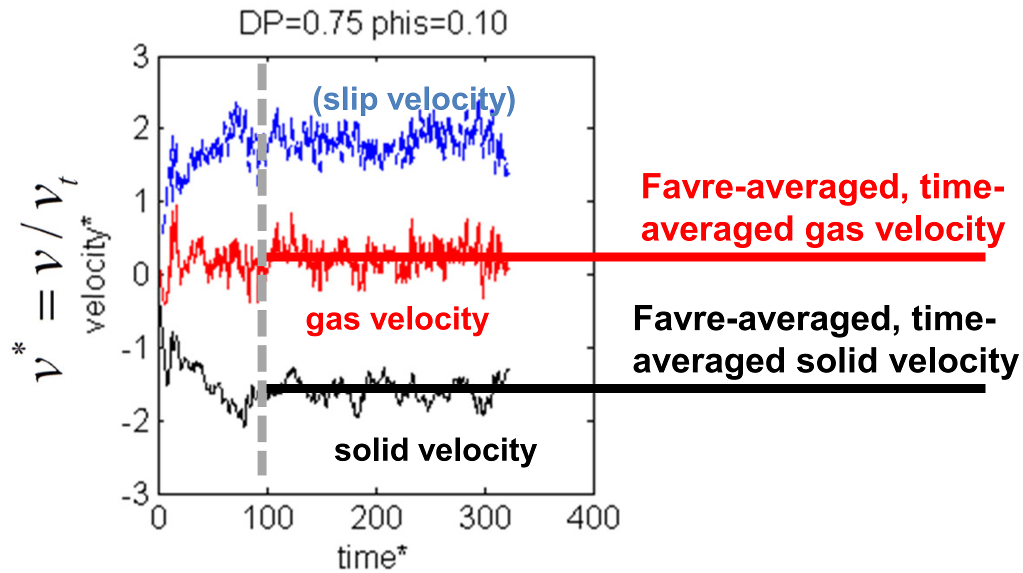
$$\phi_g=\frac{1}{V}\iiint_{CV}\phi_g^{'}dV$$

$$\phi_s=\frac{1}{V}\iiint_{CV}\phi_s^{'}dV$$

$$\phi_g v_g=\frac{1}{V}\iiint_{CV}\phi_g^{'}v_g^{'}dV$$

$$\phi_s v_s=\frac{1}{V}\iiint_{CV}\phi_s^{'}v_s^{'}dV$$

A further averaging in time is performed to obtain statistically steady state values.



$$t^*=t\left(g/v_t\right)$$

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