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Heat and Mass Transfer in Porous CO_2 Sorbent Particles

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U.S. DEPARTMENT OF ENERGY

Overview

- Introduction
- Approach
- Immersed Boundary Method
- Porous Medium Reconstruction
- Results
- Major Achievements
- Future work

Introduction

Carbon Capture and Sequestration (CCS) program

- **CO_2 capture**
- Compression and transport
- Storage

Carbon capture technology

- Pre-combustion
- **Post-combustion**
- Oxy-combustion

Post-combustion CO_2 capture

- Solvents
- **Solid sorbents**
- Membranes

Solid sorbents

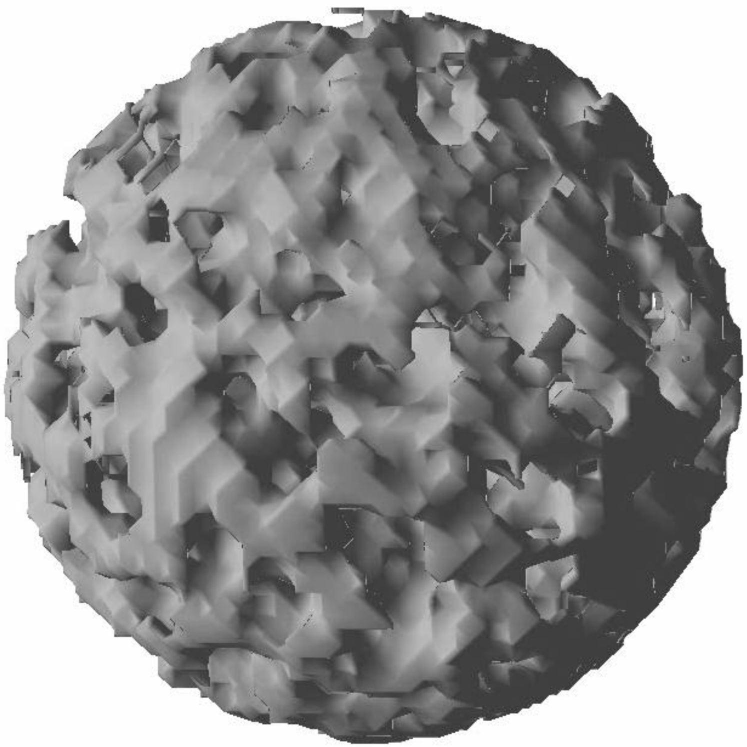
- Metal oxides, zeolites, amines …
- Enable capture from low pressure streams

Achieve 90% CO_2 capture at less than a 30% increase levelized cost of electricity (COE) of post-combustion capture for new and existing coal-fired power plants [1]

Introduction

- Transfer of heat and mass in porous particles – a problem central to solid sorbent CO_2 capture processes
- Capture of CO_2 involves modeling of species diffusion and reaction kinetics through complex porous microstructures

Quantify the flow of heat and CO_2 with other gases into the porous particles with measured porosity and microstructure



A spherical particle generated with a porosity of 0.45

Approach

Immersed boundary method (IBM)	• Capability to resolve complex geometries • Conjugate heat transfer and species transport modules
Porous reconstruction	• Use optimized stochastic reconstruction methods • Perform X-ray CT imaging to obtain statistical descriptors
Understand involved process variables	• Perform DNS calculations to resolve the porous microstructure
Help improve CO_2 capture	• Could potentially lead to design of tailored microstructures to best achieve the adsorption process

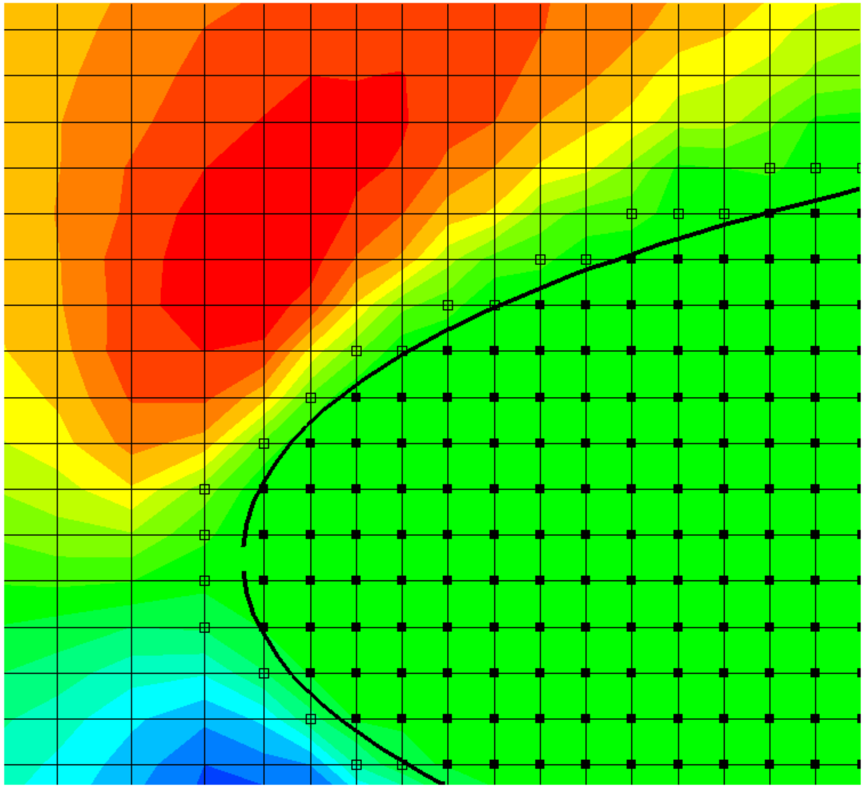
Approach

Immersed boundary method (IBM)

- *Capability to resolve complex geometries*
- *Conjugate heat transfer and species transport modules*

IBM Implementation

- Adapted from Gilmonov et al. (2003)[2]
- Steps
  - Identify the IB nodes – nodes closest to the boundary
  - Computations only on the fluid nodes (not on IB and solid nodes)
  - Change values at IB nodes – to satisfy the correct BC
- Implementation is within the framework of our in-house code – GenIDLEST



Calculation of flow over an airfoil performed on a background orthogonal mesh

IBM Implementation

GenIDLEST

- Turbulent flow on non-orthogonal meshes
- Optimized linear solvers
- Heat transfer and species transport
- Parallel framework

IBM implementation

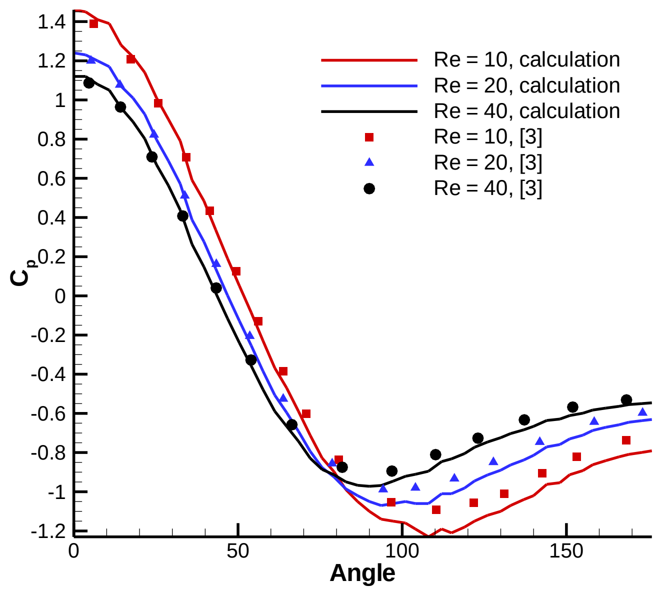
- Conjugate heat transfer
- Arbitrary solid shapes
- Movement/evolution of boundaries

GenIDLEST
+ IBM

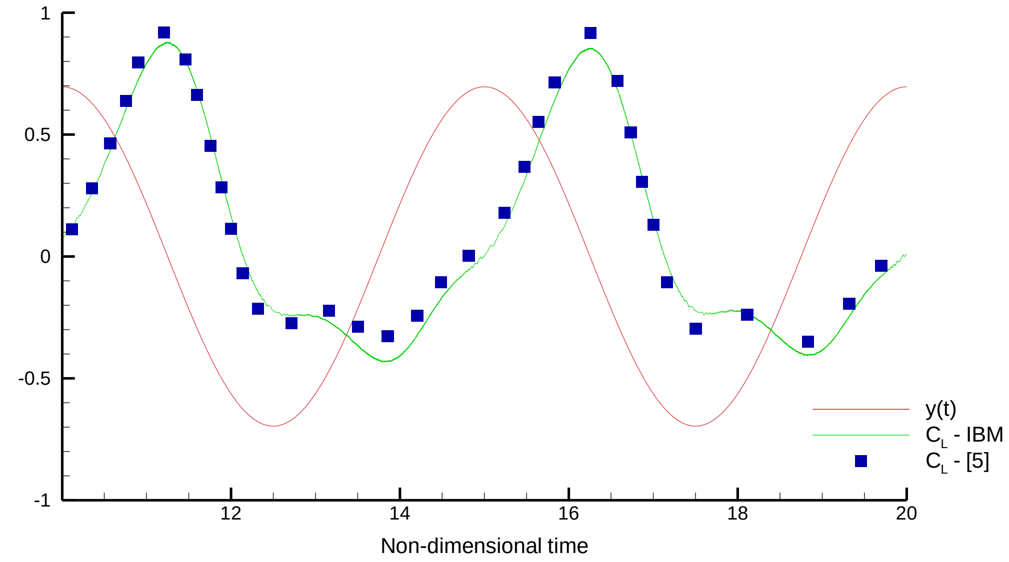
Simulation of main flow through complex geometries on non-orthogonal grids

Complex evolving porous microstructure simulation using IBM

Fluid Flow with IBM



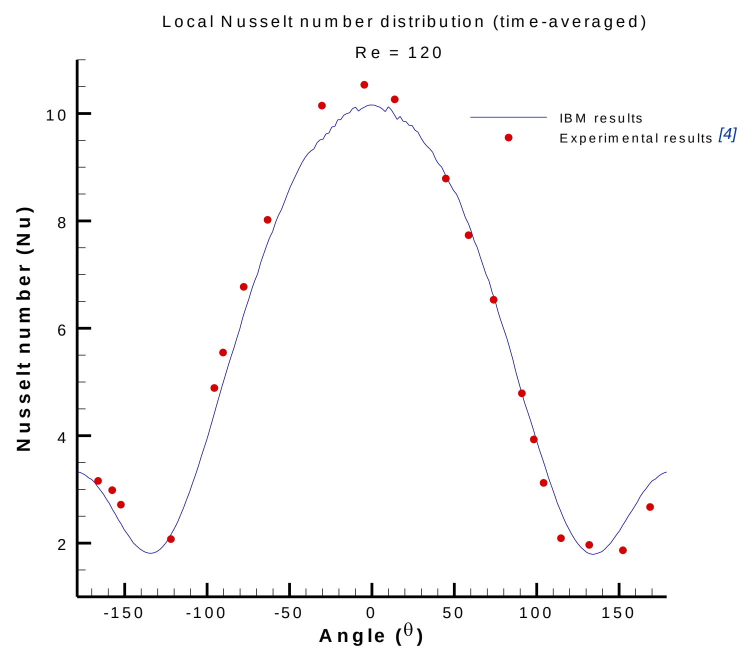
Pressure coefficients obtained for steady flow over a stationary cylinder



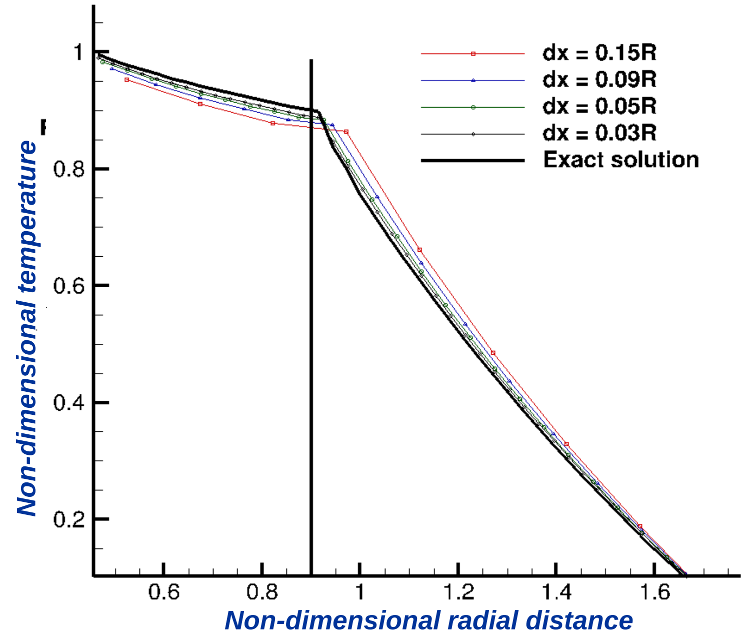
Lift coefficient comparison with experiments obtained for an oscillating cylinder at Re = 200

Validations performed for stationary and moving boundary cases for a variety of 2D and 3D problems

Heat Transfer with IBM



Time-averaged local Nusselt number distribution on a stationary cylinder at Re = 120 for iso-thermal case



Comparison of temperature fields obtained in a conjugate heat transfer setup between coannular cylinders at various grid levels

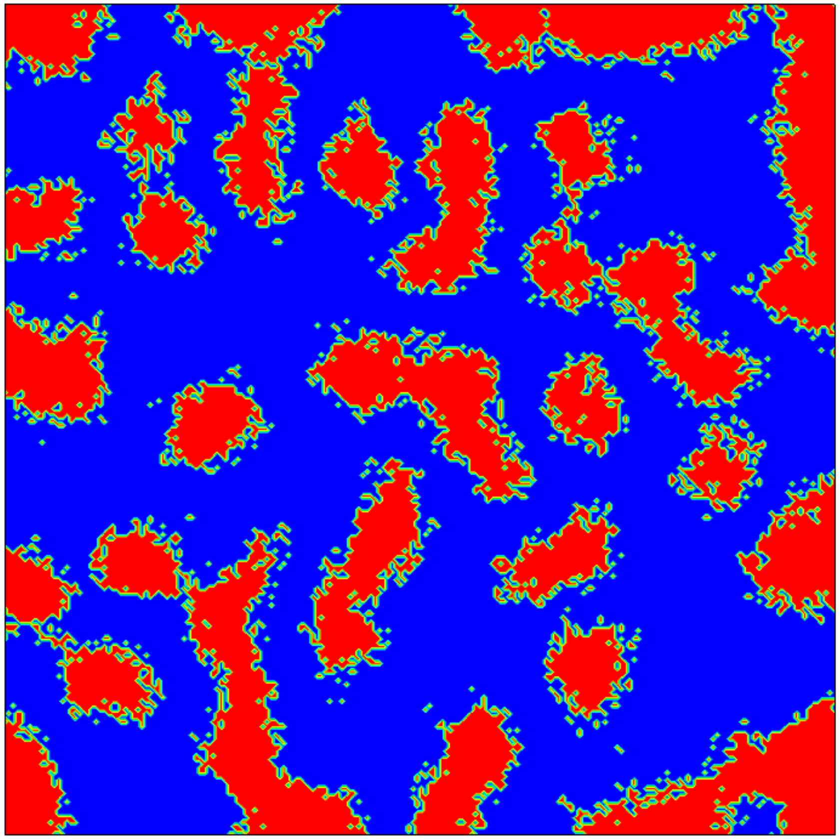
Validations and comparisons with boundary conforming code results performed check different heat transfer BCs

Approach

Immersed boundary method (IBM)	• *Capability to resolve complex geometries* • *Conjugate heat transfer and species transport modules*
Porous reconstruction	• *Use optimized stochastic reconstruction methods* • *Perform X-ray CT imaging to obtain statistical descriptors*

Porous Medium Reconstruction

- Use of stochastic reconstruction method – simulated annealing [6]
- Input – experimentally determined auto-correlation function (ACF)
- Initial – random field with desired porosity
- Final – porous structure with desired porosity and auto-correlation



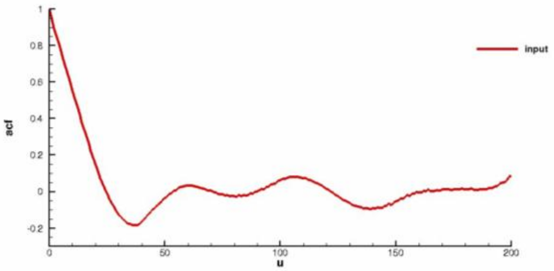
A 2D porous medium generated with a porosity of ε = 0.60

Porous Medium Reconstruction

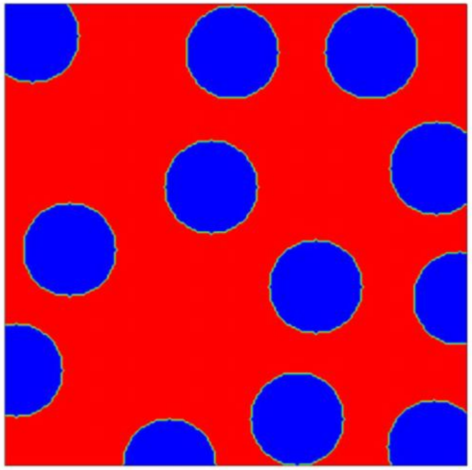
- Simulated annealing algorithm [6]
  - Obtain input ACF
  - Define a random initial distribution
  - Compute energy of the system
  - Interchange two arbitrarily chosen solid and pore nodes
  - Compute energy of the new system
  - Accept the new system based on Metropolis rule:

$$P(\Delta E) = \begin{cases} 1 & if\, \Delta E \leq 0 \\ \exp\left(\frac{-\Delta E}{T}\right) & if\ \Delta E > 0 \end{cases}$$

- Currently, arrangement of packed spheres (circles in 2D) are used for generating auto-correlation functions (2-point ACFs)



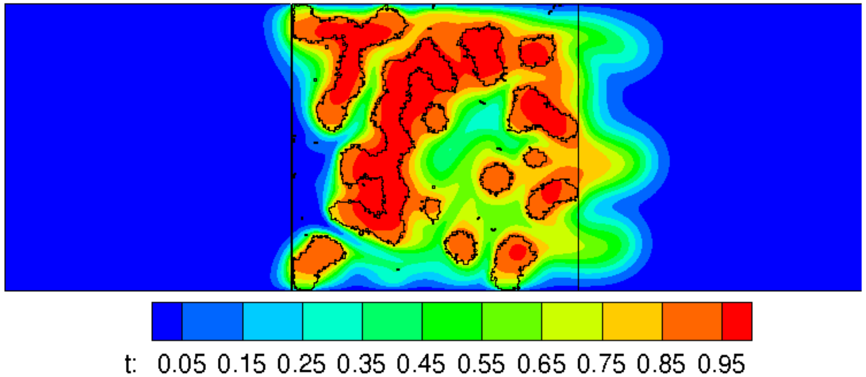
Input structure



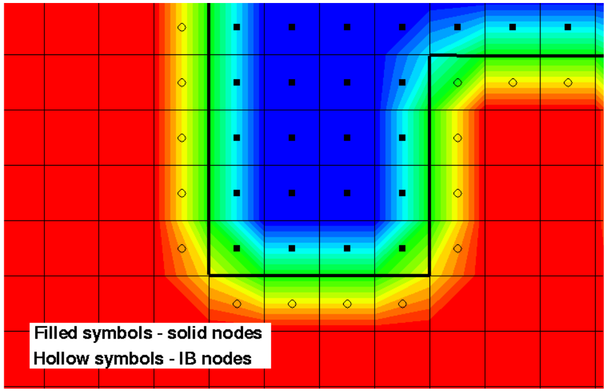
Stochastic reconstruction of a 2D porous medium with porosity of 0.75

Porous Flows with IBM

- Modified surface element detection for porous structures
- Input porous structure: Binary information (fluid – 1, solid – 0)
- Test cases
  - Comparison of pressure drops with analytical solutions
  - Species diffusion through porous particles



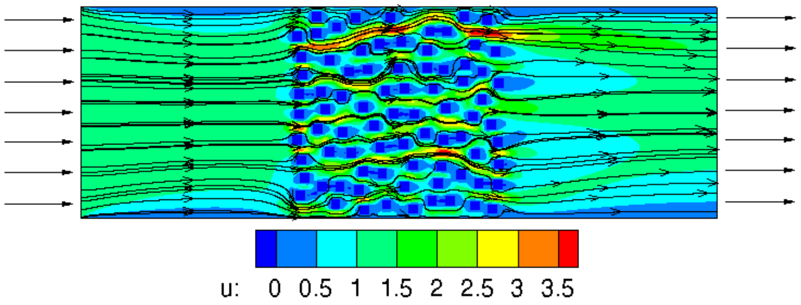
Temperature contours in a porous channel flow with conjugate heat transfer

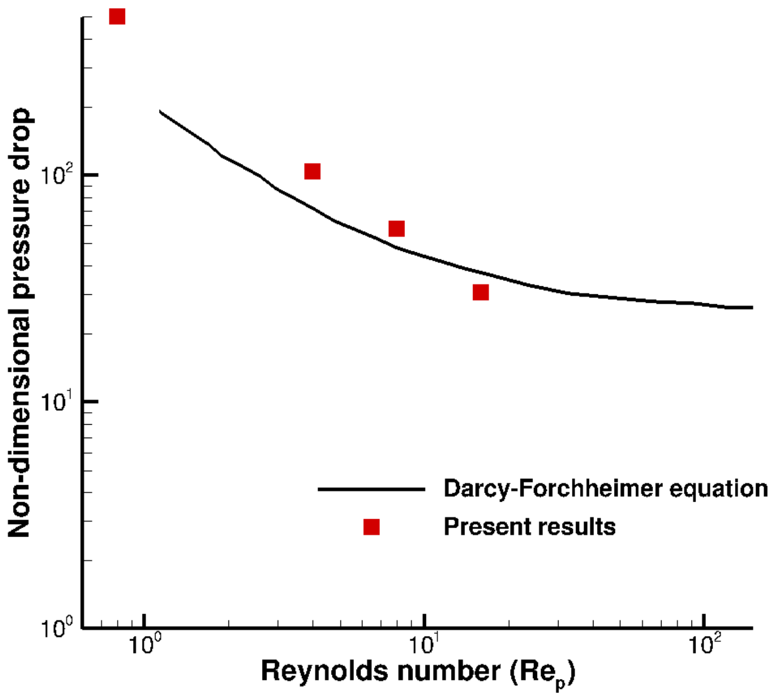


Zoomed view of the velocity field around the porous structure and the corresponding nodal identifications

Porous Flows with IBM

- Porous media used
  - Square blocks randomly placed in a channel flow
  - “Porous channel” is squeezed between the two non-porous channels
  - 2D random porous structures generated using simulated annealing
- Pressure drops obtained using Darcy-Forchheimer equation [7]



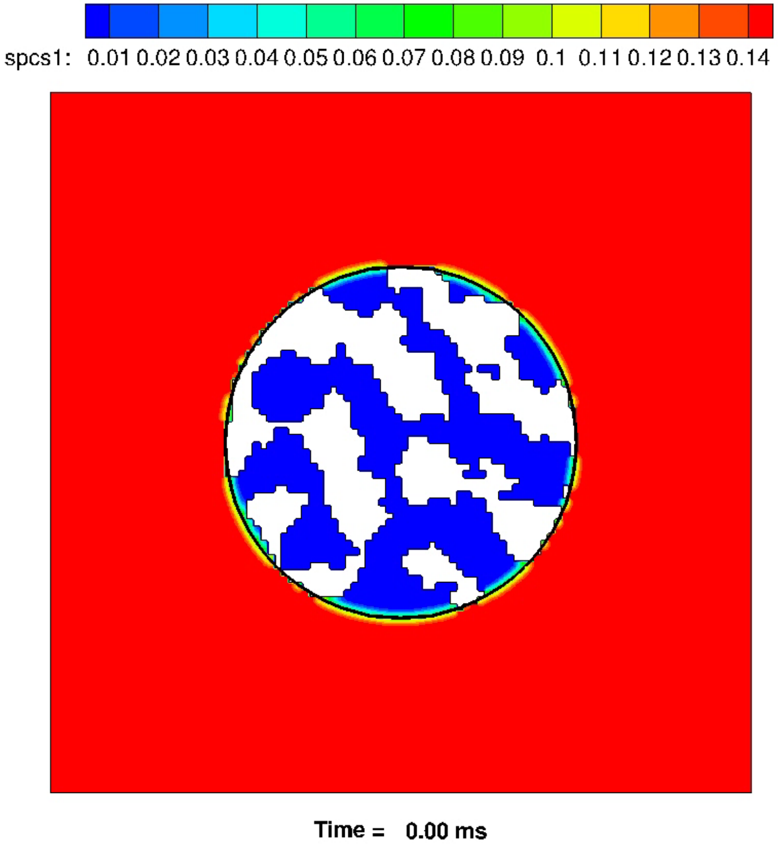


Approach

Immersed boundary method (IBM)	• *Capability to resolve complex geometries* • *Conjugate heat transfer and species transport modules*
Porous reconstruction	• *Use optimized stochastic reconstruction methods* • *Perform X-ray CT imaging to obtain statistical descriptors*
Understand involved process variables	• *Perform DNS calculations to resolve the porous microstructure*

Species Diffusion

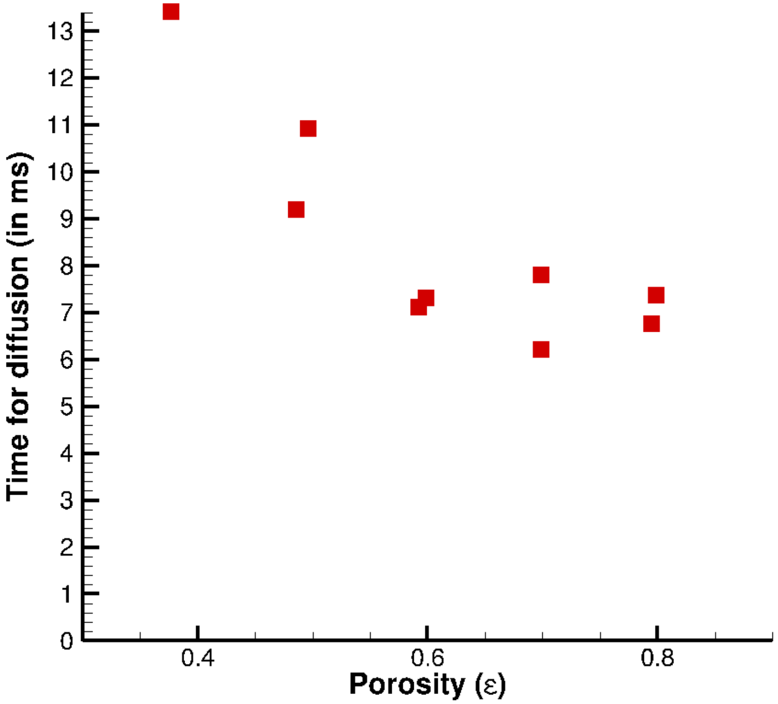
- Transport of species into porous particles (2D)
  - Square cavity with 15% CO_2 concentration at the walls
  - Zero gradient BC at the porous medium walls
  - Initial - 15% CO_2 in air outside
  - Particle diameter – 500 microns



Diffusion of CO2 into a porous 2D particle

Species Diffusion

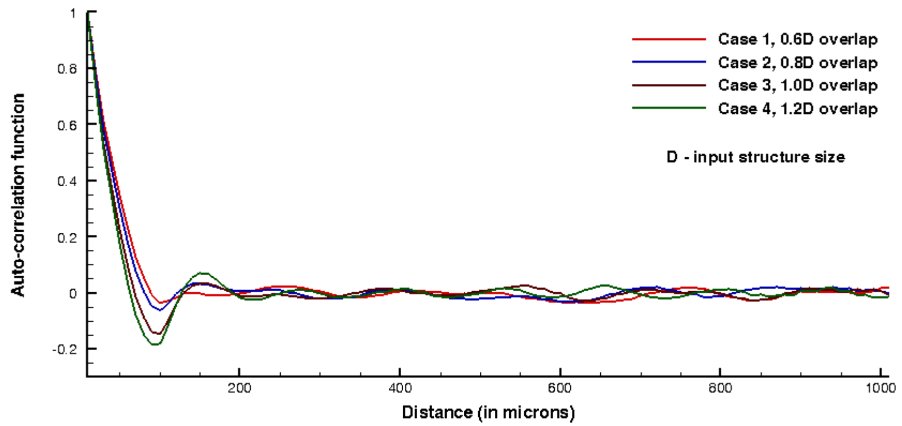
- Particle diameter (2D) - 500 microns
- Time taken for CO_2 diffusion – 95% of the ambient value
- Varying particle porosities
- Is the time affected by the structural characteristics – the auto-correlation function?



Diffusion times observed for a 500 micron 2D porous particle with varying porosities

Species Diffusion

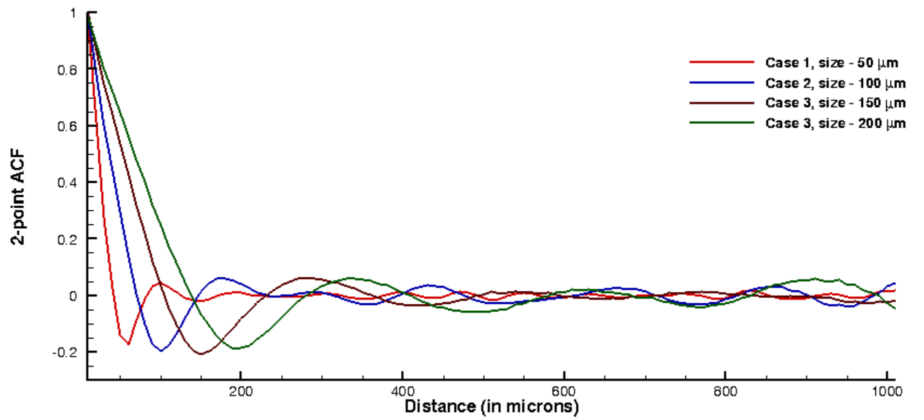
- Variation with change in the ACF
  - Overlap distance between the input structures (ε = 0.60)



Overlap	Time for diffusion (ms)
0.6 D	7.995
0.8 D	7.246
1.0 D	6.01
1.2 D	7.709

Species Diffusion

- Variation with change in the ACF
  - Overlap distance between the input structures (ε = 0.60)
  - Size of the input structures (ε = 0.75)



Size (μm)	Time for diffusion (ms)
50	6.85
100	6.66
150	6.911
200	7.29

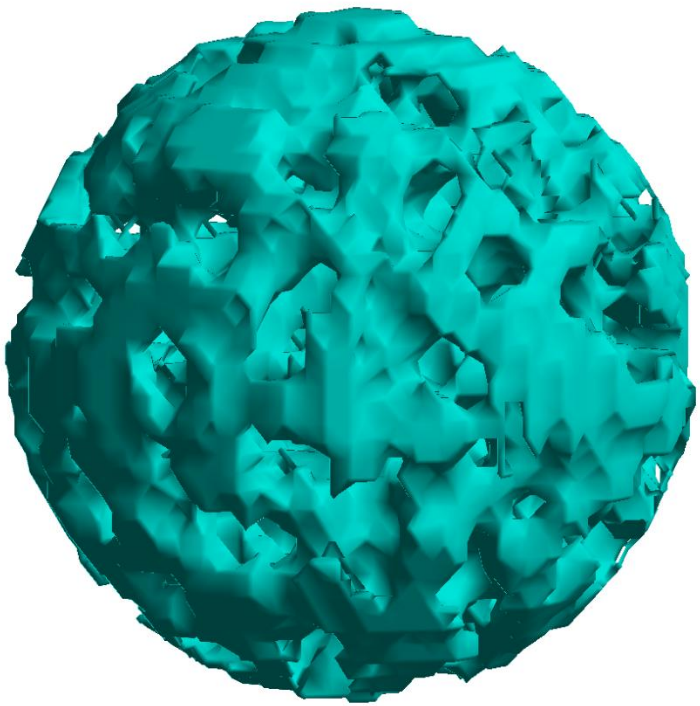
Species Diffusion

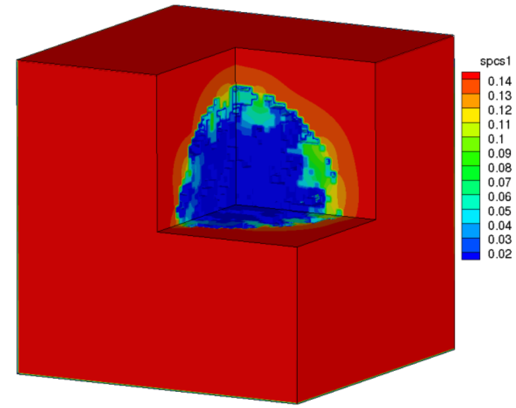
- Variation with change in the ACF
  - Overlap distance between the input structures (ε = 0.60)
  - Size of the input structures (ε = 0.75)
- No definite pattern observed so far
  - Simulations performed for ε > 0.60, for which diffusion time is in the asymptotic range

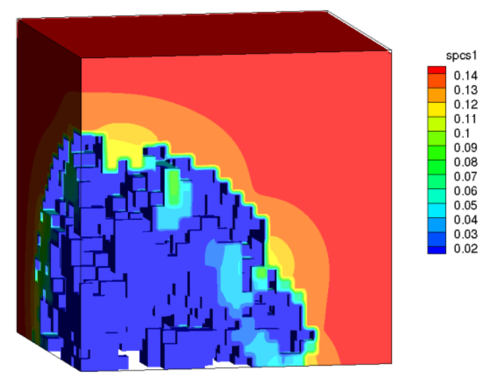
Overlap	Time for diffusion (ms)
0.6 D	7.995
0.8 D	7.246
1.0 D	6.01
1.2 D	7.709

Case	Time for diffusion (ms)
1	6.85
2	6.66
3	6.911
4	7.29

Species Diffusion







Contour plots obtained from a 3D diffusion simulation through a porous particle (ε = 0.45)

Major Achievements

- Capability to handle arbitrary 2-D and 3-D surface contours
  - Validation for stationary and moving boundary problems

- Temperature BC for heat transfer studies into IBM framework
  - Validation for uniform flow over a stationary cylinder
  - Includes implementation of conjugate heat transfer

- Porous flow simulation
  - Stochastic reconstruction of arbitrary porous structures
  - Simulation and comparison with analytical results
  - Species diffusion through 2D and 3D porous particles

Approach

Immersed boundary method (IBM)	• *Capability to resolve complex geometries* • *Conjugate heat transfer and species transport modules*
Porous reconstruction	• *Use optimized stochastic reconstruction methods* • *Perform X-ray CT imaging to obtain statistical descriptors*
Understand involved process variables	• *Perform DNS calculations to resolve the porous microstructure*
Help improve CO_2 capture	• *Could potentially lead to design of tailored microstructures to best achieve the adsorption process*

Future work

- Parallelization of IBM framework to enable faster computations (a major bottle-neck currently)
- Digital reconstruction of porous microstructure of typical sorbent particles through X-ray CT (or TEM/SEM) imaging
- Use of physical CO_2 adsorption rates in simulations depending on the local surface conditions
- Spatio-temporal evolution of the porous microstructure with adsorption

Acknowledgements

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- Multiphase Flow Research Group (MFRG) at NETL

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5. Vortex wake and energy transitions of an oscillating cylinder at low Reynolds number, Stewart, B., Leontini, J., Hourigan, K. and Thompson, M.C., ANZIAM J., Vol. 46(E), pp. C181-C195, 2005.
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Thank you!

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Stochastic Reconstruction

- **Porous medium represented by**

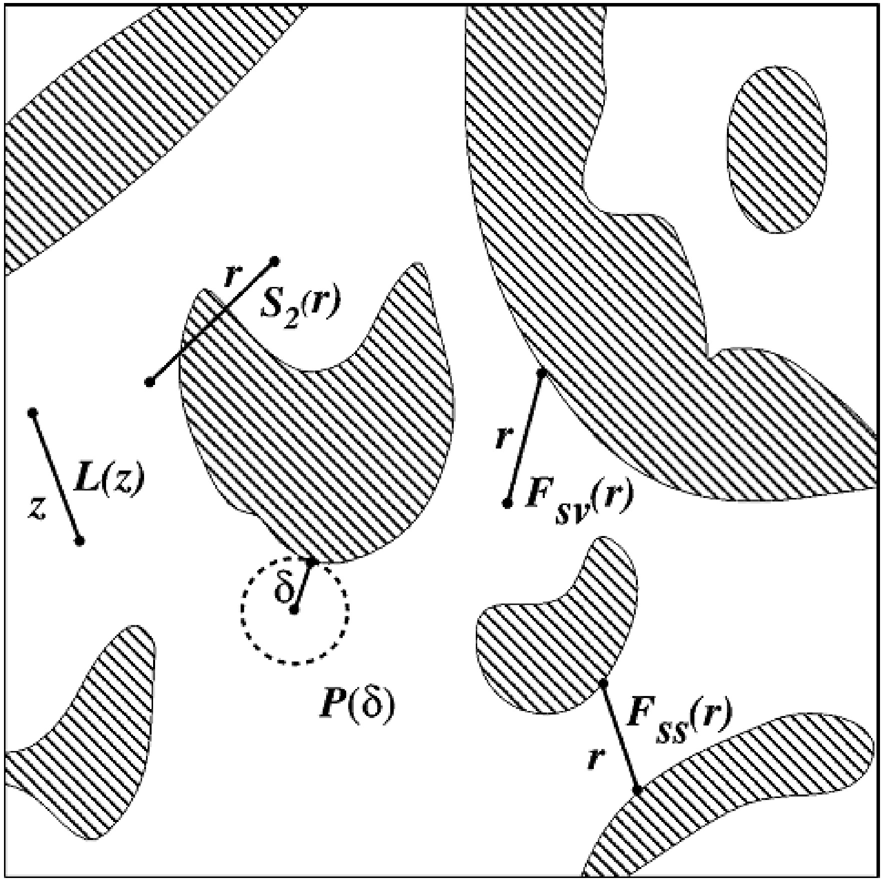
$$y(x) = \{1 \text{ for pore} | 0 \text{ for solid}\}$$

- **Porosity**

$$\varepsilon = \langle y(x) \rangle$$

- **Two point correlation**

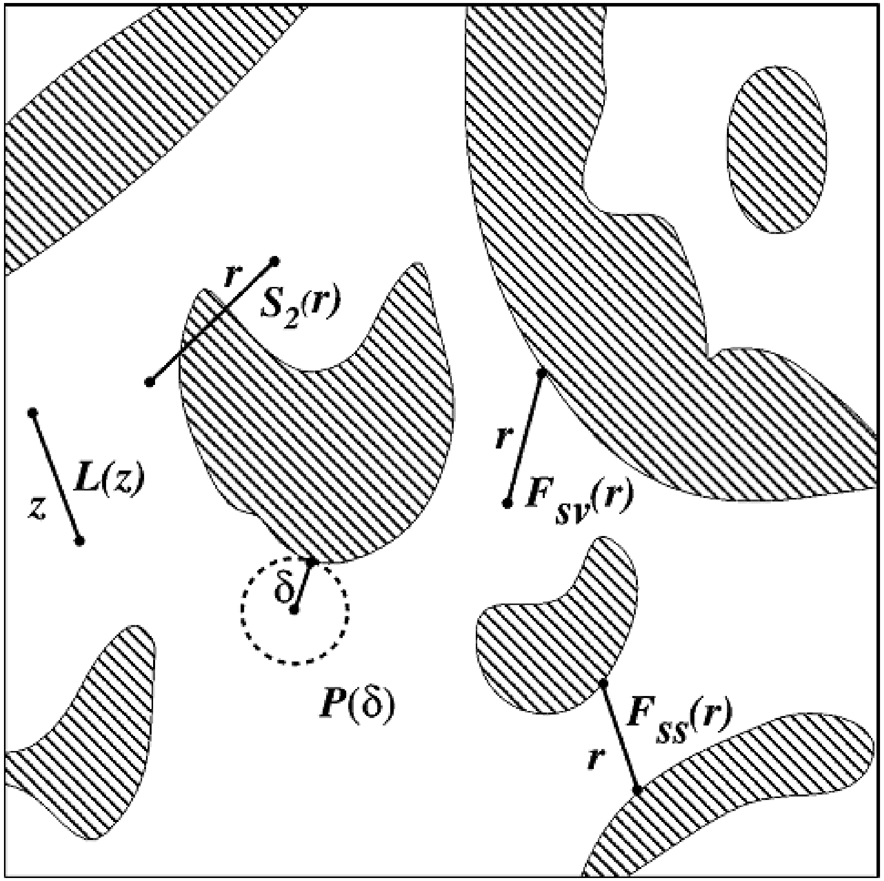
$$s_2(r) = \langle y(\vec{x}) y(\vec{x} + r) \rangle$$



Taken from Ref2

Stochastic Reconstruction

- ***Pore size distribution*** $P(\delta)$ ***- is the probability of finding pore space which lies from solid surface at a distance between*** δ ***and*** $\mathrm{d}\delta$***.***



Taken from Ref2

Simulated annealing

Steps:

$$E = \sum (f(x) - f_{ref}(x))^2 \quad (1)$$

Where f is any statistic function. In case of multiple statistic function total energy is obtained by summation with weight factor α_i

$$E = \sum \alpha_i E_i \quad (2)$$

1. Define initial distribution and find Energy (eq.1)
2. Interchange two arbitrarily chosen pore and solid
3. Compute the energy for modified system and find change in energy ($\Delta E = E_{new} - E_{old}$).
4. Accept the new configuration based on Metropolis rule(Eq.3)
5. Repeat from 2 to 4 after certain number of iteration

$$P(\Delta E) = \begin{cases} 1 & if \Delta E \le 0 \\ \exp\left(\frac{-\Delta E}{T}\right) & if\ \Delta E > 0 \end{cases} \quad (3)$$

Where T is temperature and by reducing the value as iteration progress configuration with minimum deviation(low values of E) will be generated.

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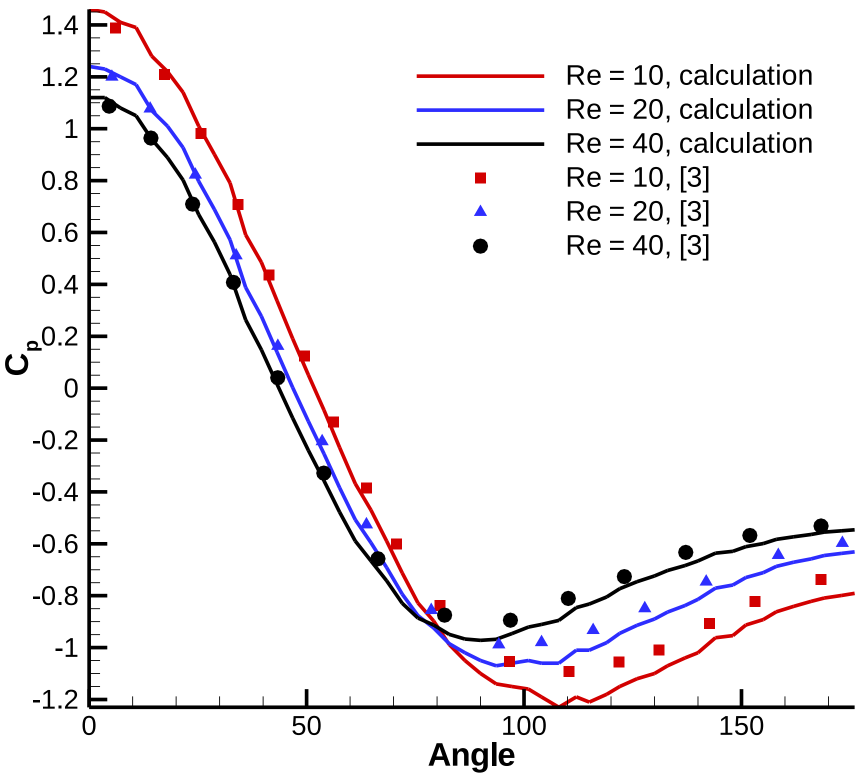
Stationary cylinder results

- **Steady case**
  - Re = 10, 20 and 40
  - Point of reattachment (L_w)
  - Coefficient of drag (C_D)
  - Comparison with Park et al. (1998)[2]

Re	C_D	C_D [3]	L_w	L_w [2]
10	2.74	2.78	0.26	0.25
20	2.02	2.01	0.94	0.95
40	1.58	1.51	2.23	2.30

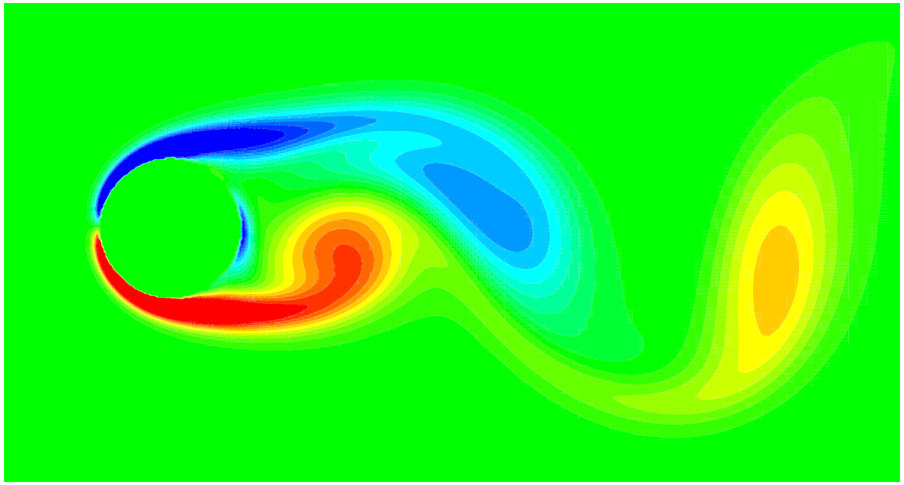


Stationary cylinder results

- **Unsteady case**
  - Karman vortex street
  - Re = 100, 150 and 200
  - Strouhal number comparison

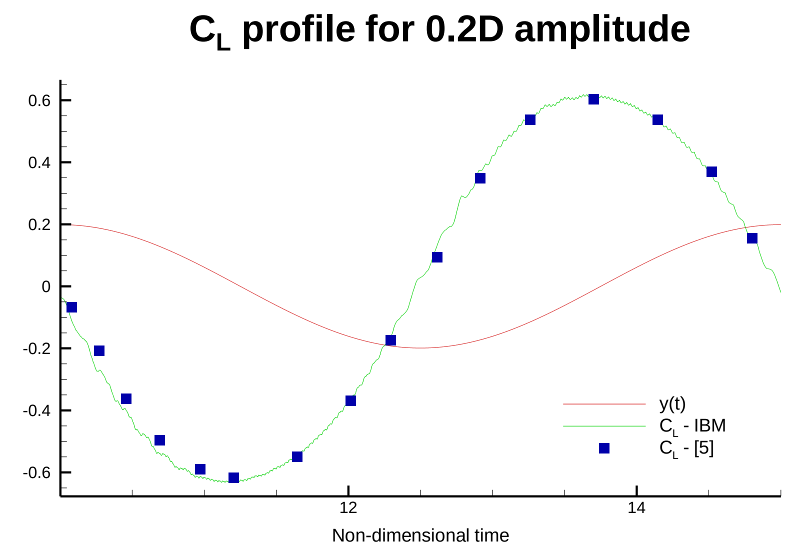
Re	St	St [3]
100	0.166	0.16
150	0.185	0.18
200	0.198	0.20

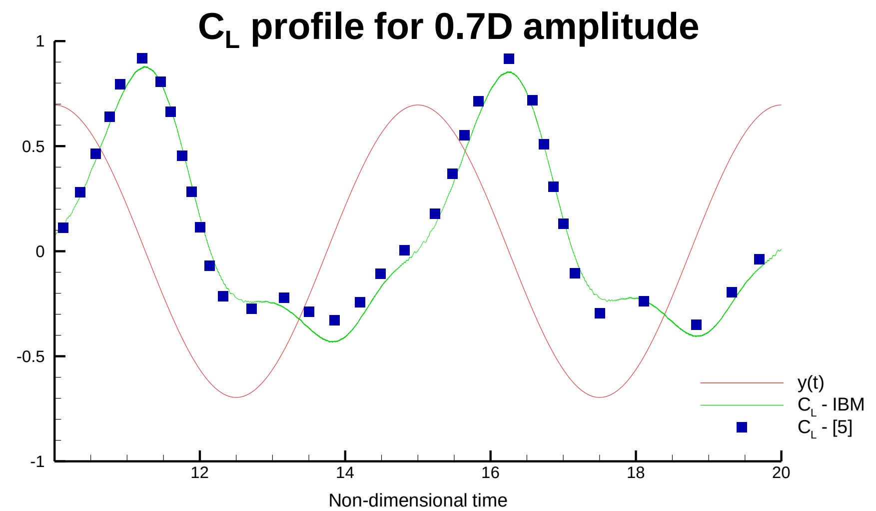
Re = 150



Oscillating Cylinder

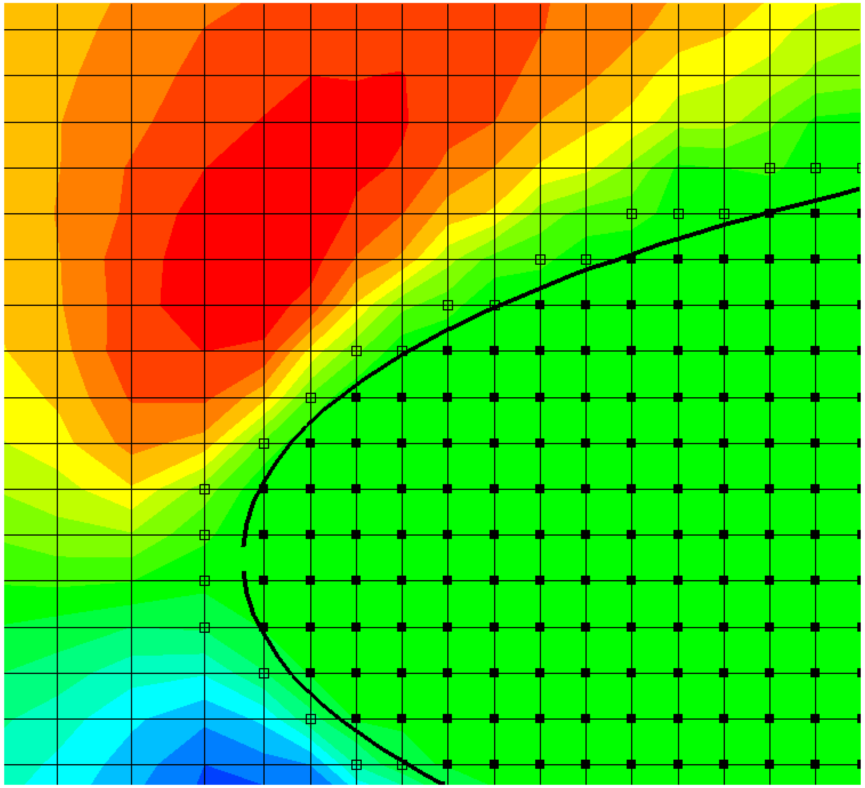
- **Re = 200**
- **Frequency – 0.2**
- **Amplitudes – 0.2D and 0.7D**
- **Grid size of 0.00625D**
- **C_L profile**
  - Correct values predicted
  - Compared with numerical results of Stewart et al.[5]
- **Correct prediction of changed vortex shedding pattern for 0.7D amplitude**





Arbitrary surface contours

- Implementation of IBM to simulate flow around solid bodies of **arbitrary shapes**
- Applicable to both **2-D and 3-D problems**



Flow over an airfoil

Heat transfer with IBM

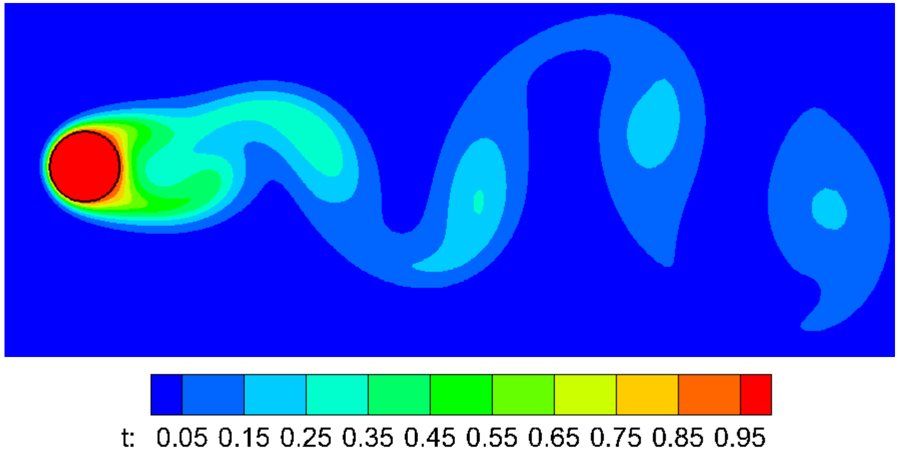
- **Temperature BC** for energy equation implemented in IBM
- **Validation** completed for uniform flow over a stationary cylinder
- Constant **heat flux** and constant **temperature** conditions implemented

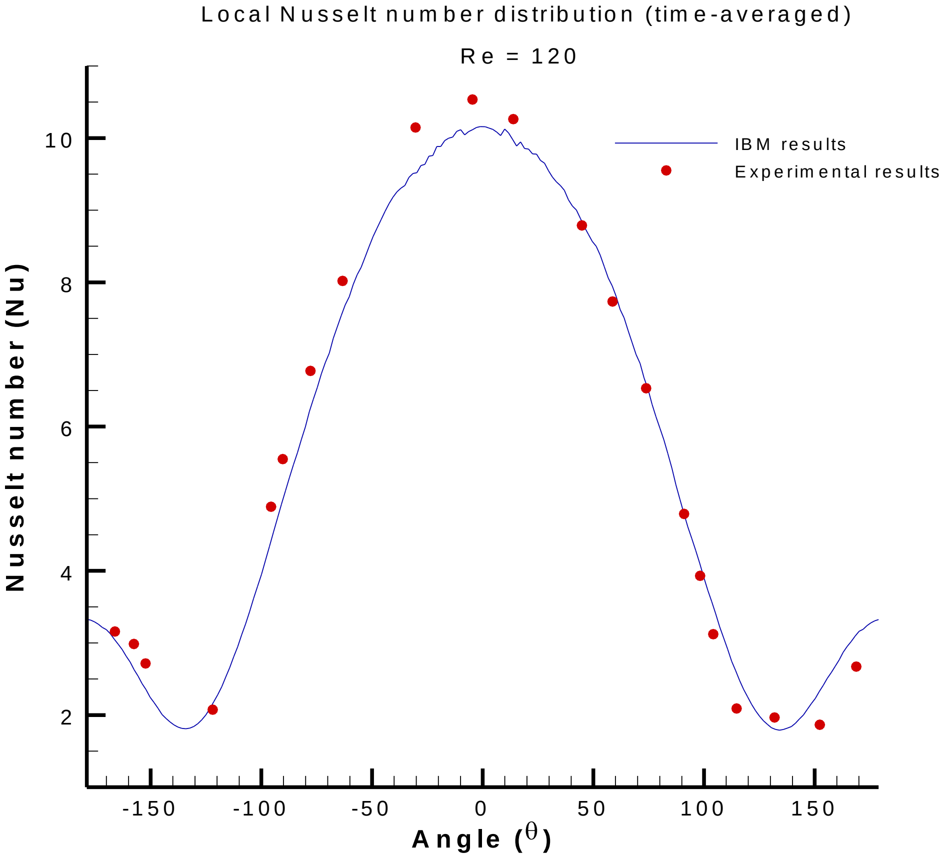
- **Implementation** of conjugate heat transfer
- Results compared with exact solution
  - Rotational flow between concentric cylinders
  - Good comparison!

Heat transfer results

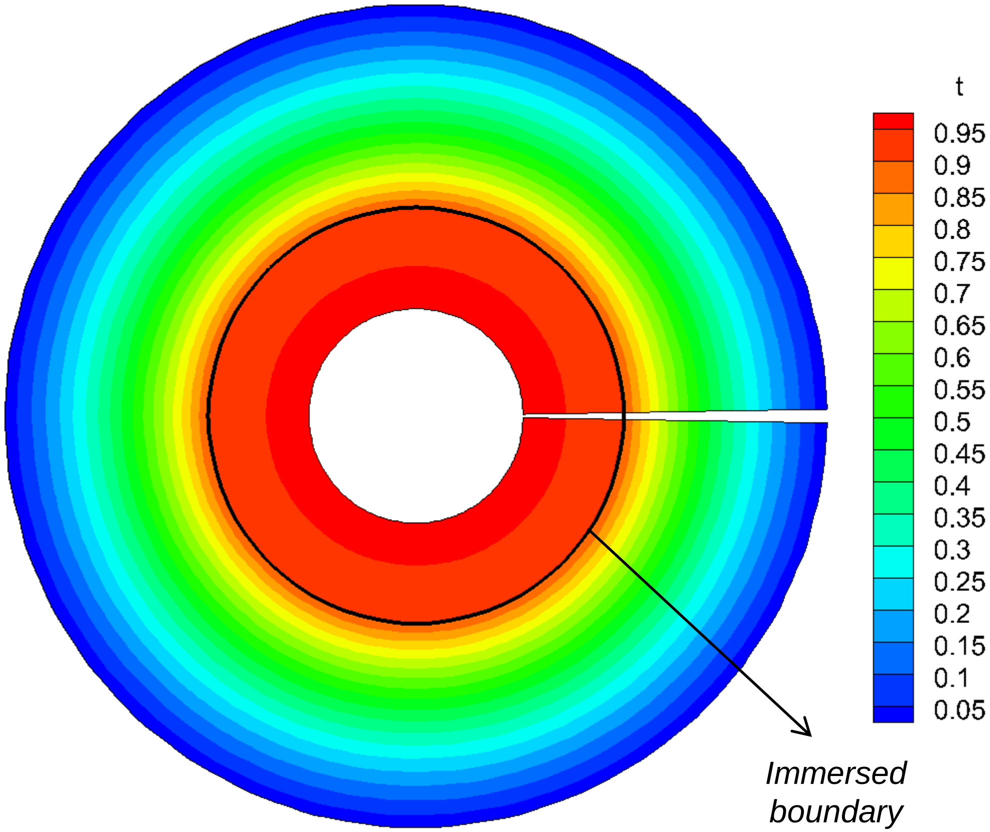
Nusselt number comparisons (iso-thermal)

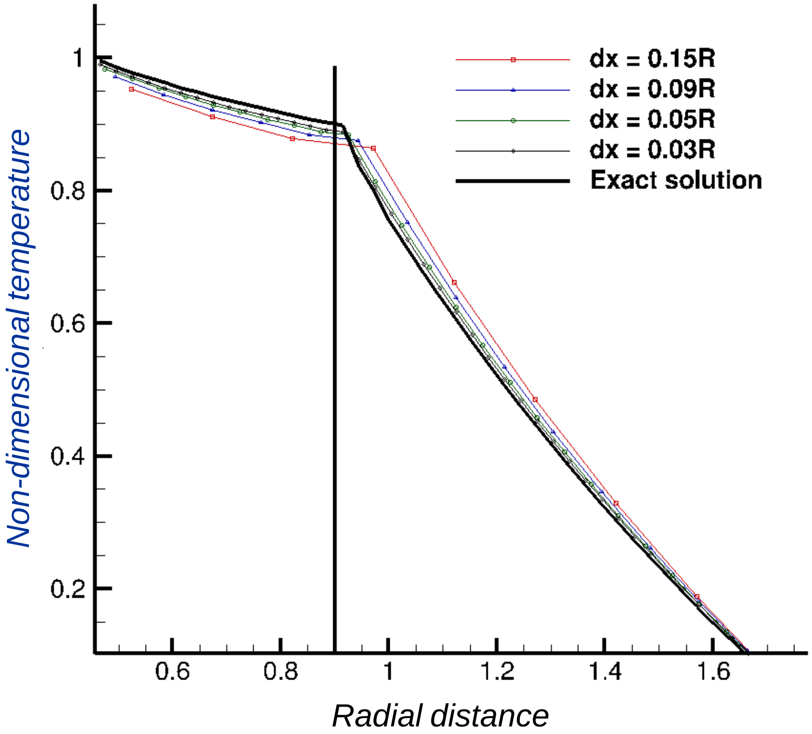
Re	Experimental results [5]	Present
10	1.80	1.83
40	3.28	3.18
120	5.69	5.56



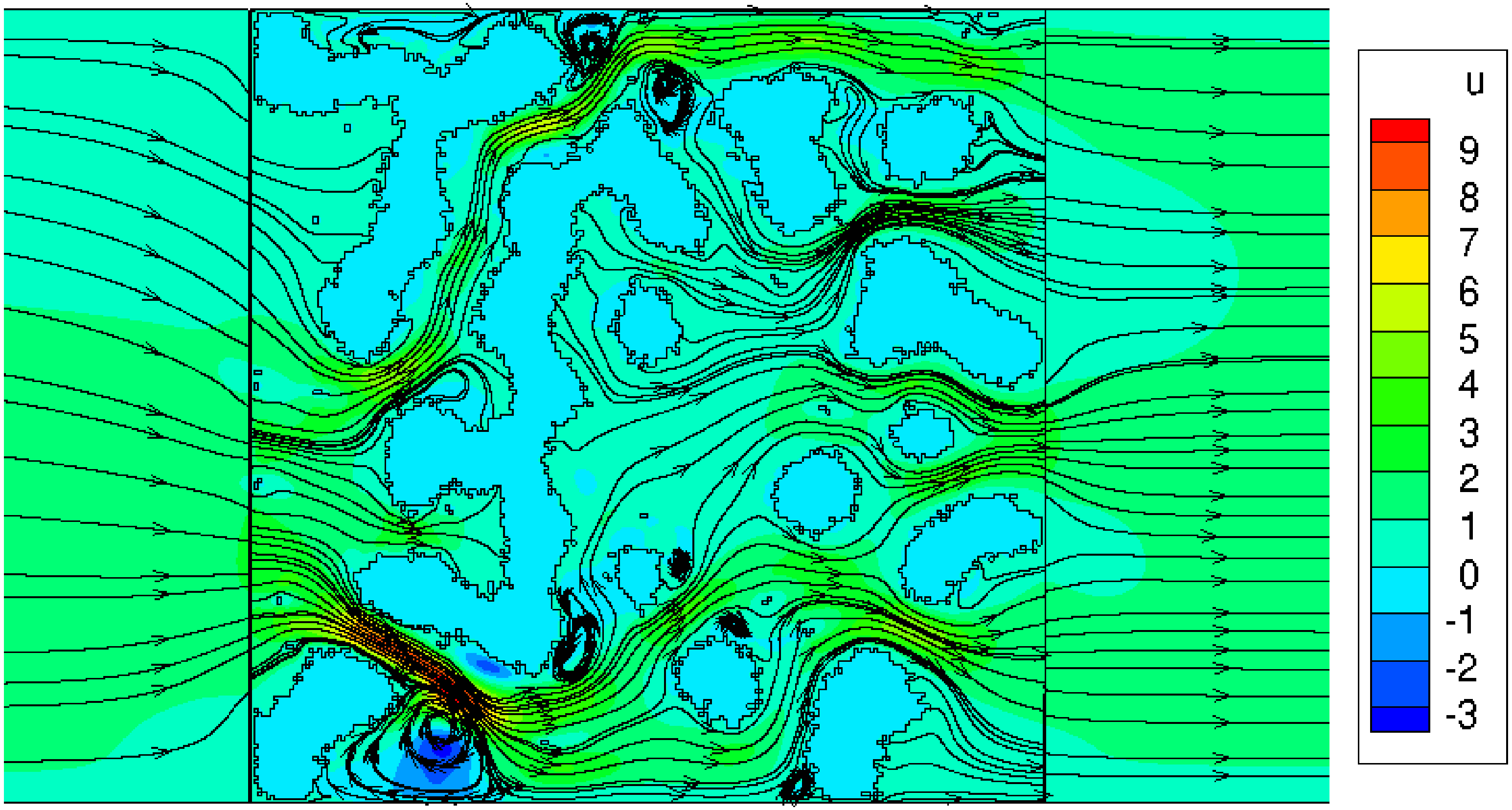


Conjugate heat transfer results





Porous flows with IBM



Porous flows with IBM