



Curtin University

Process Design using Computational Fluid Dynamics

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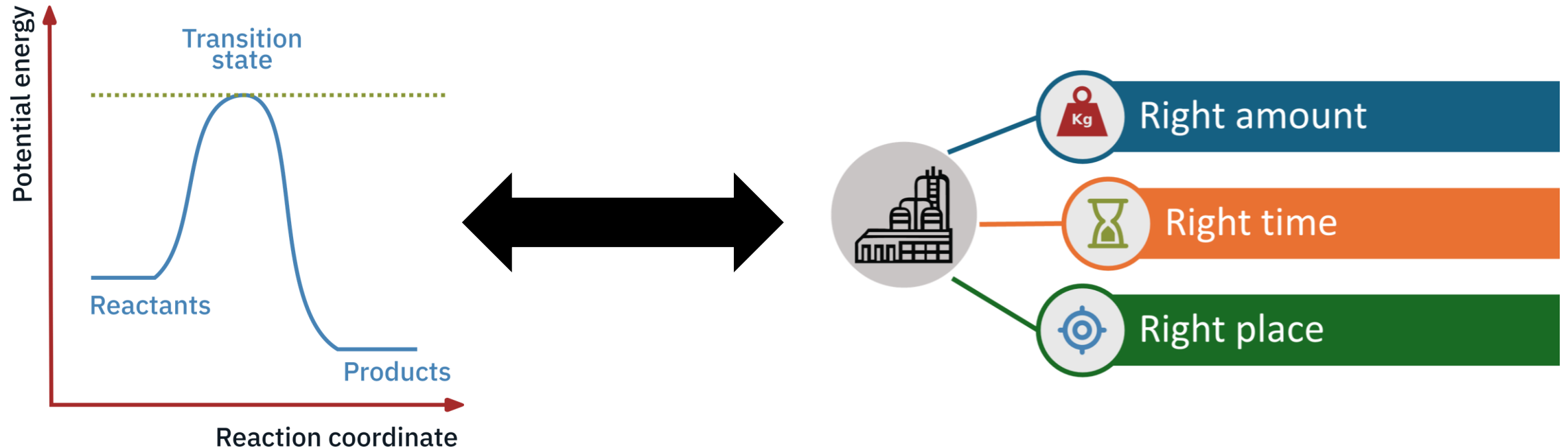
Acknowledge of Country

I acknowledge the Whadjuk Nyungar people and Traditional Custodians of the land in which Curtin University, Bentley campus is situated on.

I pay respect to Elders past, present and emerging

Process Equipment Design

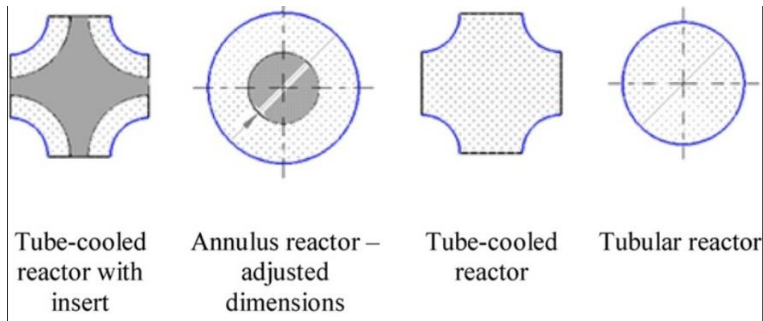
- Designing of reactors, heat exchangers, distillation columns, pumps, compressors, and vessels, ensuring that they meet the process requirements, safety standards, and economic feasibility.



One of the levers: novel geometries (in other words, optimised hydrodynamics)
 C (*any scaler, i.e., conc., temp., press.*) = $f(t, x, y, z)$

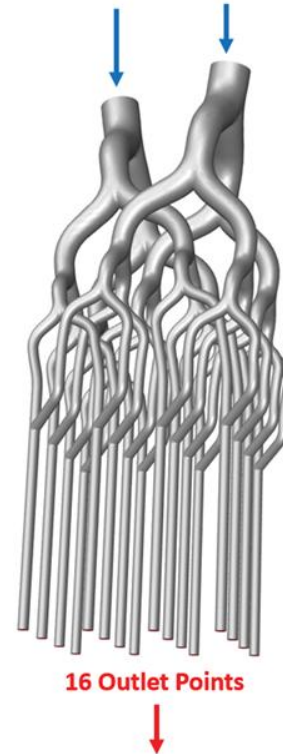
Novel geometries → Process Intensification

Example-1



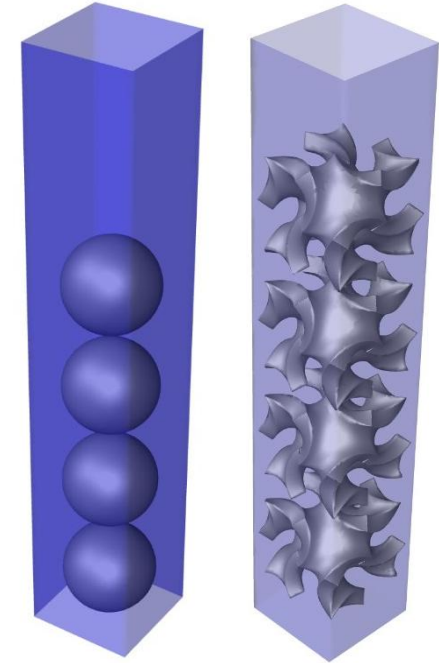
Instead of a simple tube reactor, a tube with retrofittable inserts ¹

Example-2



Fractal flow device - as a flow distributor or burner²

Example-3



Instead of spherical catalyst/packing, gyroid shaped

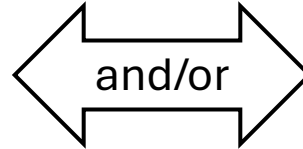
¹Redondo, B., et al. (2019). "Intensified isothermal reactor for methanol synthesis." *Chemical Engineering and Processing-Process Intensification* 143: 107606.

²Priyambodo, M. D. M., et al. (2022). "Numerical evaluation of an additively manufactured uniform fractal flow mixer." *Chemical Engineering and Processing-Process Intensification* 179: 109047

How we test intensified designs?

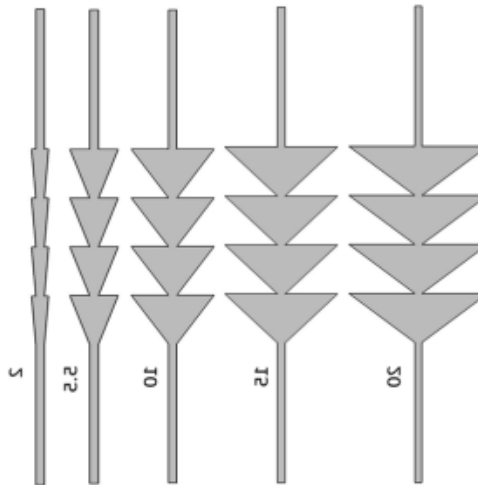
Experiments:

Expensive,
time consuming,
can't be performed at real conditions,
measurement limitations,
do not provide distributed parameters



CFD:

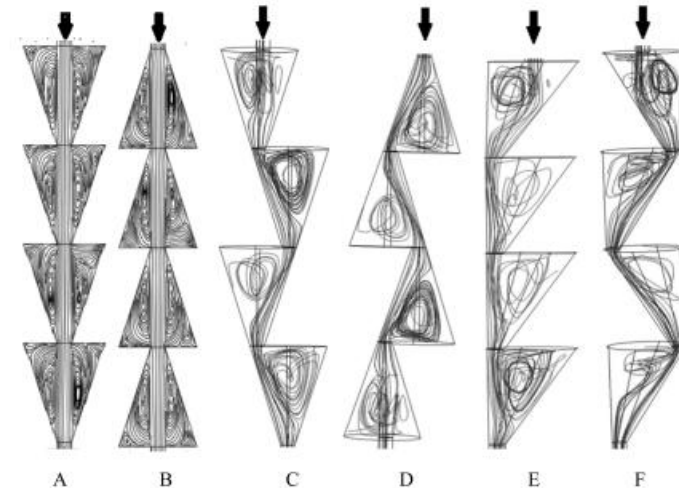
Provides information of all parameters,
Unlimited attempts as per availability
of computational resources



Conceptual designs¹



Exp. of one design¹



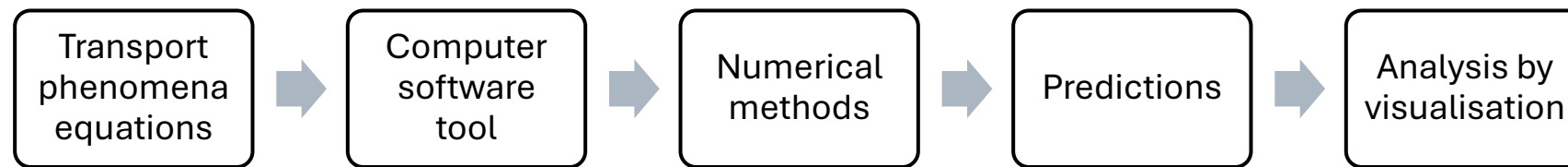
CFD – flow streamlines¹

¹Sharma, M., et al. (2014). "3D flow reactors: flow, hydrodynamics, and performance." *Industrial & Engineering Chemistry Research* **53(5)**: 1916-1923.

What is CFD? How it works?

CFD

- A computer-based software tool which can *predict fluid flow and associated transport phenomena*.



Inlet fluid

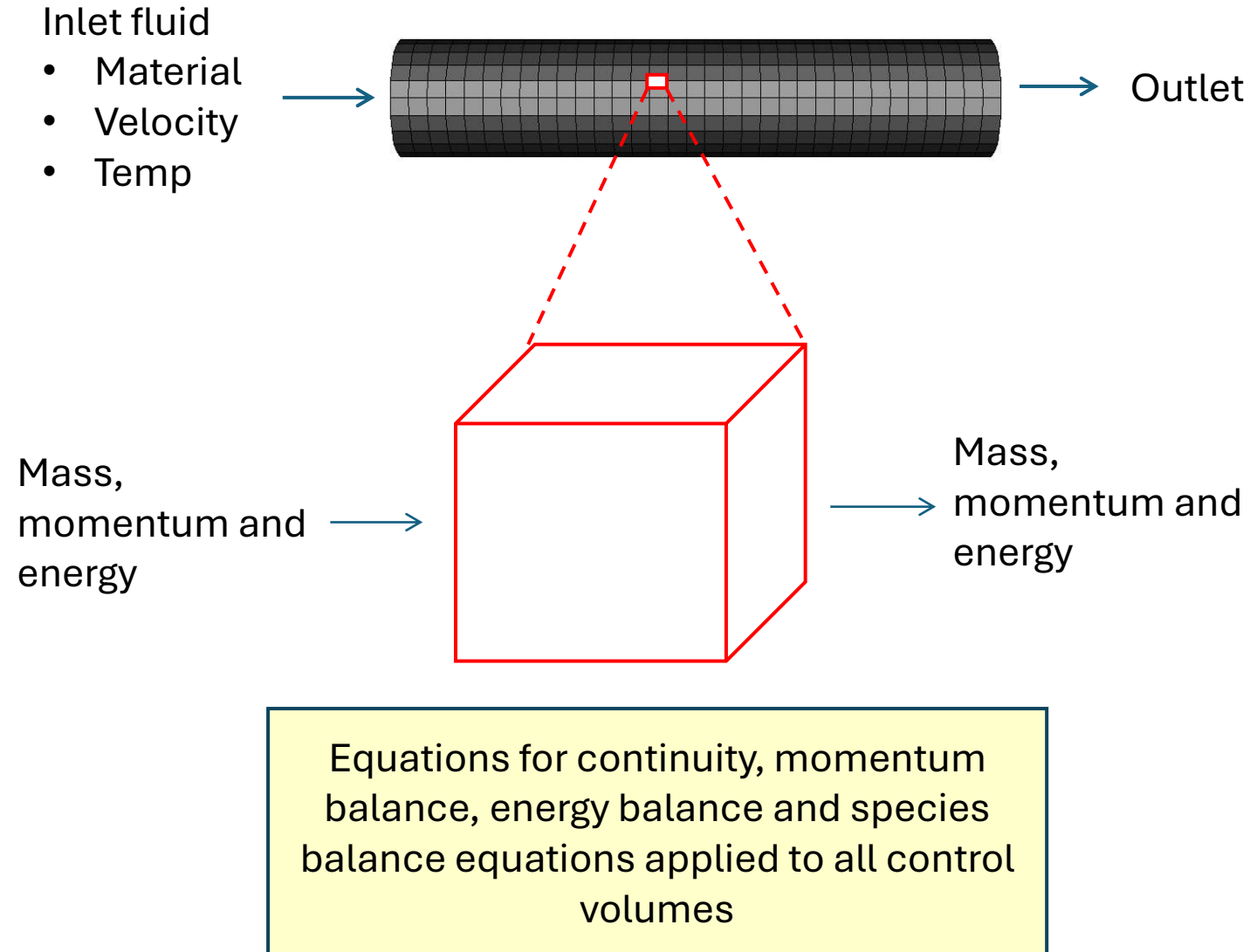
- Material
- Velocity
- Temp



Outlet

Required solution:
What will be the velocity field, pressure profiles, temperature distributions in the flow domain?

What is CFD? How it works?



What is CFD? How it works?

- Continuity equation

$$\frac{\partial \rho}{\partial t} = - \left(\frac{\partial \rho u_x}{\partial x} + \frac{\partial \rho u_y}{\partial y} + \frac{\partial \rho u_z}{\partial z} \right) + S_m$$

- Momentum balance equations

$$\rho \left(\frac{\partial u_x}{\partial t} + u_x \frac{\partial u_x}{\partial x} + u_y \frac{\partial u_x}{\partial y} + u_z \frac{\partial u_x}{\partial z} \right) = - \frac{\partial p}{\partial x} + \mu \left[\frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial y^2} + \frac{\partial^2 u_x}{\partial z^2} \right] + \rho g_x + F$$

m. b. in y-direction

m. b. in z-direction

- Energy balance equation

$$\rho \hat{C}_p \left(\frac{\partial T}{\partial t} + u_x \frac{\partial T}{\partial x} + u_y \frac{\partial T}{\partial y} + u_z \frac{\partial T}{\partial z} \right) = k \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) + S$$

- Species balance equation (for species A)

$$\frac{\partial c_A}{\partial t} + v_x \frac{\partial c_A}{\partial x} + v_y \frac{\partial c_A}{\partial y} + v_z \frac{\partial c_A}{\partial z} = D_{AB} \left(\frac{\partial^2 c_A}{\partial x^2} + \frac{\partial^2 c_A}{\partial y^2} + \frac{\partial^2 c_A}{\partial z^2} \right) + R_A$$

Case study: Settling tank for produced water treatment



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A novel settling tank for produced water treatment: CFD simulations and PIV experiments



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Context:

<https://www.youtube.com/watch?v=vuuMcaSv59k>

<https://www.youtube.com/watch?v=KwP8mdwvE2A>

Objective:

Design a tank that not only works as produced water storage but also a settling tank which can separate heavy particles from produced water.

Case study: Settling tank for produced water treatment

Task: design a settling tank for settling of heavy particles (sand and heavier, micron size particles) from produced water

Reference design/size/data:

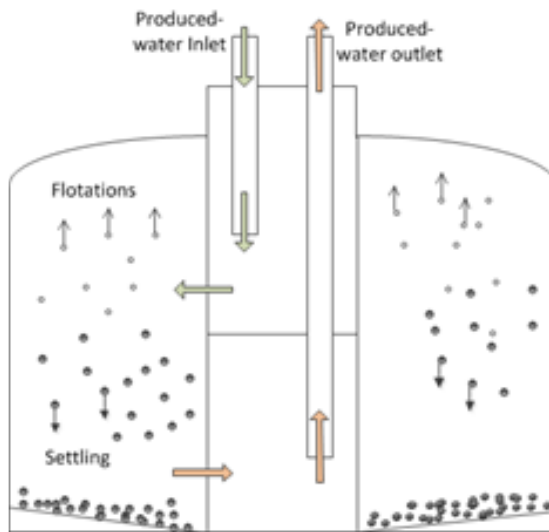


Table-1: Dimensions, flow rates and particle properties: SSU tank¹.

<u>Dimensions</u>		<u>Solids</u>		<u>Size distribution</u>	
Height	20 m	Type	Sand	<u>Range</u>	<u>Mass frac.</u>
Diameter	25 m	Density	2500 kg/m ³	0.01-0.1 µm	5%
Hatch dia.	1 m	Terminal velocity	0.00223 m/s	0.1-1 µm	10%
<u>Flow rates</u>		Avg. particle size	50 µm	1-10 µm	35%
Water	55.2 kg/s			10-100 µm	45%
Solids conc.	100 ppb			100-1000 µm	5%

Design constraints:

- (i) inlet and outlet must be located in the central hatch
- (ii) perforations on hatch wall at inlet and outlet for a flow to-and-from bulk of the tank and hatch
- (iii) no internal allowed

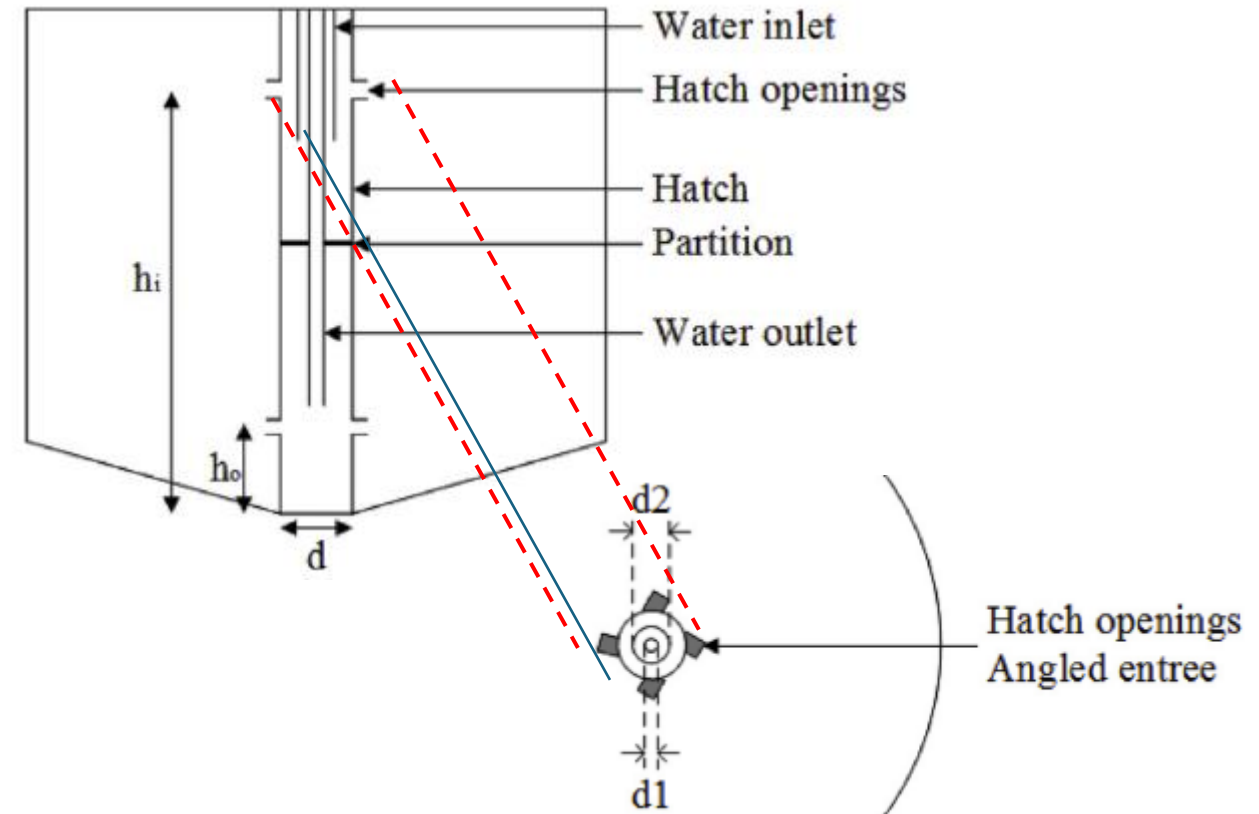
Case study: Settling tank for produced water treatment

Hypothesis:

“The tea-leaf paradox refers to the migration of tea leaves toward the centre of a teacup when the water is put in rotation by a spoon.”



Conceptual tanks design:



Case study: Settling tank for produced water treatment

Pre-processing: geometry, meshing, boundary condition, materials

Solver: model parameters, boundary conditions

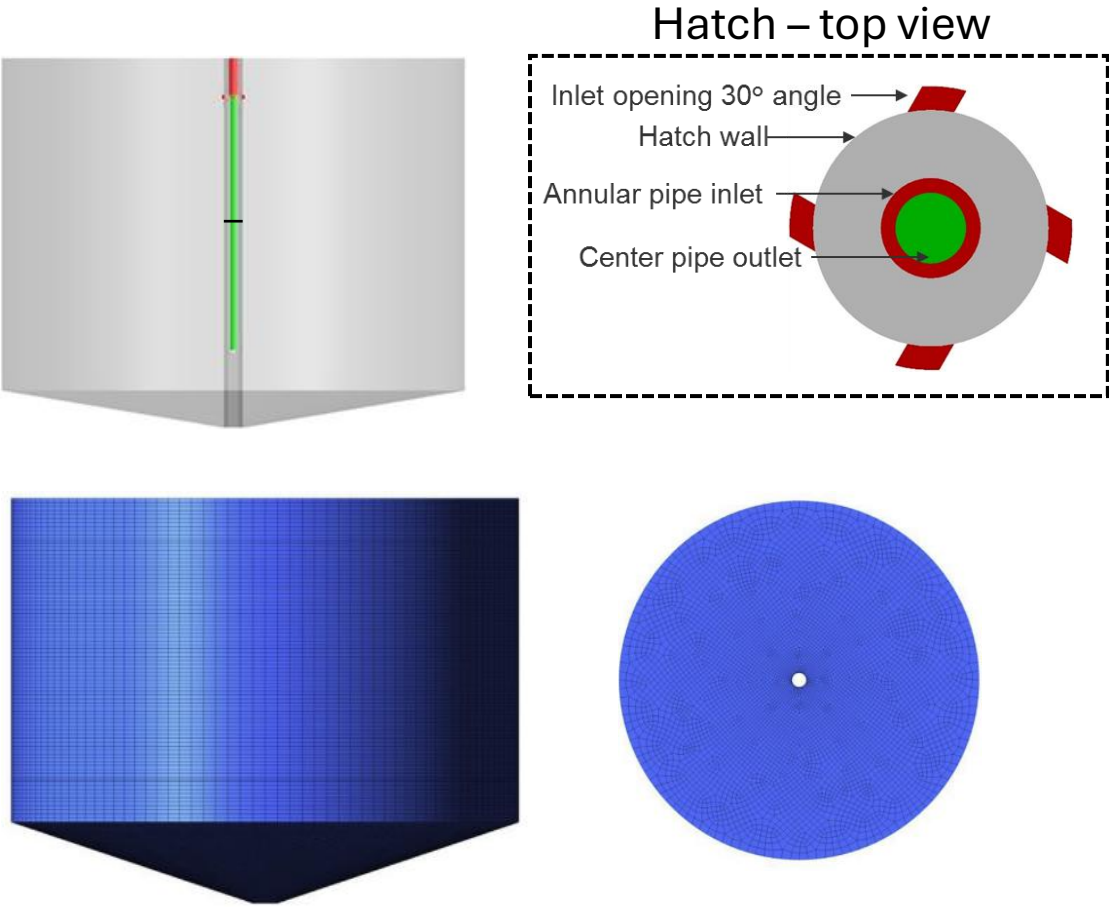
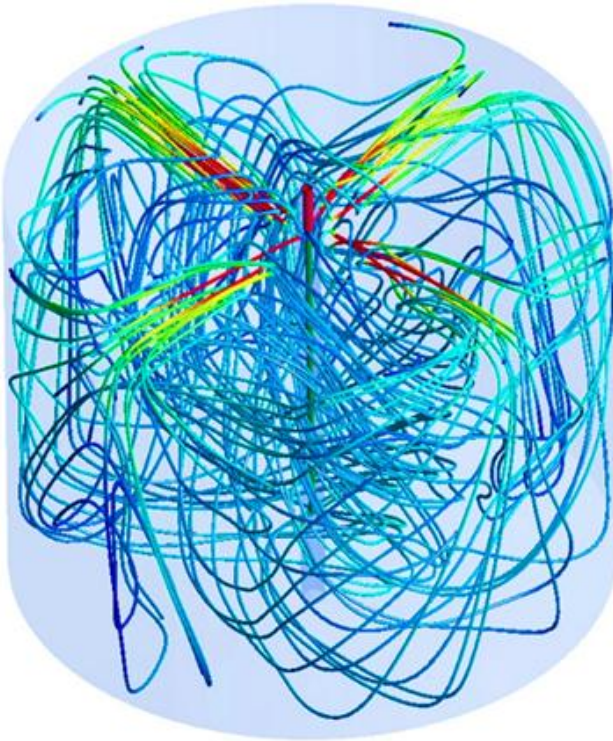


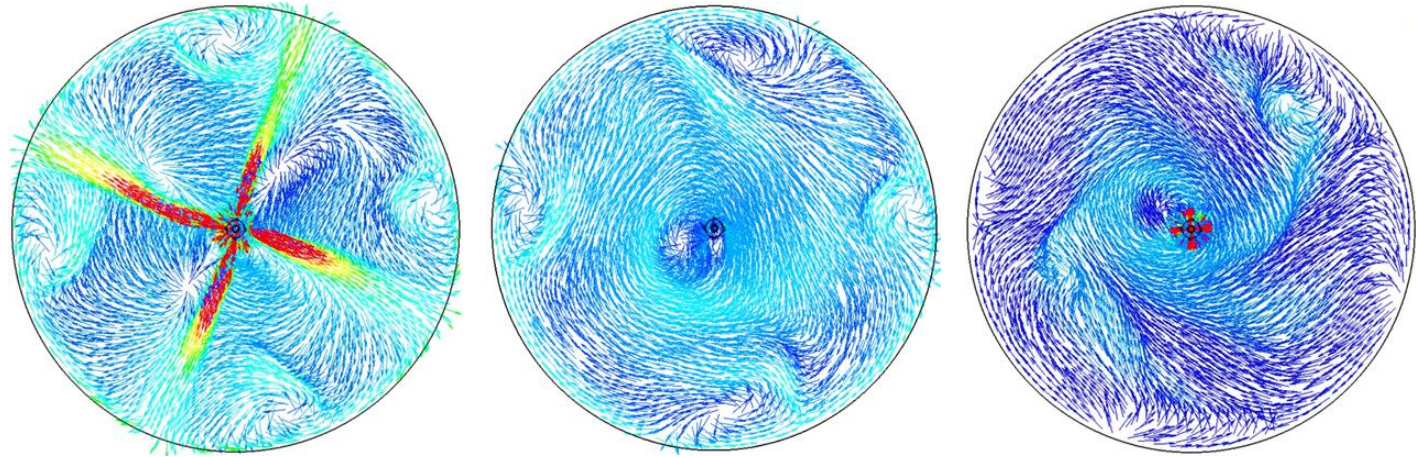
Table-2: CFD model	
Model	3D, Single phase, steady state
Number of cells	2.2 million
Turbulent model	K-ε or K-Ω-SST
Boundary conditions	
Inlet	Velocity inlet
Outlet	Pressure outlet
Outer walls	Wall
Centre hatch walls	Wall
Flow of solids	DPM, coupled with flow, steady state and transient
Size distribution	Rosin-Rammler linear particle size distribution
DPM Boundary cond.	
Bottom wall	Reflection co-efficient 0.4 or trap
Inlet	Reflect
Outlet	Escape
Walls	Reflect

Case study: Settling tank for produced water treatment

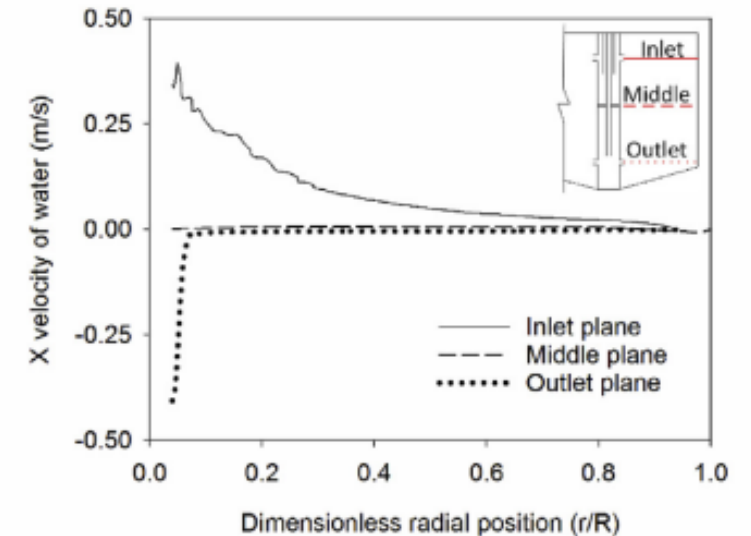
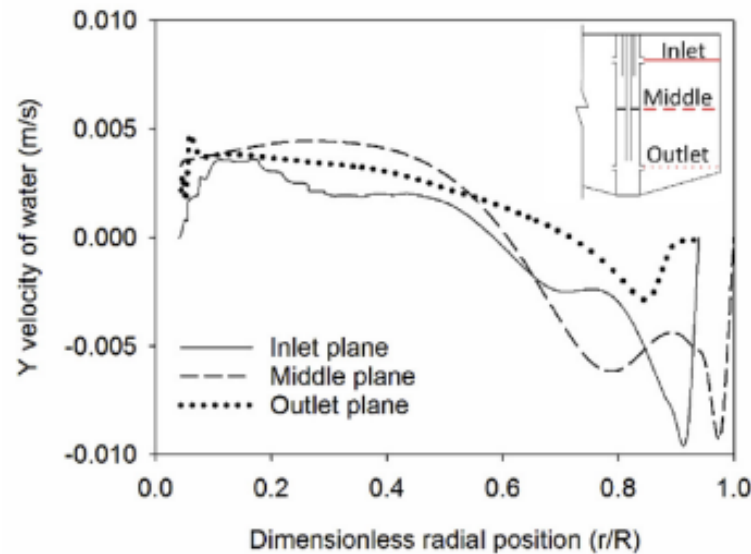
Post processing:



Velocity path lines

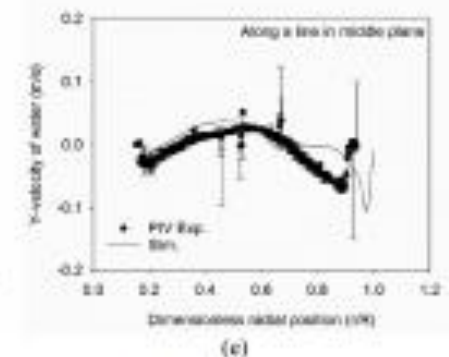
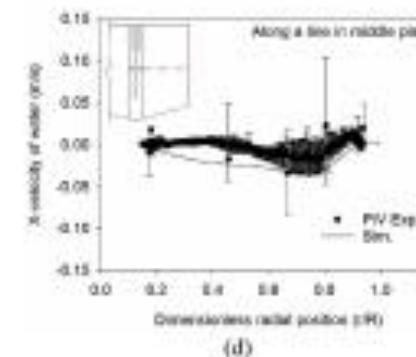
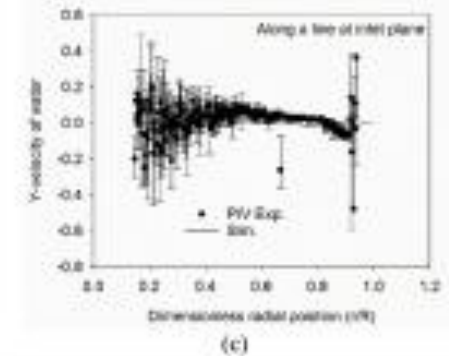
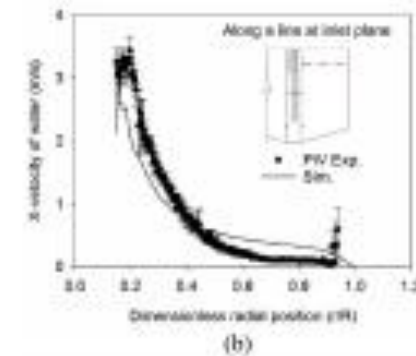
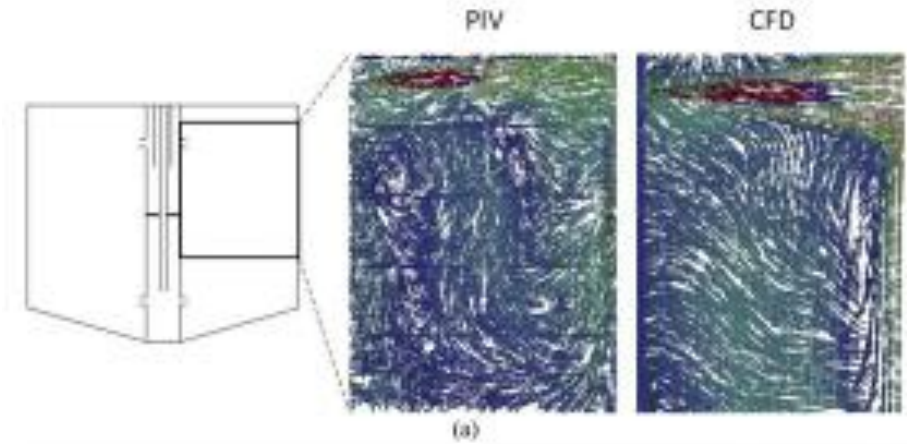
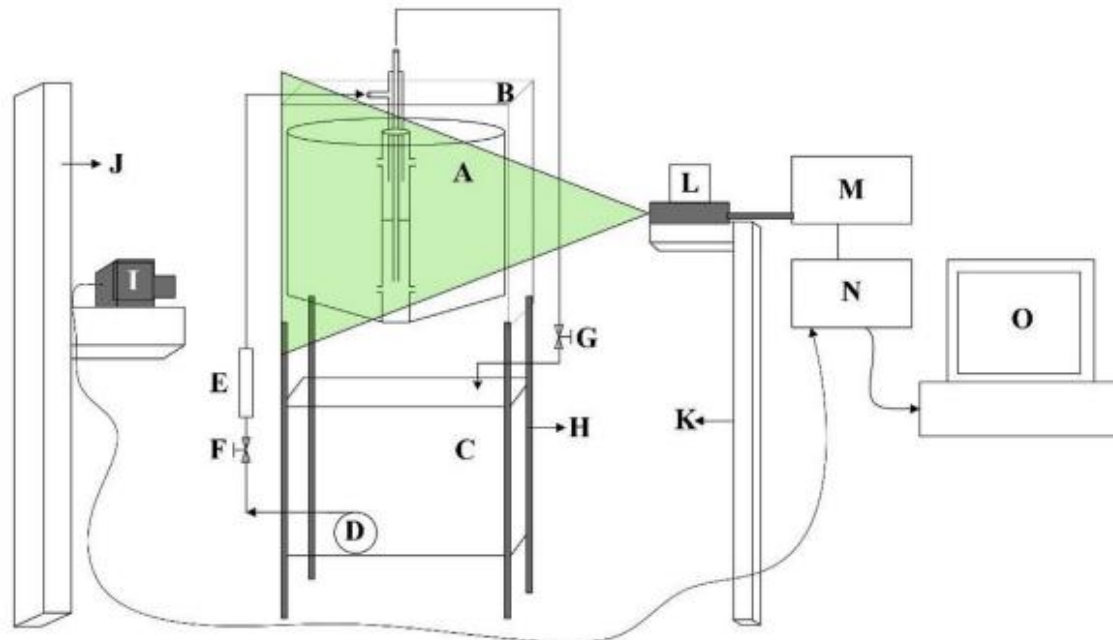
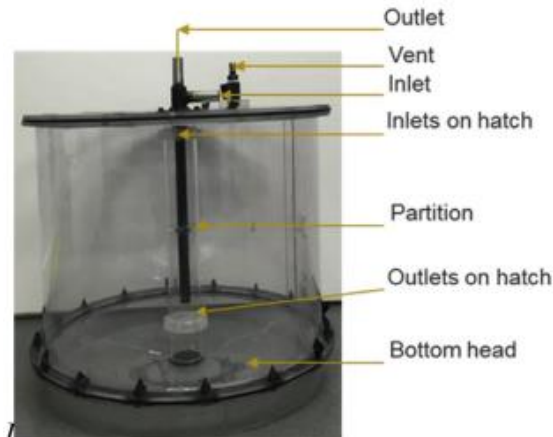


Velocity vectors



Case study: Settling tank for produced water treatment

Validation: comparison with experimental data



Case study: Settling tank for produced water treatment

Post processing: particle tracks (from DPM model)



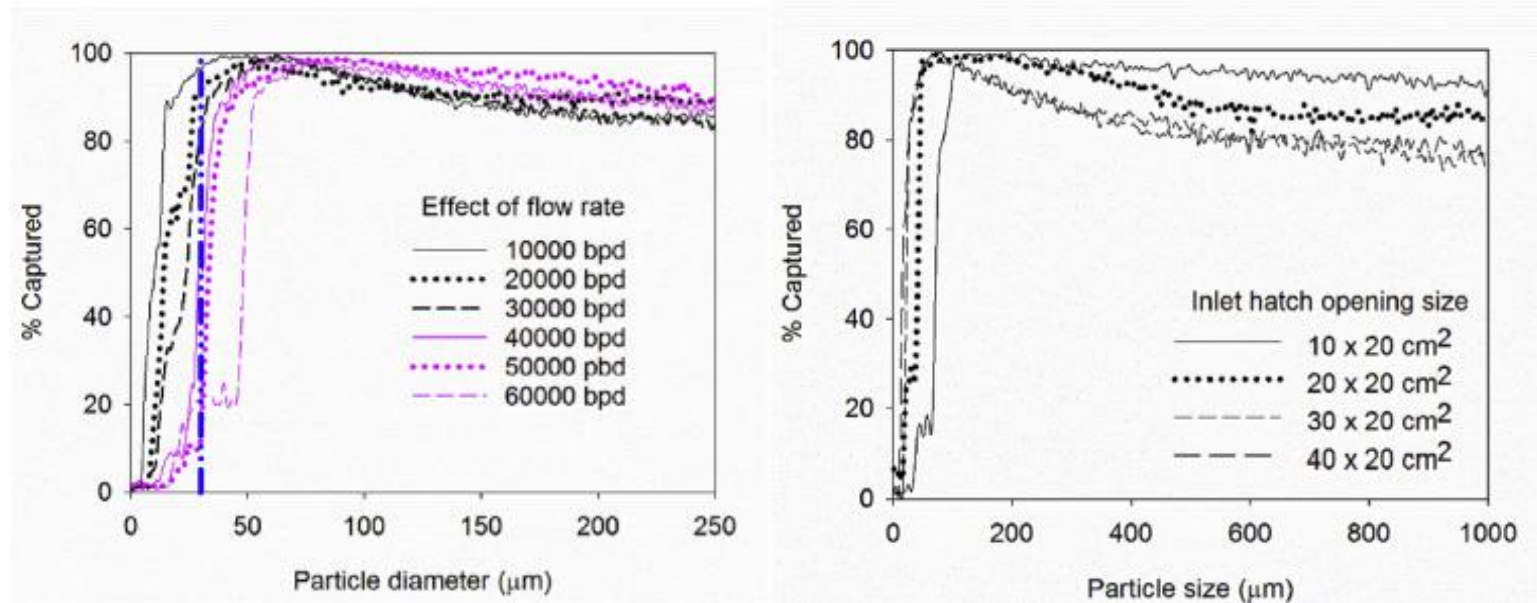
Iso-contour of axial velocity $\geq$
particle terminal velocity



Particle tracks

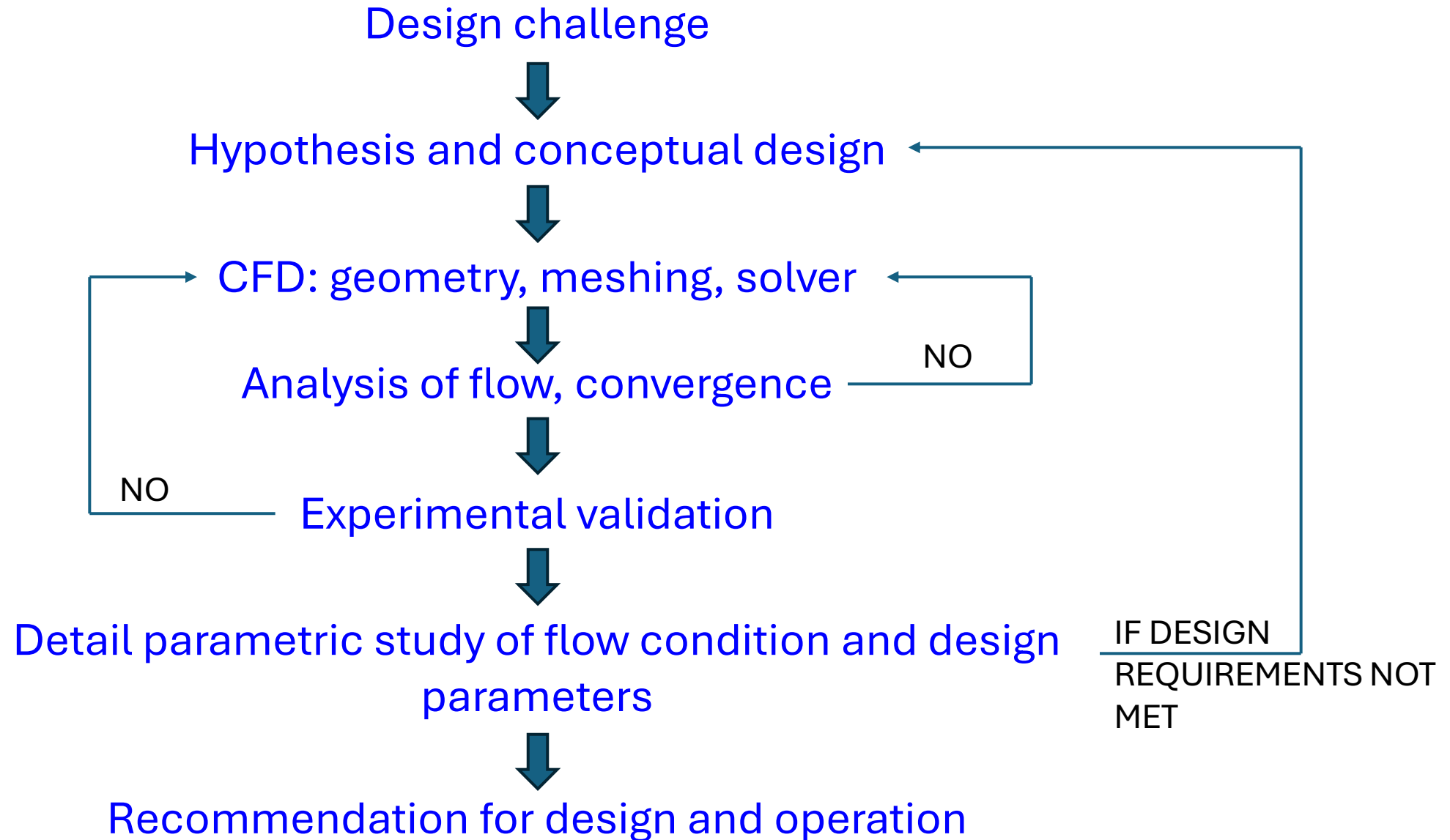
Case study: Settling tank for produced water treatment

Final recommended design and performance:



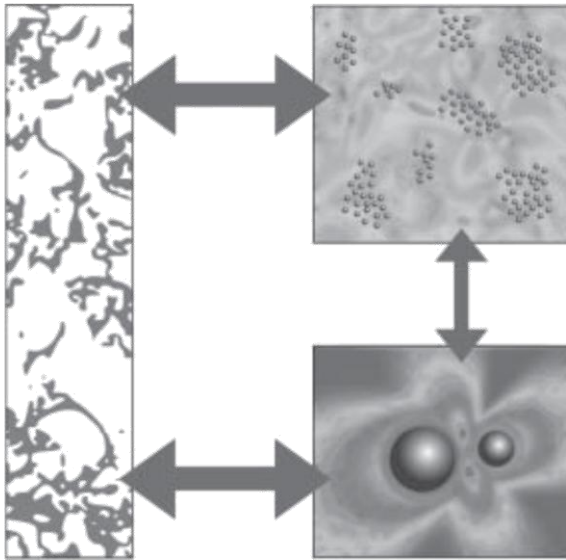
For inlet openings of $40 \times 20 \text{ cm}^2$, the simulations predicted capture of more than 80% particles having a size range of 30–1000 μm at an operating flow rate of 3000 barrels per day

Case Study: Workflow



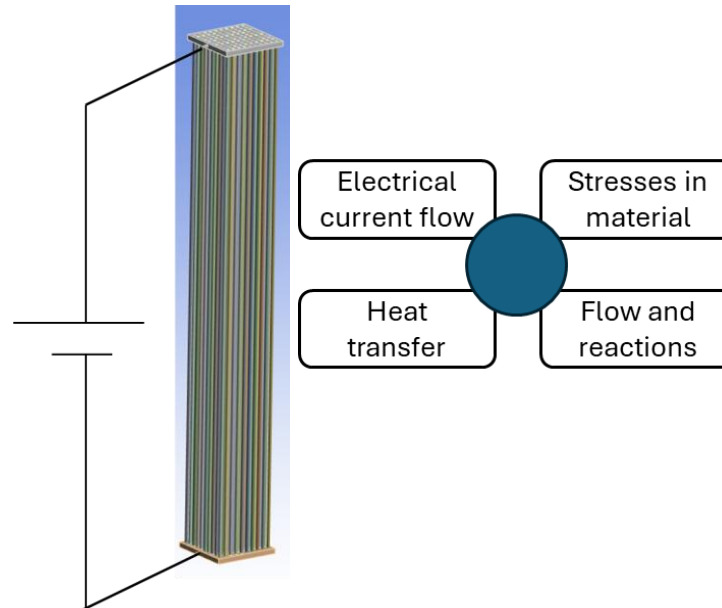
Challenges

Multi-scale of a process



- Immature closure models
- Empirical constants require tuning

Multi-physics nature of system



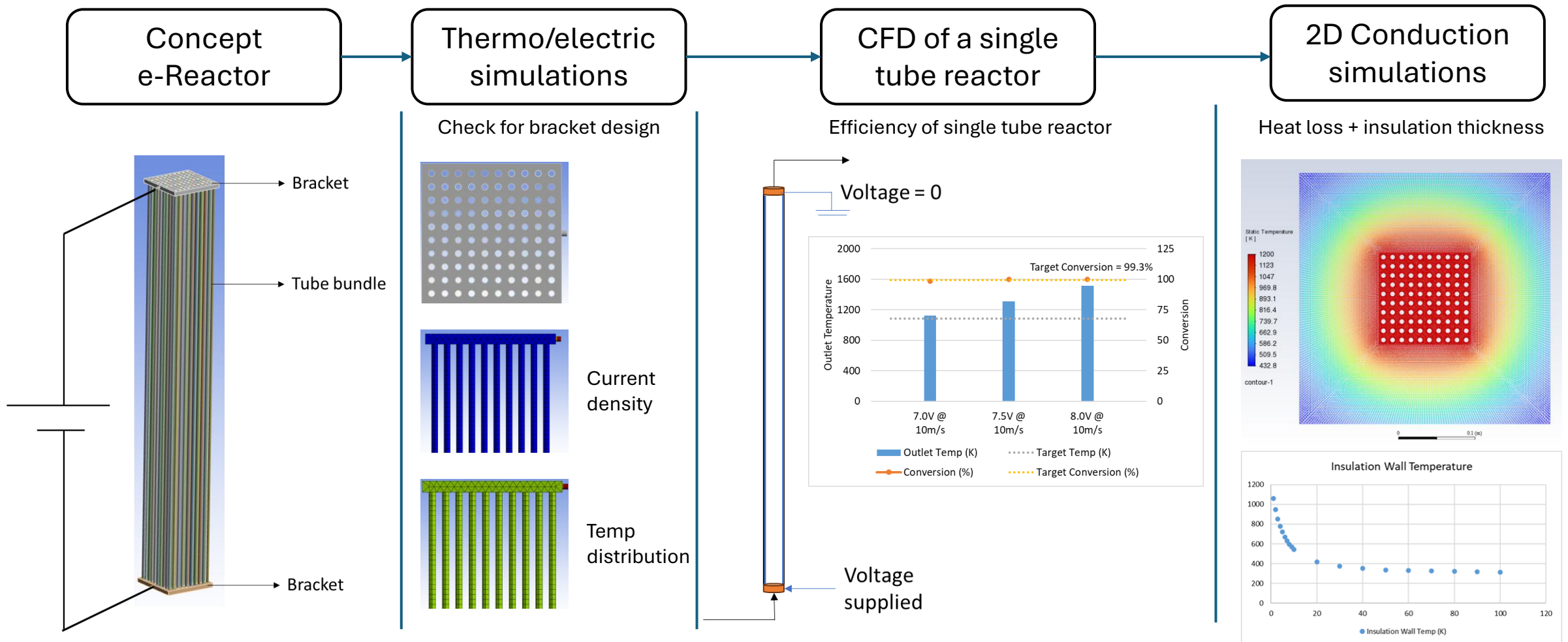
- CFD tool alone – not sufficient
- Tools to resolve different physics - required

Computational power



- Expensive
- Requires cloud computing

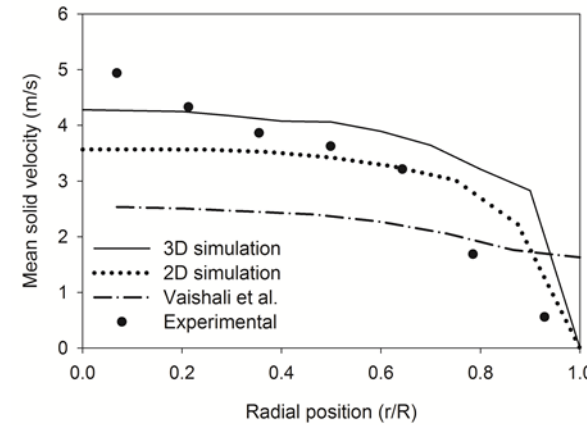
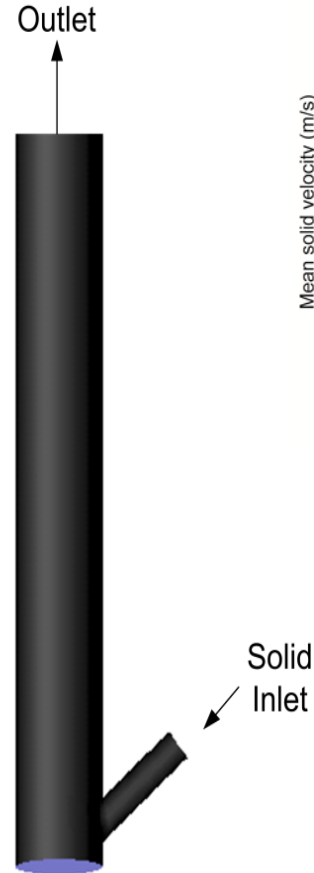
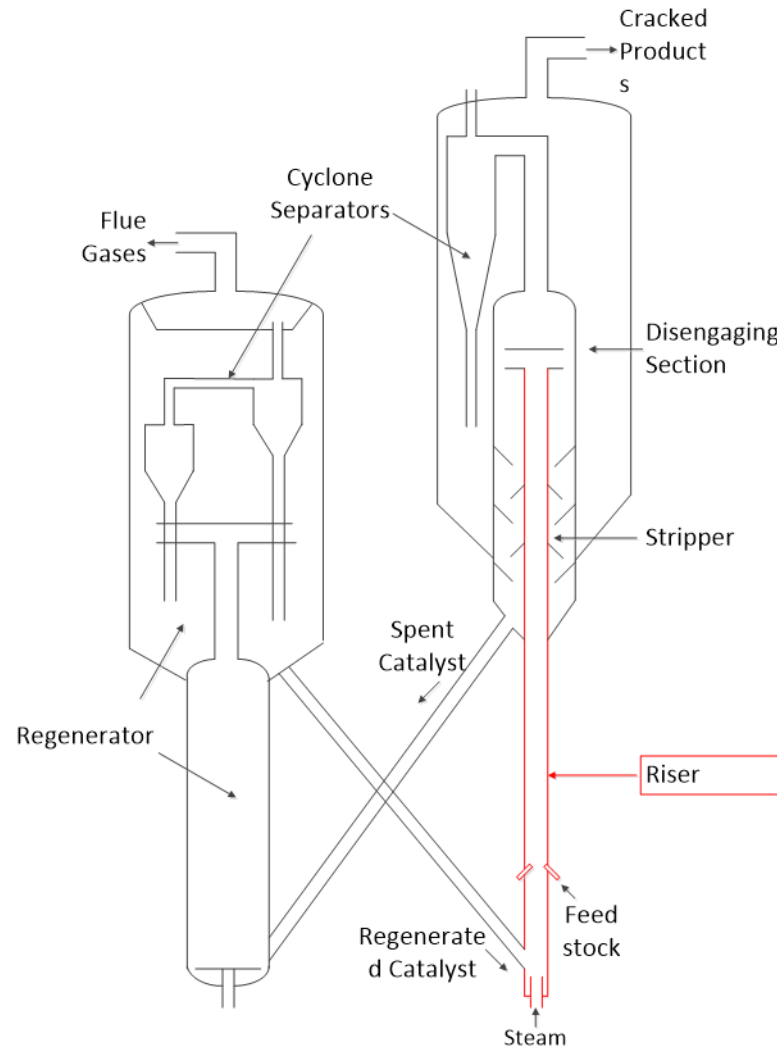
Example: multi-physics simulations of e-Reactor



100 tubes e-Reactor, size = 1 x 1 m², capacity = 40 kg H₂/day, Kanthal (FeCrAl) tubes, copper bracket, electrical and thermal insulation, 7.5-volt potential, 3451 Amp current, total energy to be supplied = 25.88 kW + 226.2 W/m²

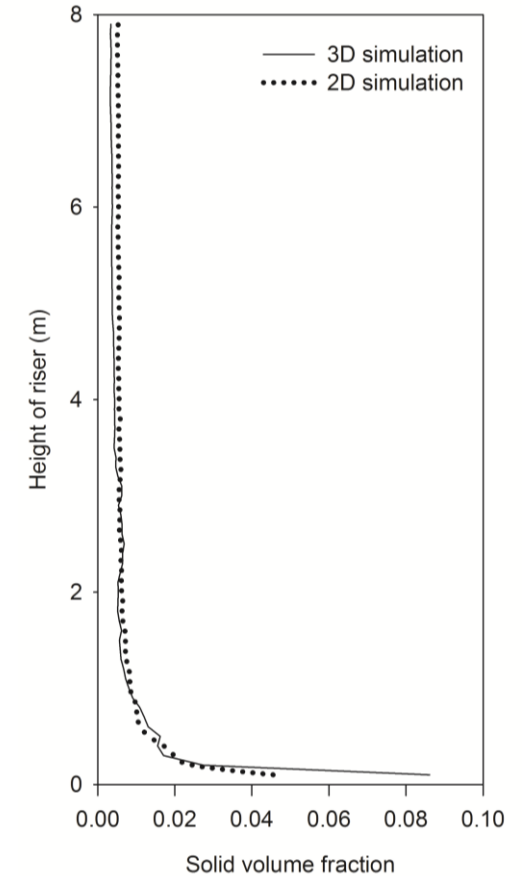
Efficiency = 98%

Example: multi-scale simulations of riser

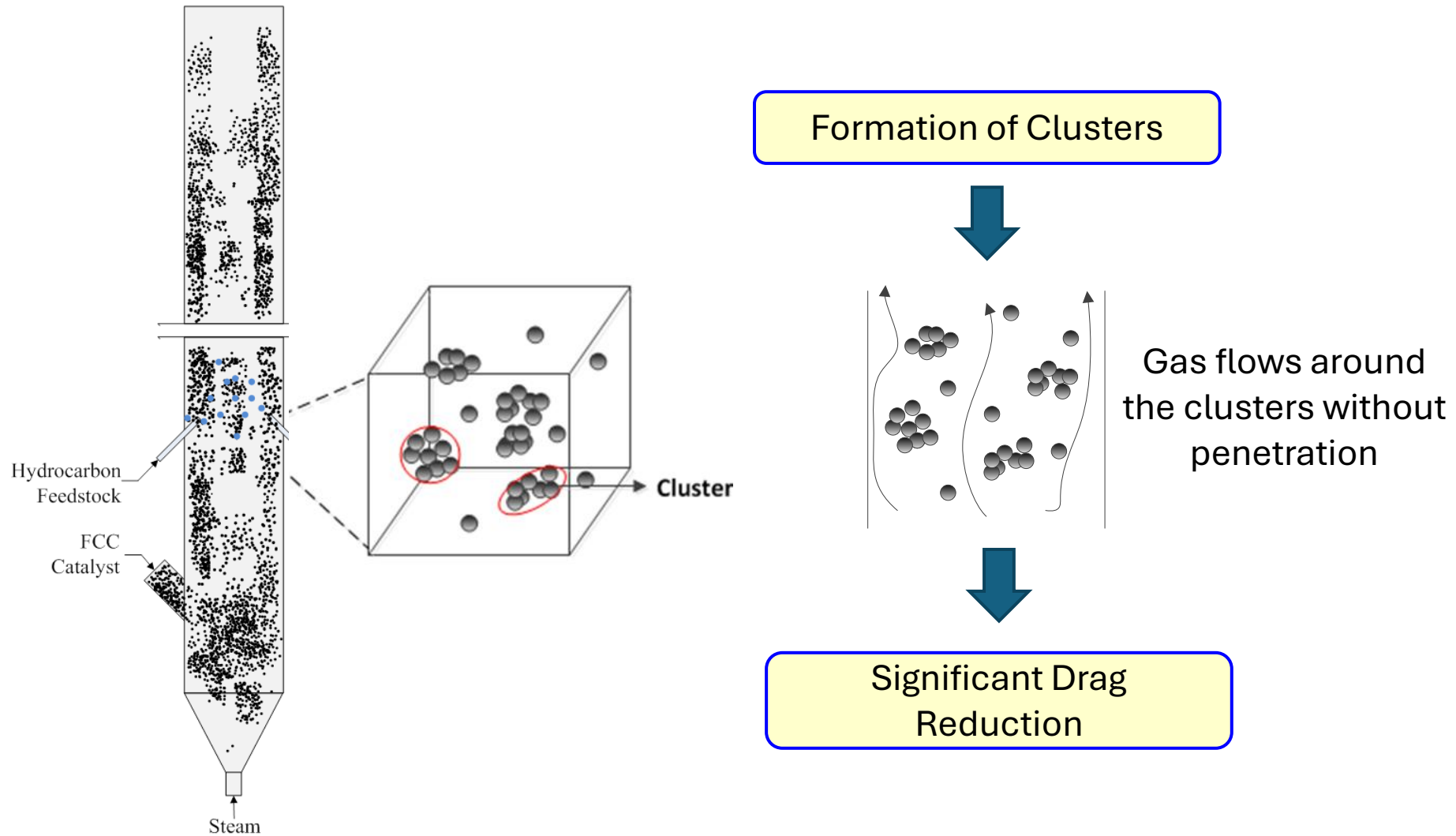


2D, 3D, coarse grid, or fine grid CFD simulations of riser could predict radial profile, but not the s-shape axial profile.

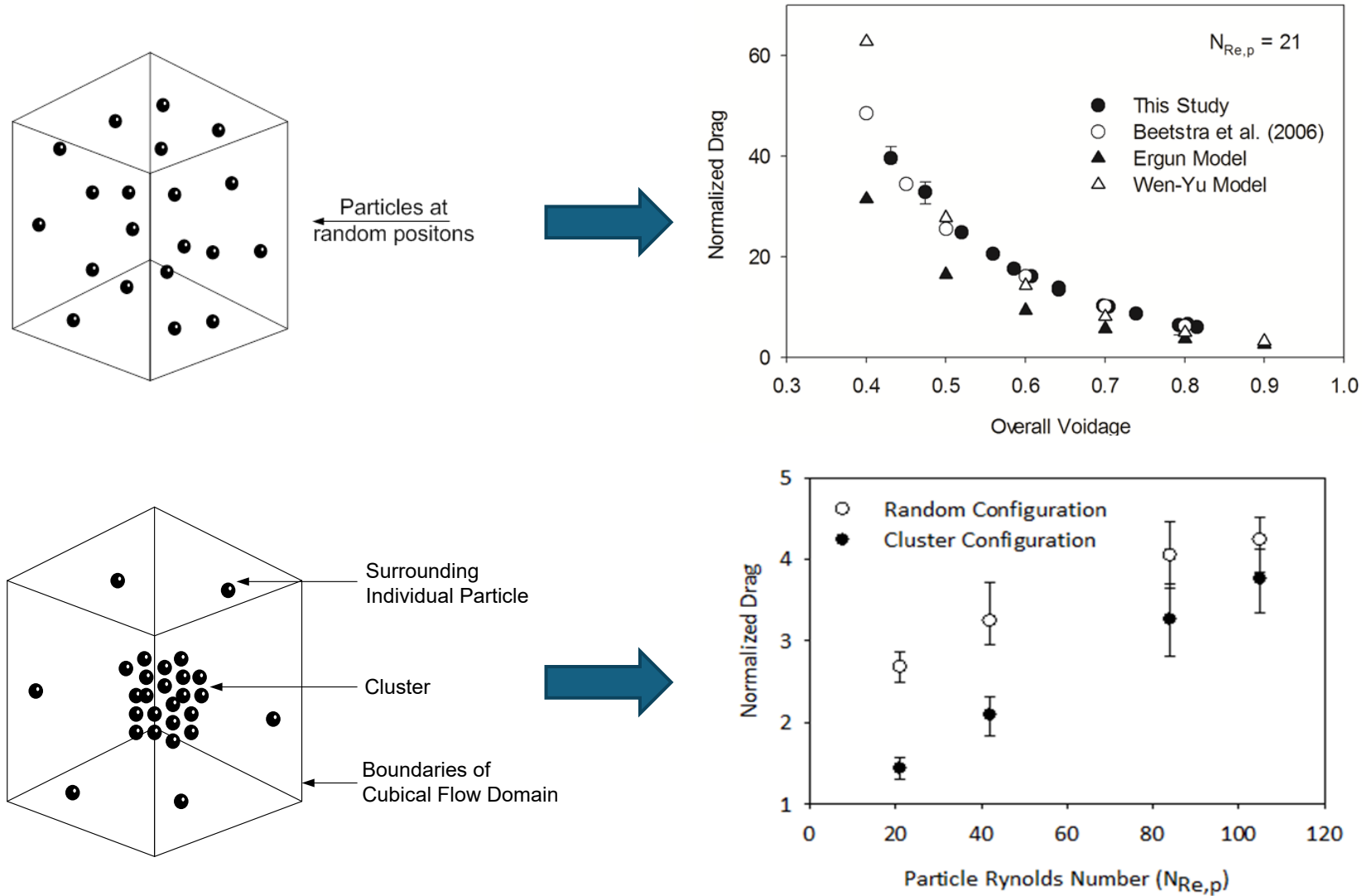
Why?



Example: multi-scale simulations of riser

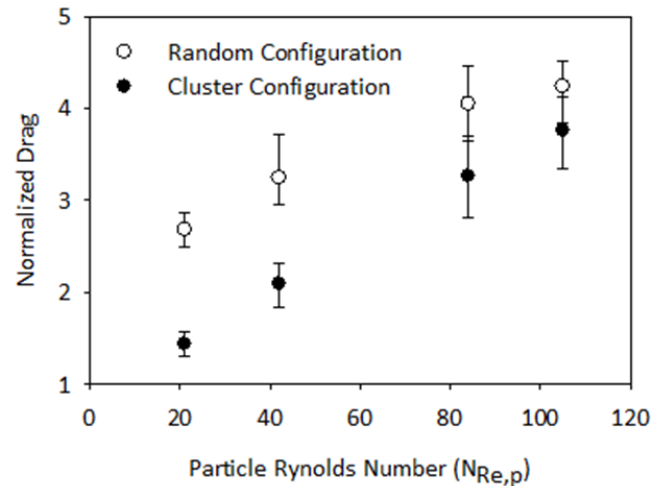
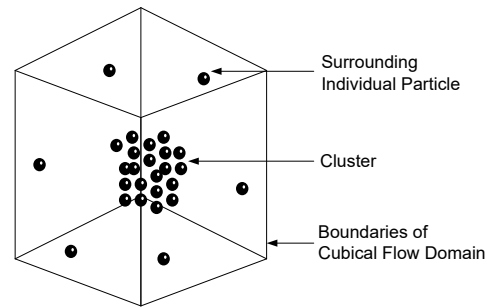


Example: multi-scale simulations of riser



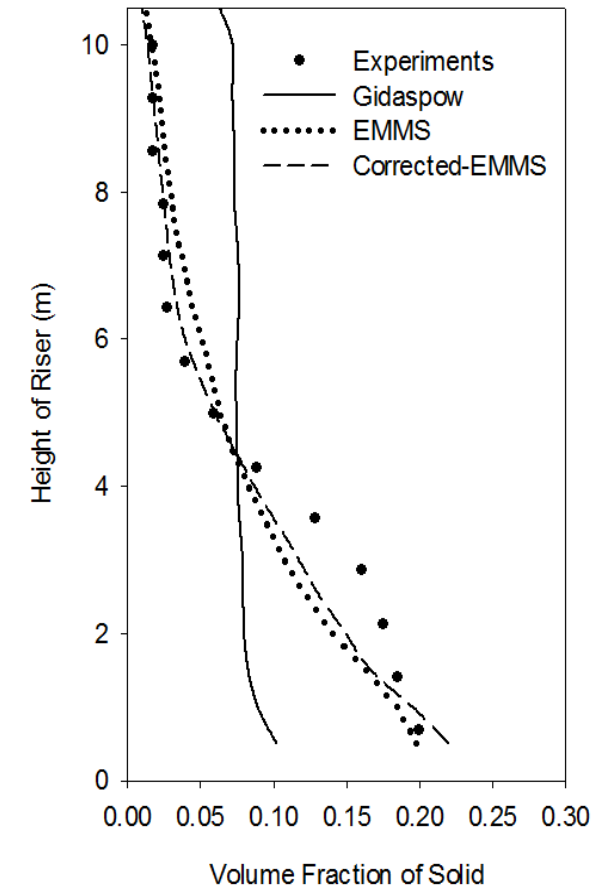
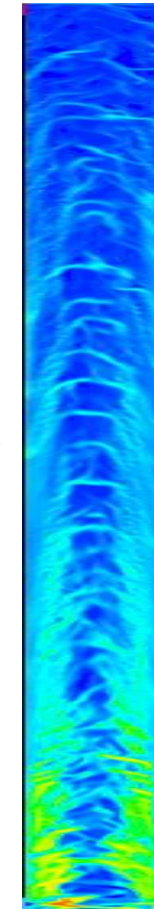
Example: multi-scale simulations of riser

DNS: direct numerical simulations



Drag model for dilute gas-solid flow of fine powder

Industrial-scale FCC riser



Multi-scale approach: Meso scale is analysed first using DNS and information from meso-scale simulation is passed to the larger scale simulations.

Summary

Background: Euler equations, Navier-Stokes equations, Reynolds number equation, Boundary layer theory by Prandtl (1904), Solution of simple flow systems

CFD as a distinct discipline: Finite volume method, First CFD codes applied by NASA and academic institutions (may be in aerodynamics)

High Performance Computing, DNS and LES at moderate Reynolds number, Multi-physics and multi-scale simulations

Late 19th
and early
20th
Century

Mid 20th
Century

1960s-
1970s

1980s –
1990s

2000
onwards

Birth of CFD: Finite difference methods for solving PDEs

Birth of commercial CFD codes (Fluent, CFX, STAR-CD, COMSOL)

case studies
presented
here

- Real time simulations
- Cloud-based CFD
- AI/ML based solver acceleration