EPIC
Enabling Process Innovation through Computation

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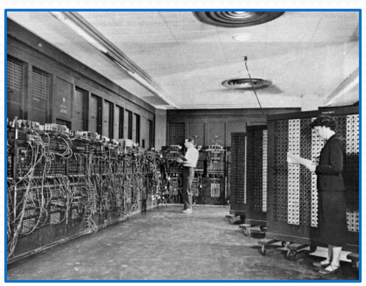
Technology as a transformative agent

Automotive

Aeronautical



ICT

Achieved through sustained, incremental improvement, rapid innovation cycle, use of advanced development tools.

Not so in Chemical Processes – why?

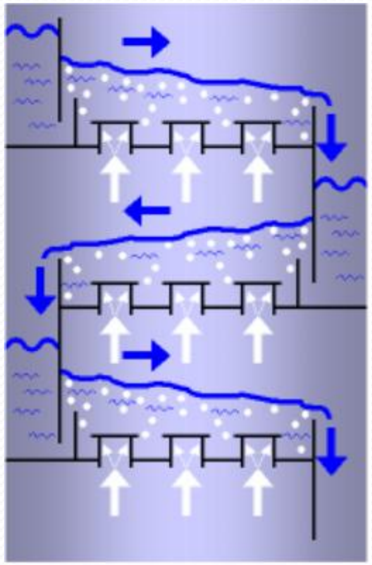
Certainly innovation has helped in mass producing chemicals, fertilizers, and pharmaceuticals, pesticides etc.

But sustained improvements in technology have been very slow – why?

The challenges are indeed greater!

1940

2000

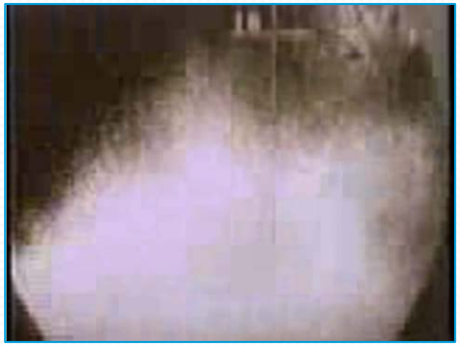


Two phase vapor-liquid contact device

Examples - Tray hydraulics on sieve tray

Films courtesy of FRI Inc.


Weeping

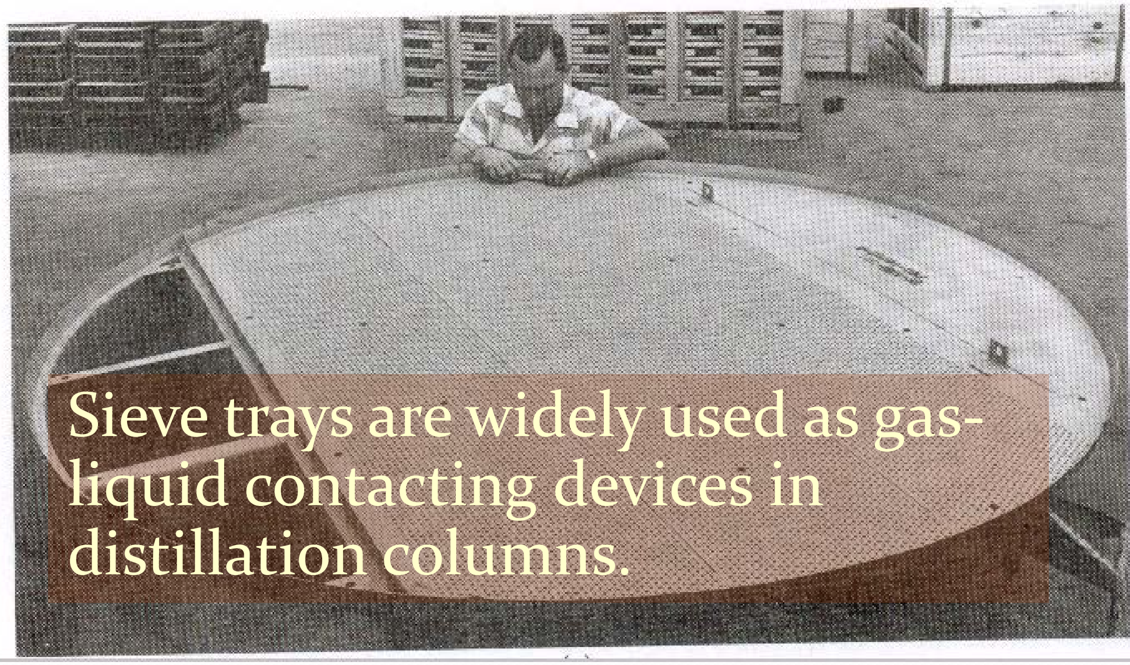

Froth


Spray

Increasing vapor flow rate

Enabling Process Innovation through Computation

Examples - Tray hydraulics on sieve tray



$$\left.\begin{aligned}&\rho_L \frac{d\mathbf{u}}{dt} = \rho_L \mathbf{g} + \nabla \bullet \boldsymbol{\sigma}\\ &\nabla \bullet \mathbf{u} = 0\end{aligned}\right\} in \quad \Omega \setminus \bar{P}(t)$$

The NSE is valid in all these scales, but can we compute such complex multiphase flows?

Modeling at appropriate scale - Hierarchy of models

Overview of interrelations among models on various scales

Pilot scale Experiments → Lumped, homogeneous, input/output models; Equipment scale (ASPEN/HYSYS) → Process Perofrmance

$$\sum m_i = 0$$

Lab Experiments → Tray efficiency | overall heat/mass transfer

Volume averaged equations: Eulerian-Eulerian models
Time averaged equations: Turbulence models
Eulerian-Lagrangian models: Discrete Particle Models
Interpenetrating continuua scale (FLUENT/MFiX)

Lab Experiments → Drage/lift forces | Interface heat/mass transfer

Stoksian Dynamics, Macro Particle Direct Numerical Simulation

Navier-Stokes equation
Continuum scale (FLUENT/OpenFOAM/MFiX)

$$\rho \frac{\mathfrak{D}v}{\mathfrak{D}t} = -\nabla p + \rho g + \mu \nabla v^2;$$

Lab Experiments → Material Properties | viscosity, density, surface tension

MD simulation
Molecular scale (GROMACS)

$$m\frac{du}{dt} = \sum F$$

Lab Experiments → Intermolecular Interaction potential

Direct Numerical Simulations

Rigid particles in a Newtonian fluid

Fluid

$$\left.\begin{aligned}\rho_L \frac{d\mathbf{u}}{dt} &= \rho_L \mathbf{g} + \nabla \bullet \boldsymbol{\sigma} \\ \nabla \bullet \mathbf{u} &= 0\end{aligned}\right\} in \quad \Omega \setminus \overline{P}(t)$$

$$IC: \ \mathbf{u}\big|_{t=0} = \mathbf{u}_0 \quad in \quad \Omega \setminus \overline{P}(0)$$

$$BC: \quad \mathbf{u} = \mathbf{u}_\Gamma(t) \quad on \quad \Gamma$$

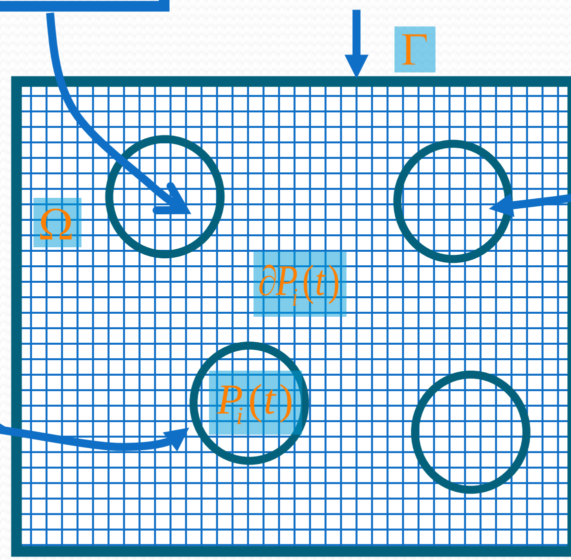
Solid

$$\left.\begin{aligned} M_i \frac{d\mathbf{U}_i}{dt} &= M_i \mathbf{g} + \mathbf{F}_i \\ I_i \frac{d\varpi_i}{dt} + \varpi_i \times I_i \varpi_i &= \mathbf{T}_i \end{aligned}\right\} \quad in \quad \overline{P}(t)$$

$$\frac{d\mathbf{X}_i}{dt} = \mathbf{U}_i$$

$$\frac{d\theta_i}{dt} = \varpi_i$$

$$IC: \ X_i\big|_{t=0} = X_{i,o}; \ \theta_i\big|_{t=0} = \theta_{i,o}$$



Coupling

$$\mathbf{u} = \mathbf{U}_i + \varpi_i \times \mathbf{r}_i \quad on \quad \partial P_i(t), i = 1..N$$

$$\mathbf{F}_i = \int_{\partial P_i(t)} \boldsymbol{\sigma} \cdot \mathbf{n}\, dS;$$

$$\mathbf{T}_i = \int_{\partial P_i(t)} \mathbf{r}_i \times \boldsymbol{\sigma} \cdot \mathbf{n}\, dS$$

C. Veeramani, P. D. Minev and K. Nandakumar, A Fictitious Domain Formulation for Flows with Rigid Particles: A non-Lagrange multiplier version, *J. Comp. Physics* **224**(2) *(2007)*, 867-879.

Direct Numerical Simulations – DNS-LS

Deformable droplets/bubbles (Newtonian fluid)

Fluid 1

$$\left.\begin{aligned} \frac{D\mathbf{u}_1}{Dt} &= \mathbf{f}_1 + \nabla \bullet \boldsymbol{\sigma}_1 \\ \nabla \bullet \mathbf{u}_1 &= 0 \end{aligned}\right\} in \quad \Omega_1$$

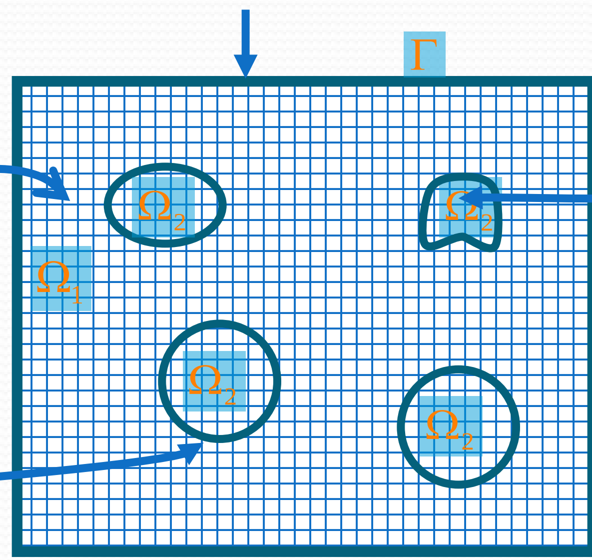
$$\boldsymbol{\sigma}_i = p_i \boldsymbol{\delta} + 2/\mathrm{Re}_i\, \mathbf{D}[\mathbf{u}_i]$$

$$\mathbf{D}[\mathbf{u}_i] = 0.5[\nabla \mathbf{u}_i + (\nabla \mathbf{u}_i)^T]$$

$$BC: \ \mathbf{u}_1 = \mathbf{u}_{1,\Gamma}(t) \ \ on \ \ \Gamma$$

Fluid 2

$$\left.\begin{aligned} \lambda \frac{D\mathbf{u}_2}{Dt} &= \mathbf{f}_2 + \nabla \bullet \boldsymbol{\sigma}_2 \\ \nabla \bullet \mathbf{u}_2 &= 0 \end{aligned}\right\} in \quad \Omega_2$$



Coupling

$$(\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2) \cdot \mathbf{n} = \frac{1}{We} \kappa \mathbf{n}, \quad \mathbf{u}_1 = \mathbf{u}_2 \quad on \ \ \Sigma$$

$$\frac{\partial \Sigma}{\partial t} + (\mathbf{u} \bullet \nabla)\Sigma = 0$$

$$Re_1 = \frac{\mathrm{U} R \rho_1}{\mu_1}$$
$$Re_2 = \frac{\mathrm{U} R \rho_1}{\mu_2} = \eta Re_1$$
$$We = \mathrm{U} R \rho_1 / \sigma$$
$$\lambda = \rho_1 / \rho_2$$

Chen, T., P. D. Minev and K. Nandakumar, A projection scheme for incompressible multiphase flow using adaptive Eulerian grid: 3D validation, *Int. J. Numerical Methods in Engineering* **48** (2005) pp 455-466

Two-fluid models

Continuity

$$\frac{\partial}{\partial t}(\gamma_\alpha \rho_\alpha) + \nabla \cdot (\gamma_\alpha \rho_\alpha \mathbf{U}_\alpha - \Gamma_\alpha \nabla \gamma_\alpha) = 0 \qquad \alpha = L,\ \mathrm{G}$$

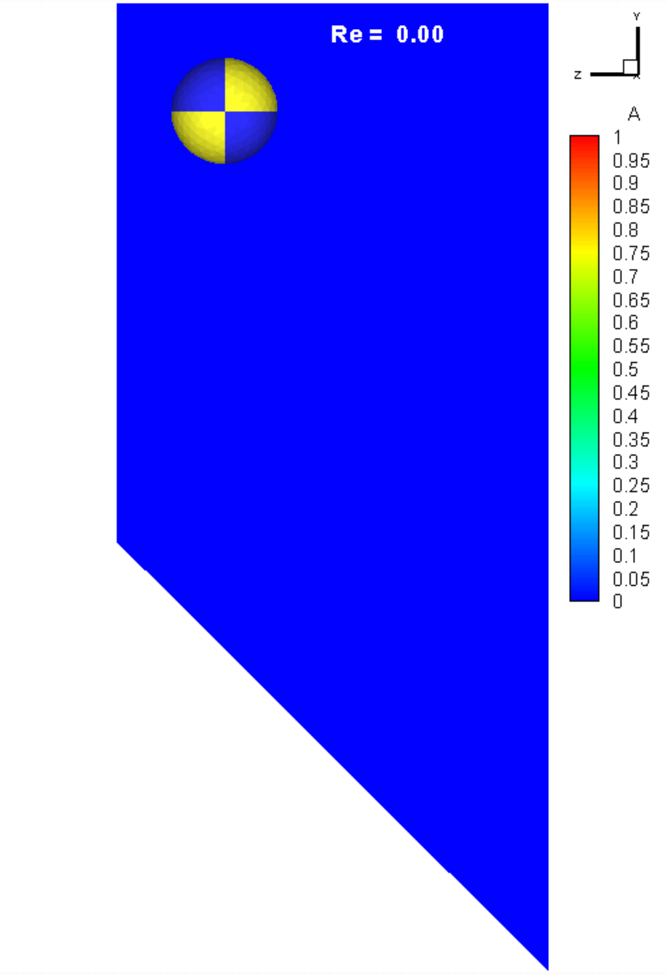
Momentum

$$\frac{\partial}{\partial t}(\gamma_\alpha \rho_\alpha \mathbf{U}_\alpha) + \nabla \cdot \left\{ \gamma_\alpha \left[\rho_\alpha \mathbf{U}_\alpha \otimes \mathbf{U}_\alpha - \mu_{e\alpha} \left(\nabla \mathbf{U}_\alpha + (\nabla \mathbf{U}_\alpha)^T \right) \right] \right\} = \gamma_\alpha (\mathbf{B}_\alpha - \nabla p) + \mathbf{F}_\alpha \qquad \alpha = L,\ \mathrm{G}$$

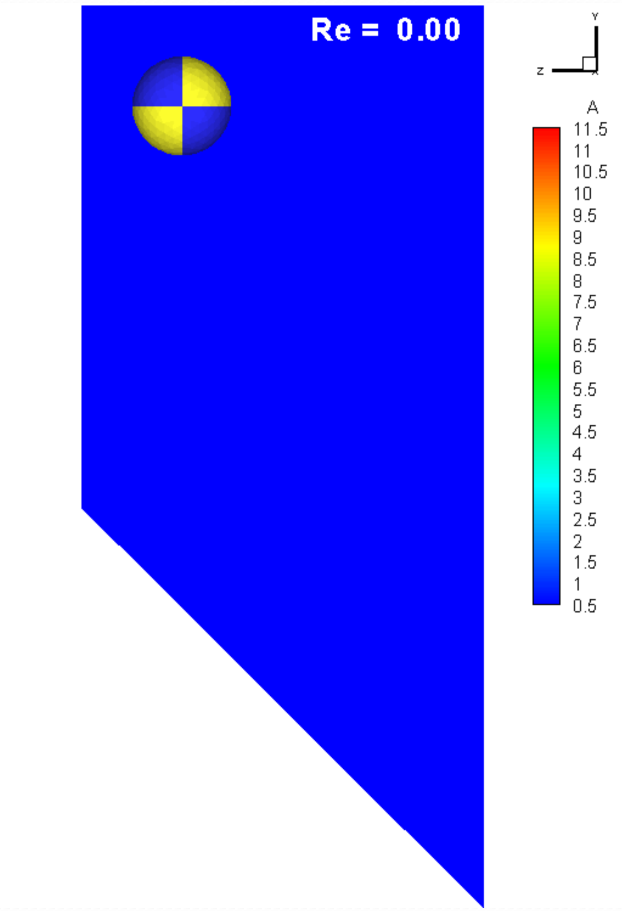
Species conservation

$$\frac{\partial}{\partial t}(\gamma_\alpha \rho_\alpha Y_{i\alpha}) + \nabla \cdot \left[\gamma_\alpha \left(\rho_\alpha \mathbf{U}_\alpha Y_{i\alpha} - \Gamma_{i\alpha} \nabla Y_{i\alpha} \right) \right] = \sum_{\beta=1,\ \beta\neq\alpha}^{N} \dot{m}^i_{\alpha\beta} \qquad \alpha = L,\ \mathrm{G} \qquad i = 1, \cdots\cdots, N_C$$

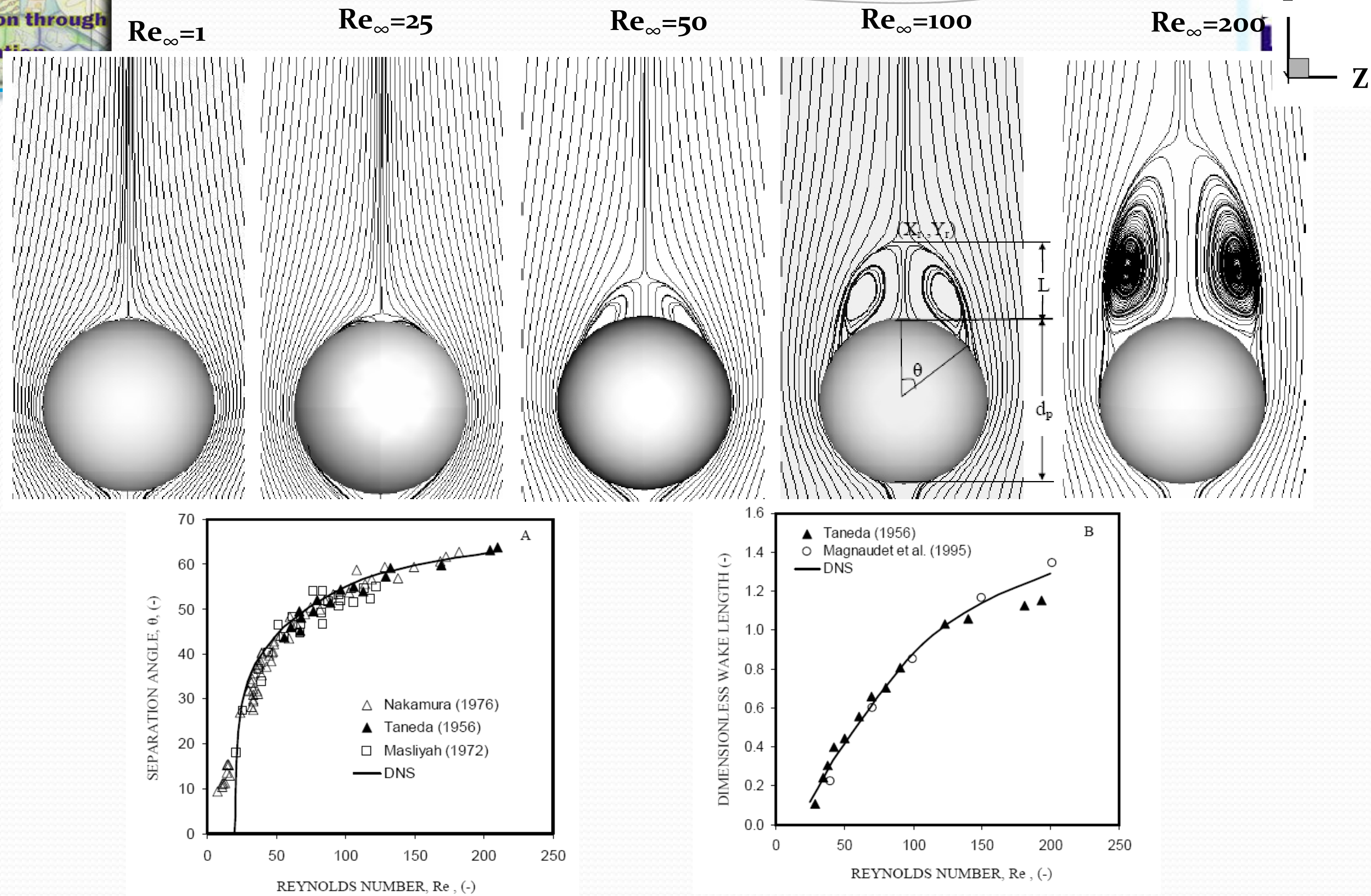
Impact on an inclined wall – pvc ball



Impact on an inclined wall – steel ball

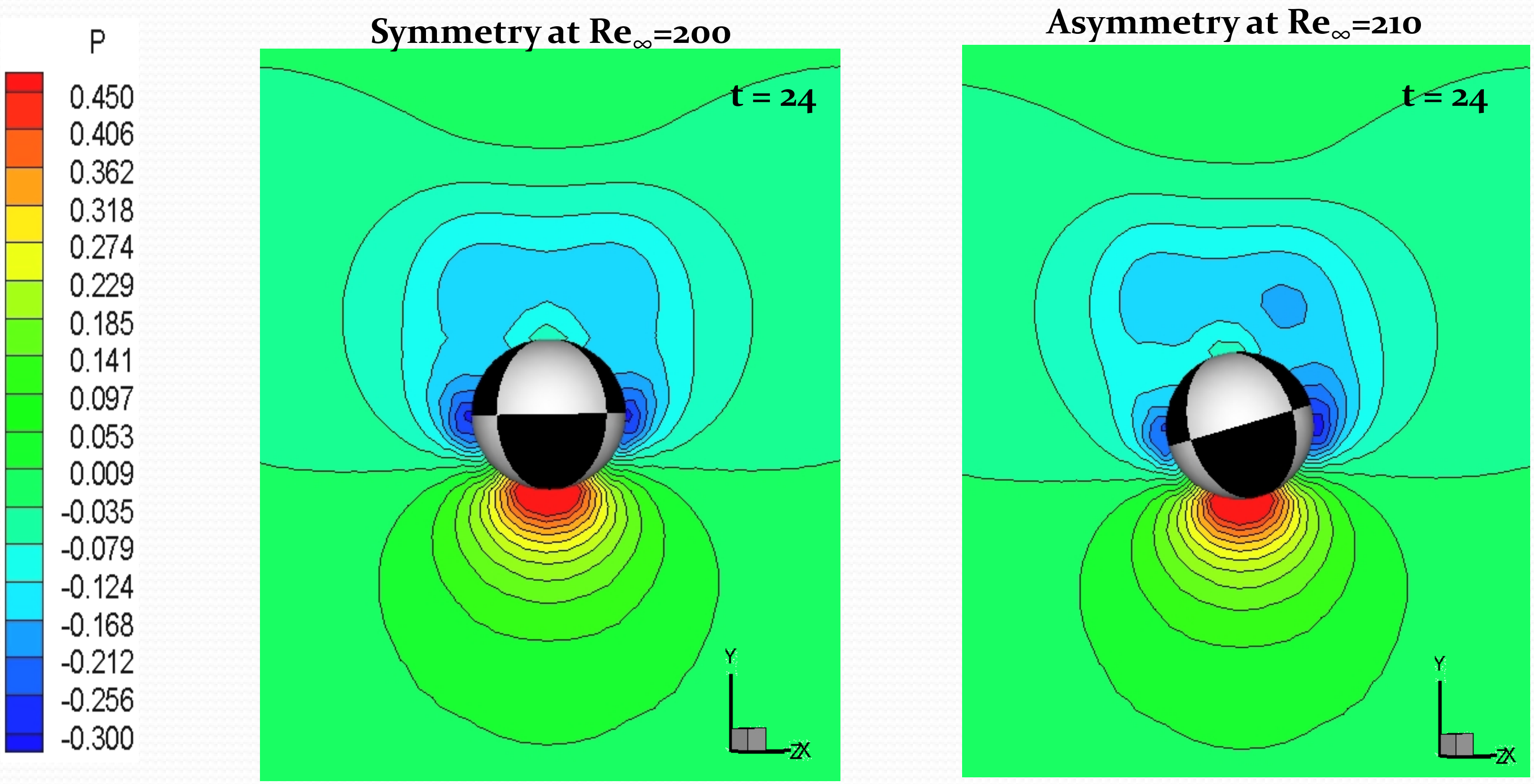


Wake length and separation angle



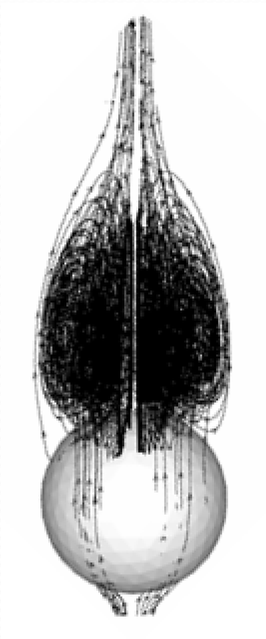
Breaking of axisymmetry at Re_∞ = 210

Contours of pressure



The onset of instability leads to the beginning of the rotation of the sphere and the lift force, which occurs due to breakage of steady axisymmetric wake

Comparison with experimental observations

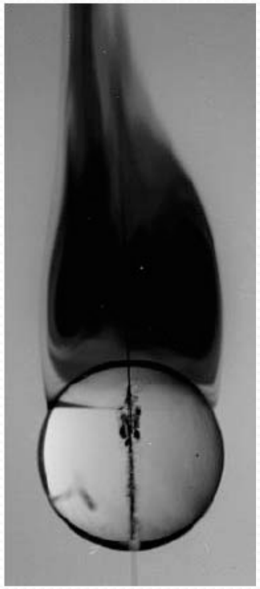


DNS

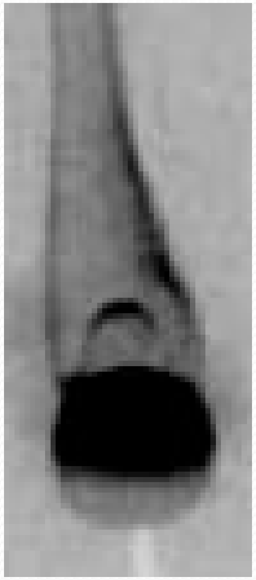
Magarvey and MacLatchy (1965)

Johnson and Patel (1999)

DNS



Johnson and Patel (1999)



Schouveiler and Provansal (2002)

Experimental results of Lee et al. (2007) in Journal of fluid Mechanics

Diameter of the particle is **3.1 mm**.

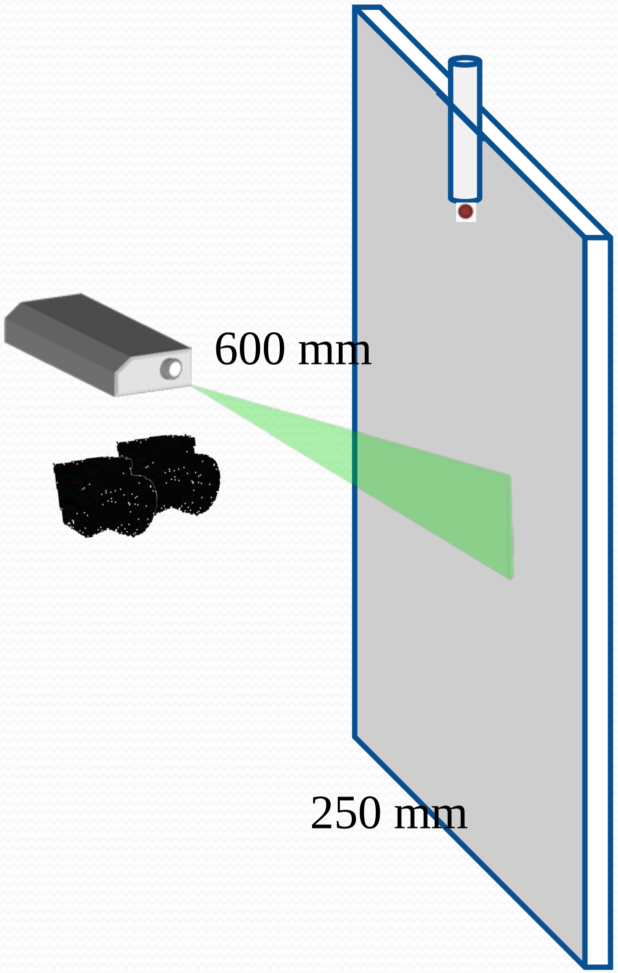
Density if the particles are **2500 and 3070 kg /m^3**

Range of Reynolds number ($d_p\ V_{s\infty}\ \rho_L / \mu_L$) is from **43.5 to 375.**

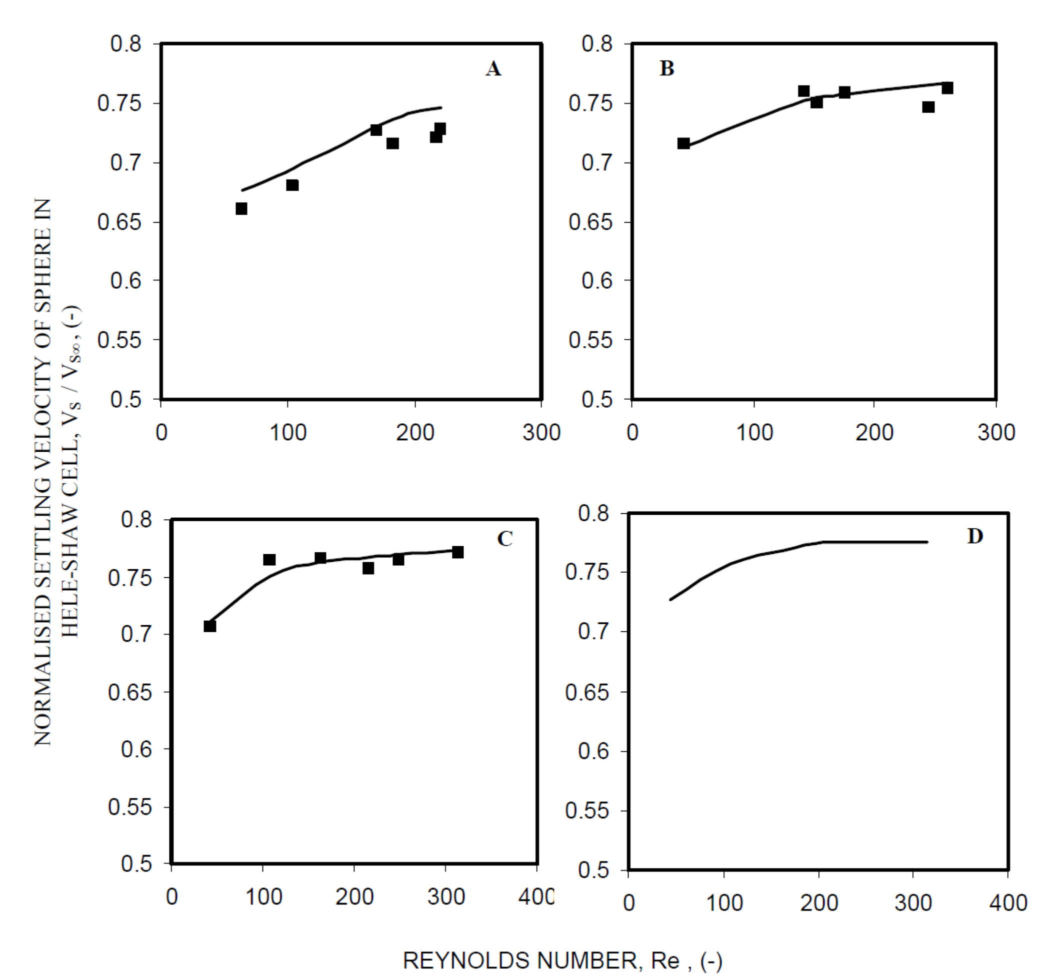
The desired range of Reynolds number was achieved using dense aqueous solutions of an inert salt, sodium metatungstate

Experimental set up is 600 mm height and 250 mm wide

The gap between the parallel plates varied from **1.014 d$_p$ to 1.4d$_p$** (3.1 mm to 4.34 mm)



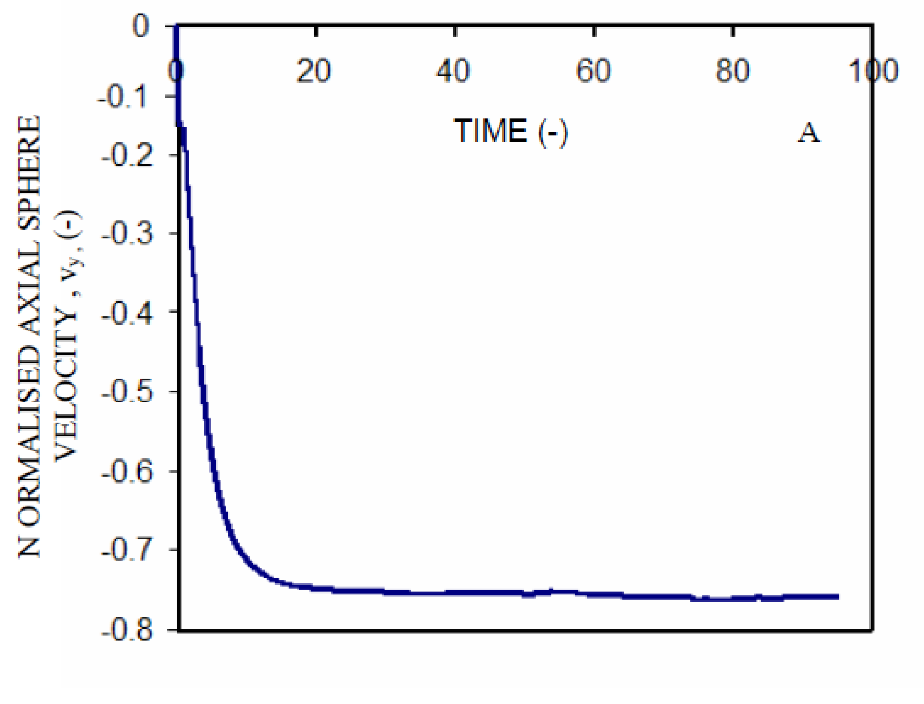
Comparison of the simulated settling velocity of sphere with experimental results



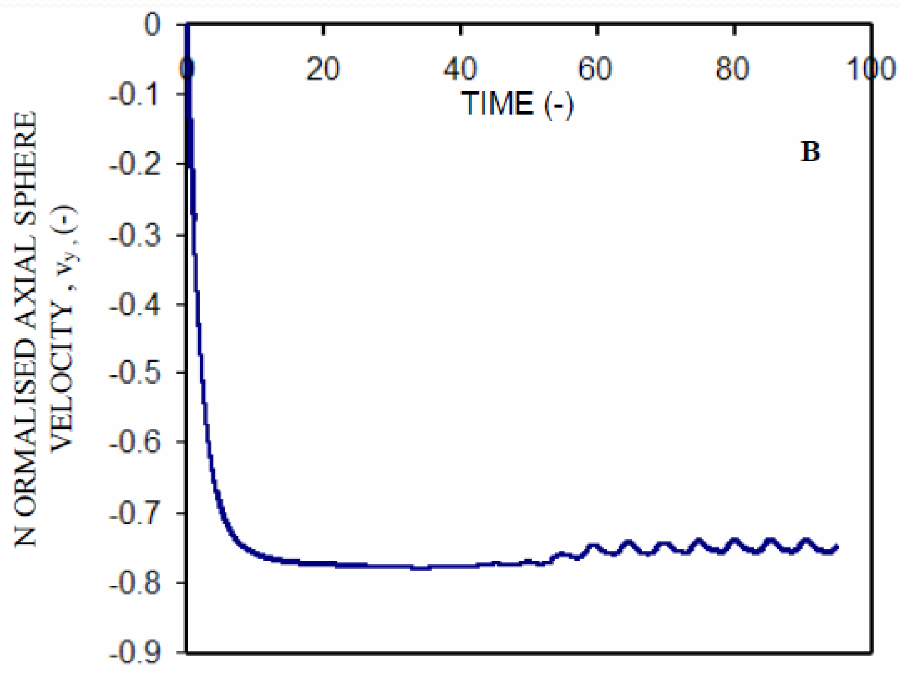
(A) gap of 1.2 d_p
(B) gap of 1.3 d_p
(C) gap of 1.4 d_p
(D) gap of 1.5 d_p;
, DNS;
■, Lee et al. (2007)

Axial velocities (V_y) of the freely falling sphere with respect to time at the gap of 1.4 d_p

Re = 108



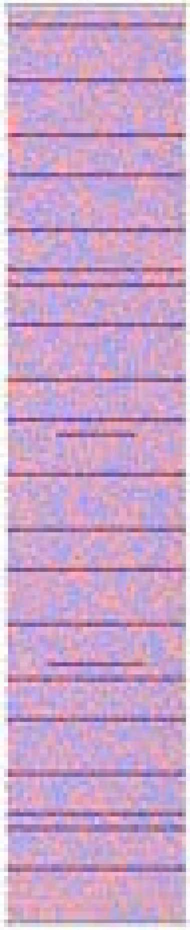
Re = 163



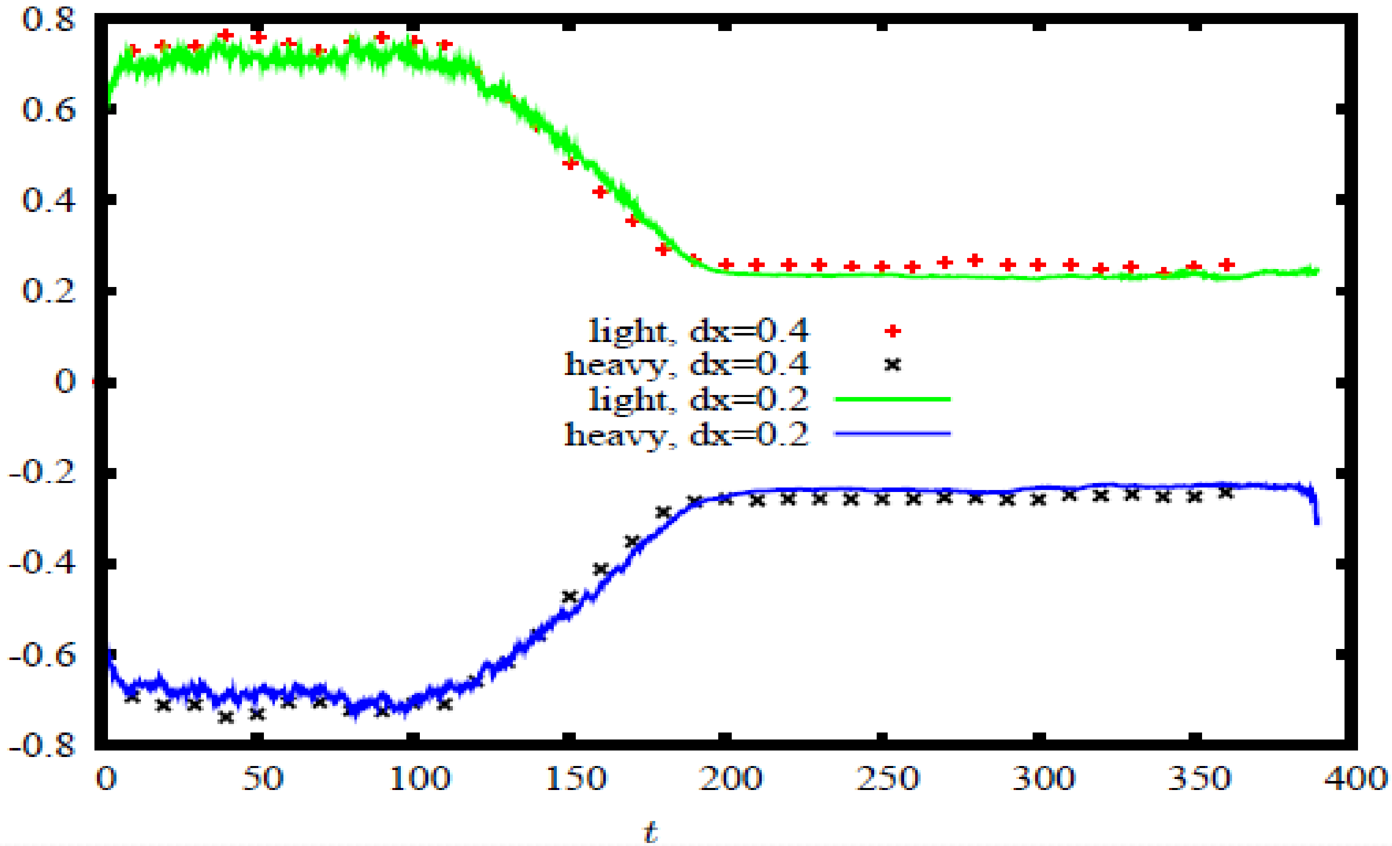
Comparison of the computed results with experimental results of Lee et al. (2007)

S.No.	d_p (mm)	P_L kg m^{-3}	P_p kg m^{-3}	Viscosity kg m^{-1} s^{-1}	$V_{S\infty}$ (m s^{-1})	Re_∞	Velocity of the particle in the presence of the walls (m s^{-1})		Experiment St_Y	DNS St_Y	Experiment St_Z	DNS St_Z
							Experiment	DNS				
1	**3.175**	**2523**	**2418**	**0.0059**	**0.0334**	**43.5**	**0.0236**	**0.0228**	**-**	**-**	**-**	**-**
2	**3.175**	**2523**	**2282**	**0.0045**	**0.0663**	**108**	**0.0507**	**0.0505**	**-**	**-**	**-**	**-**
3	**3.175**	**2523**	**2190**	**0.0037**	**0.0870**	**163**	**0.0667**	**0.0672**	**0.225**	**0.241**	**0.112**	**0.063**
4	**3.175**	**2523**	**2128**	**0.0032**	**0.1014**	**215**	**0.0768**	**0.0805**	**0.222**	**0.243**	**0.111**	**0.06**
5	**3.175**	**2523**	**2070**	**0.0030**	**0.1130**	**249**	**0.0864**	**0.089**	**0.222**	**0.249**	**0.111**	**0.075**
6	**3.175**	**2523**	**1993**	**0.0026**	**0.1293**	**314**	**0.0997**	**0.1025**	**0.113**	**0.252**	**0.113**	**0.078**
Different density of sphere												
8	**3.175**	**3073**	**2282**	**0.0045**	**0.1400**	**227**	**0.109**	**0.1036**	**0.214**	**0.231**	**0.107**	**0.063**
9	**3.175**	**3073**	**2190**	**0.0037**	**0.1577**	**295**	**0.1225**	**0.1297**	**0.109**	**0.123**	**0.109**	**0.069**
10	**3.175**	**3073**	**2128**	**0.0032**	**0.1707**	**362**	**0.1323**	**0.141**	**0.109**	**0.126**	**0.110**	**0.072**

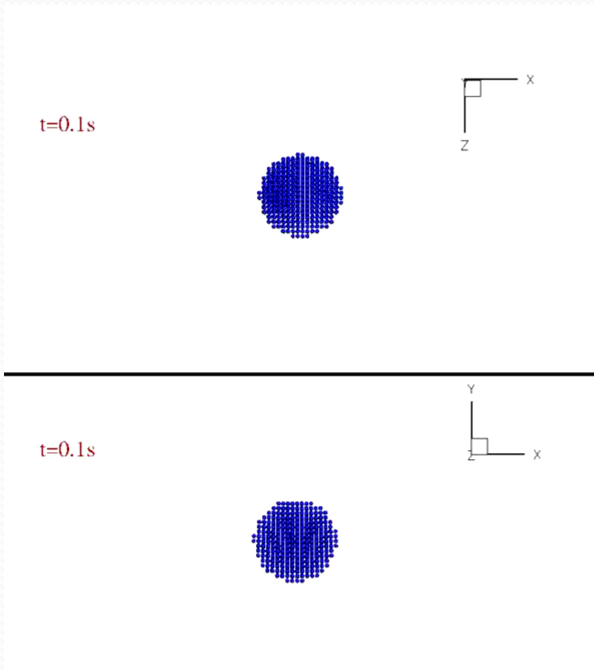
21336 particles - bidisperse



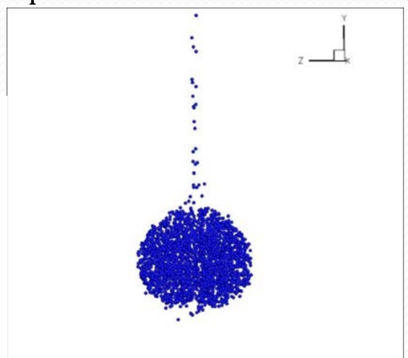
Average settling velocity of suspension

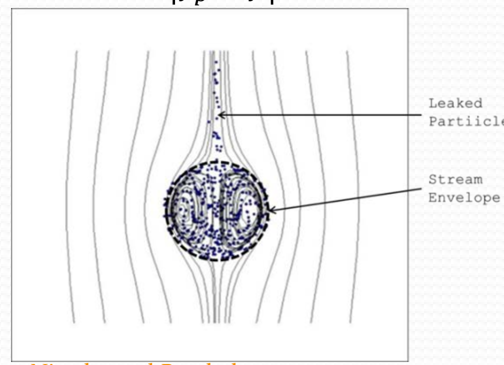


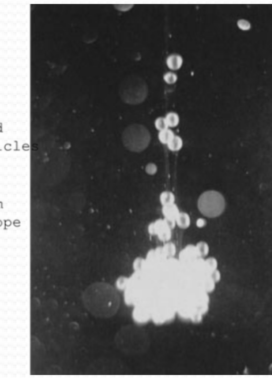
Particle Leakage At low Re_c



Leaked particle must subscribe to this criterion $|y_p - \bar{y}| > 1.2R$



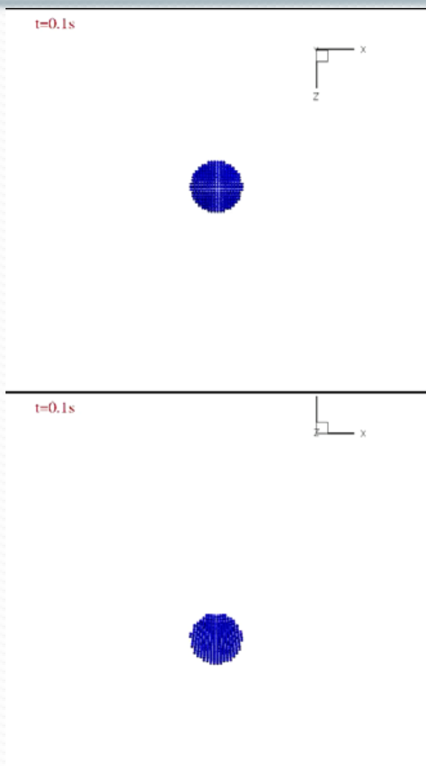


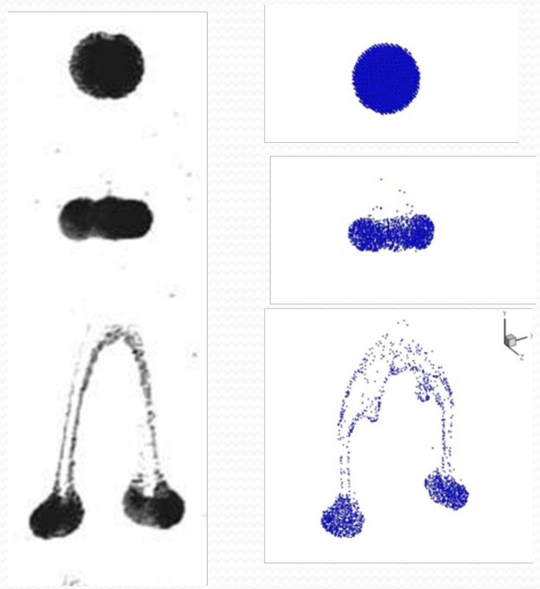


Nitsche and Batchelor 1997

- ❑ Particle Cross Boundaries of blob due to Hydrodynamic interactions
- ❑ Conveyed to rear by background streamlines
- ❑ Slower than Aggregate

Break-up At Moderate Re_c



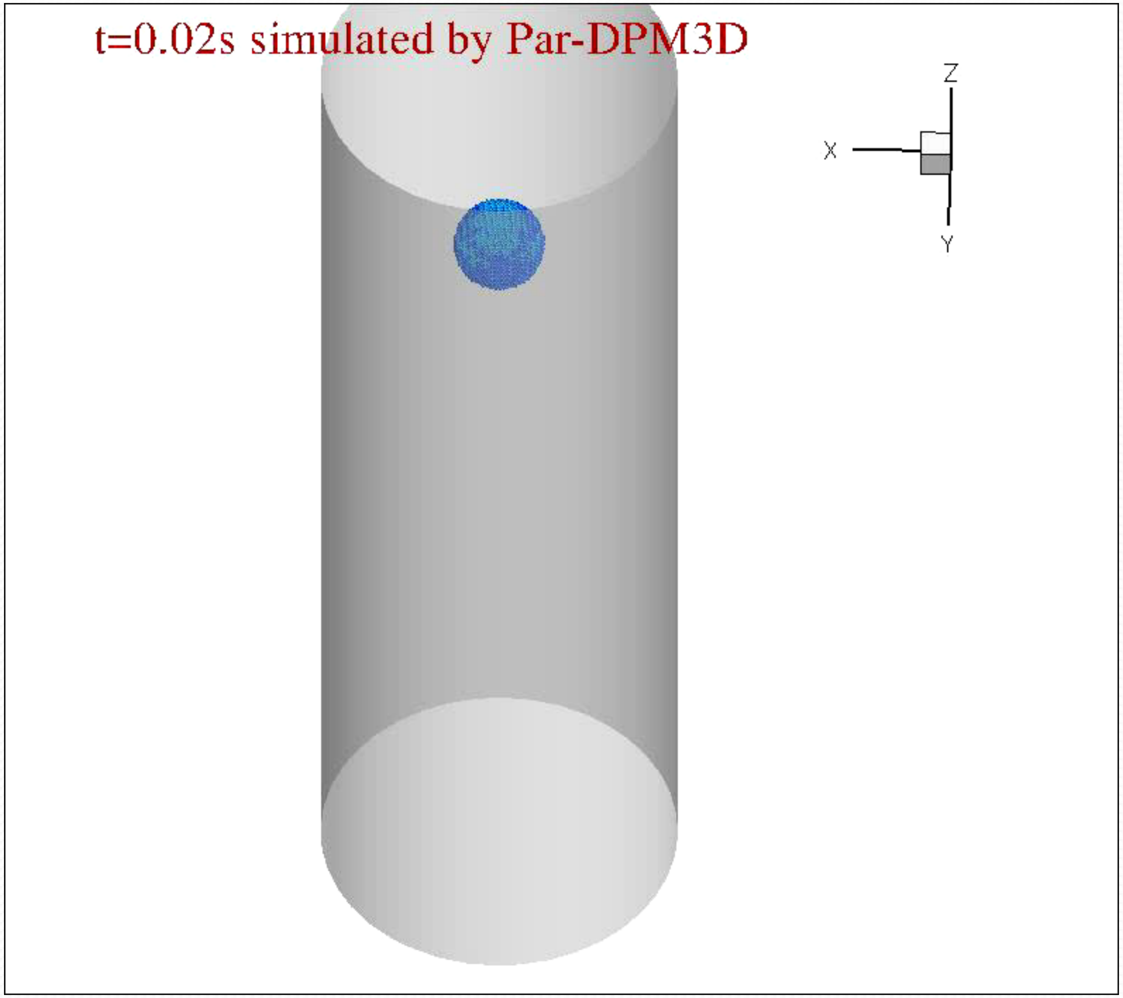


Qualitative comparison with Experiments of
Machu, Meile et al. 2001

- Leakage is reduced
- Torus is intermediate shape of Blob
- Torus is an unstable structure

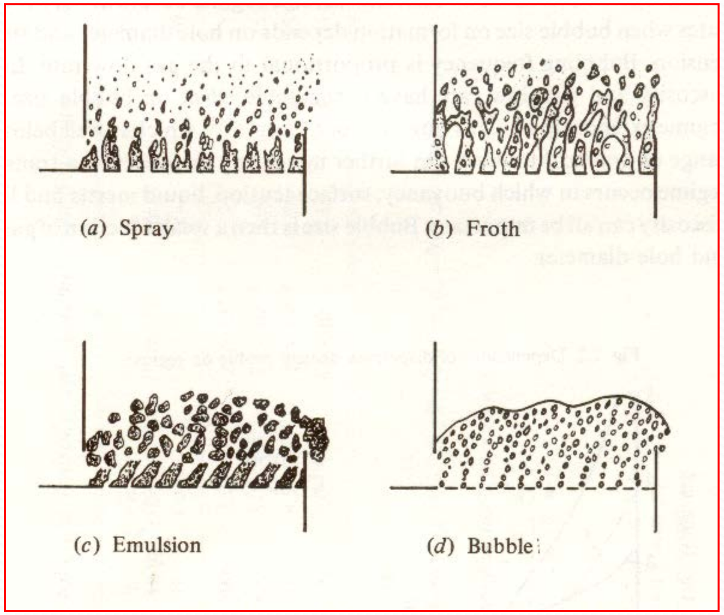
- Number of Secondary Drops??

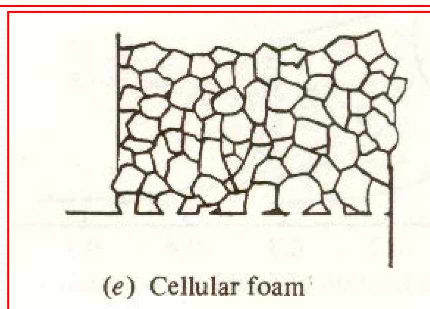
Cloud of settling suspension
Medium fidelity simulation - DPM

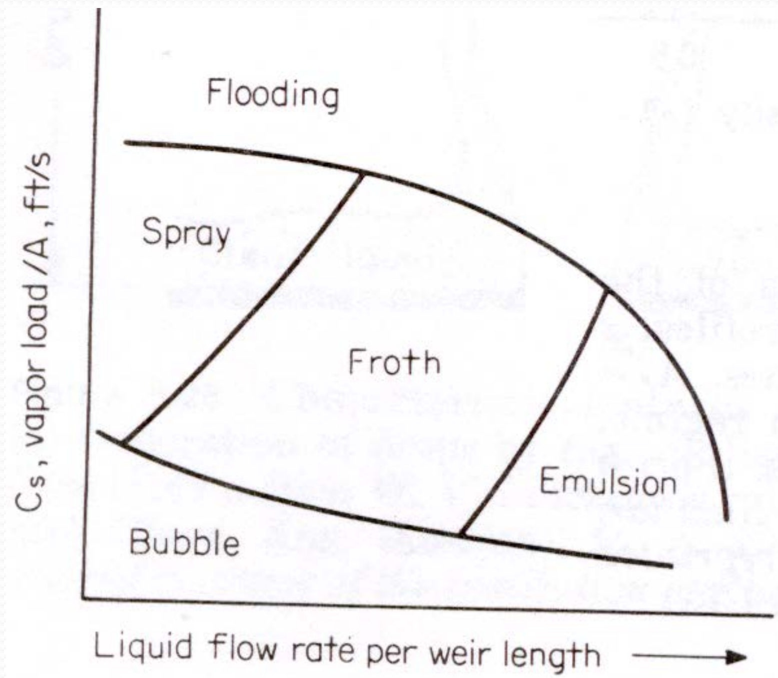


Tray hydraulics on sieve tray

Flow Regimes on Sieve Trays







Divide and conquer
G. K. Batchelor

Graphical method of McCabe-Thiele

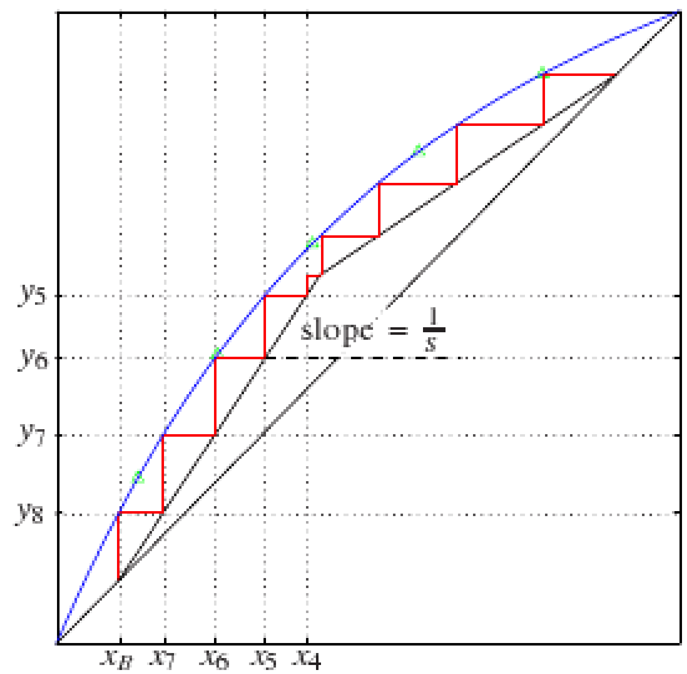
http://en.wikipedia.org/wiki/McCabe%E2%80%93Thiele_method

The **McCabe-Thiele method** was presented by two graduate students at Massachusetts Institute of Technology (MIT), Warren L. McCabe and Ernest W. Thiele in 1925.

Assumptions:

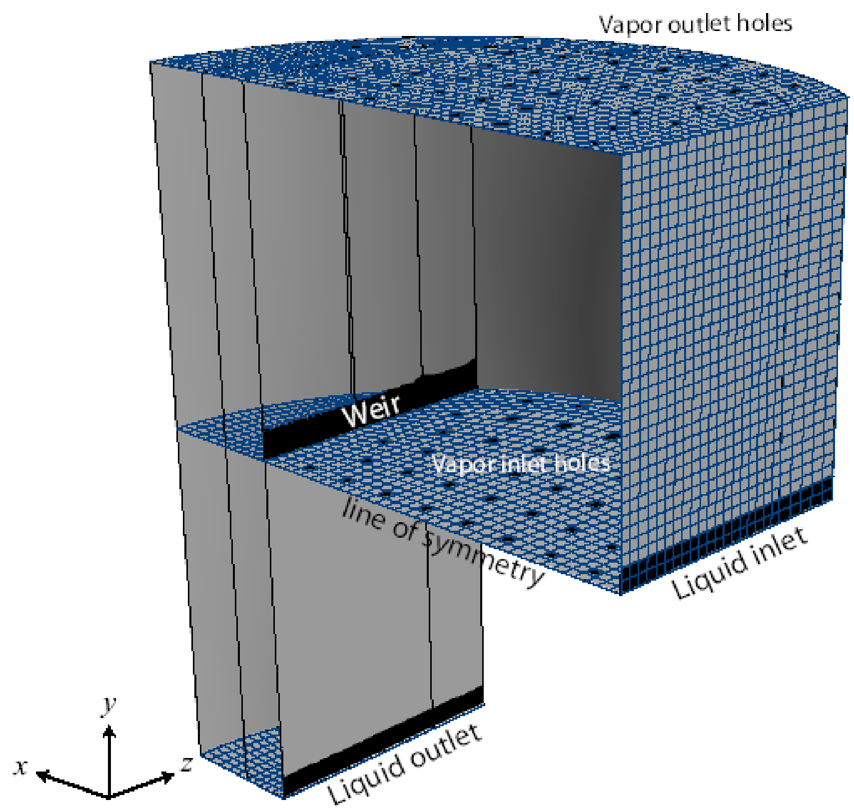
Constant molar over flow – makes the operating line a straight line? Is that always true or needed in the age of computers? NO! ASPEN/HYSYS in fact removes this assumption

Well mixed stage. Composition is uniform in a tray? Is that true or needed in the age of computers? NO! Advanced CFD modeling can remove that! [That should be the focus of our collective efforts]



$$y_i = x_0 \frac{1}{1+R} + x_{i-1} \frac{R}{1+R}, \qquad i \in [1, n]$$

Tray hydraulics on sieve tray - TFM



Getye Gesit, K. Nandakumar and Karl T. Chuang*AIChEJ*. **49** (2003) pp 910-924.

Closures for Standard two-fluid model in CFX

$$M_{GL} = \frac{3}{4}\frac{C_D}{d_G} r_G \rho_L |V_G - V_L|(V_G - V_L) \quad (8)$$

The drag coefficient, C_D, has been estimated using the drag correlation of Krishna et al. (1999a), a relation proposed for the rise of a swarm of large bubbles in the churn turbulent regime

$$C_D = \frac{4}{3}\frac{\rho_L - \rho_G}{\rho_L} g d_G \frac{1}{V_{\text{slip}}^2} \quad (9)$$

where the slip velocity, $V_{\text{slip}} = |V_G - V_L|$, is estimated from the gas superficial velocity, V_S, and the average gas holdup fraction in the froth region is estimated as

$$V_{\text{slip}} = \frac{V_S}{r_G^{\text{average}}} \quad (10)$$

For the average gas holdup fraction, two correlations were considered. One was the correlation of Bennett et al. (1983)

$$r_G^{\text{average}} = 1 - \exp\left[-12.55\left(V_S\sqrt{\frac{\rho_G}{\rho_L - \rho_G}}\right)^{0.91}\right] \quad (11)$$

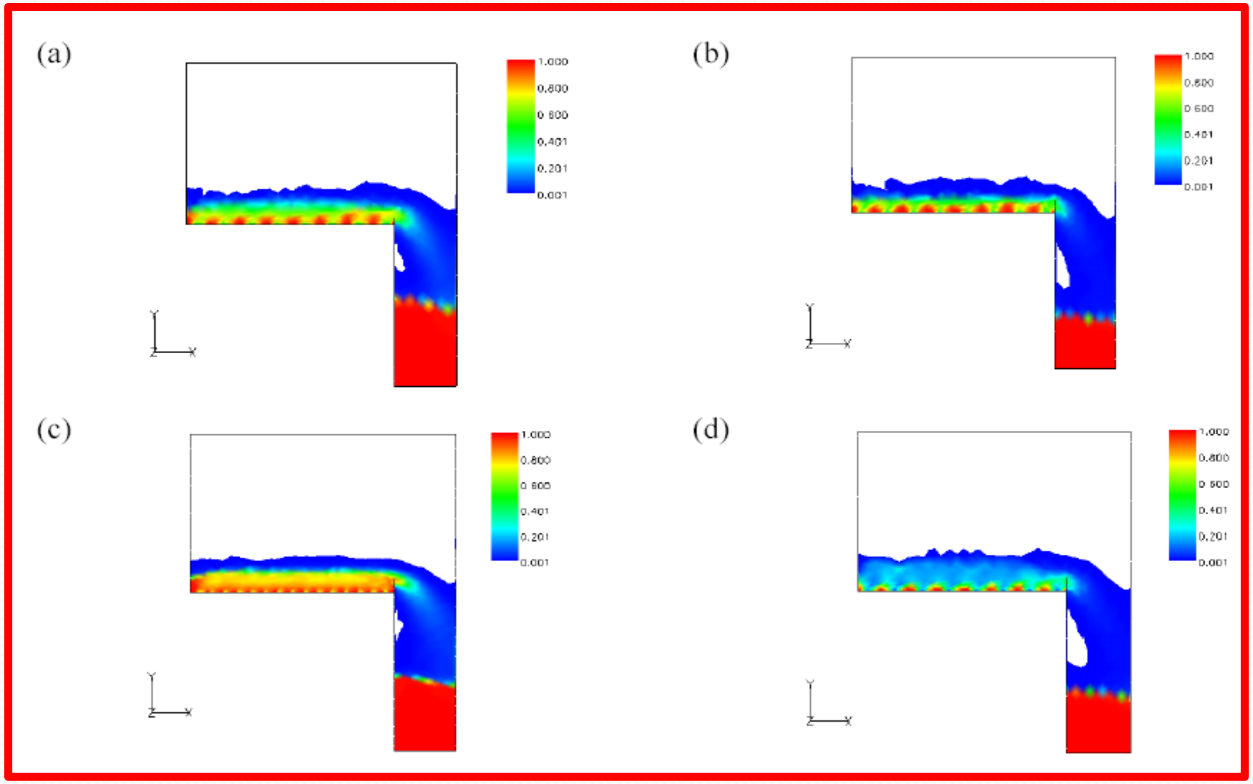
The second one was Colwell's (1979)

$$r_G^{\text{average}} = 1 - \frac{1}{1 + 12.6\left[\left(\frac{\rho_G}{\rho_L - \rho_G}\right)\frac{V_S^2}{g h_L}\right]^{0.4}\left(\frac{A_H}{A_B}\right)^{-0.25}} \quad (12)$$

Enabling Process Innovation through Computation

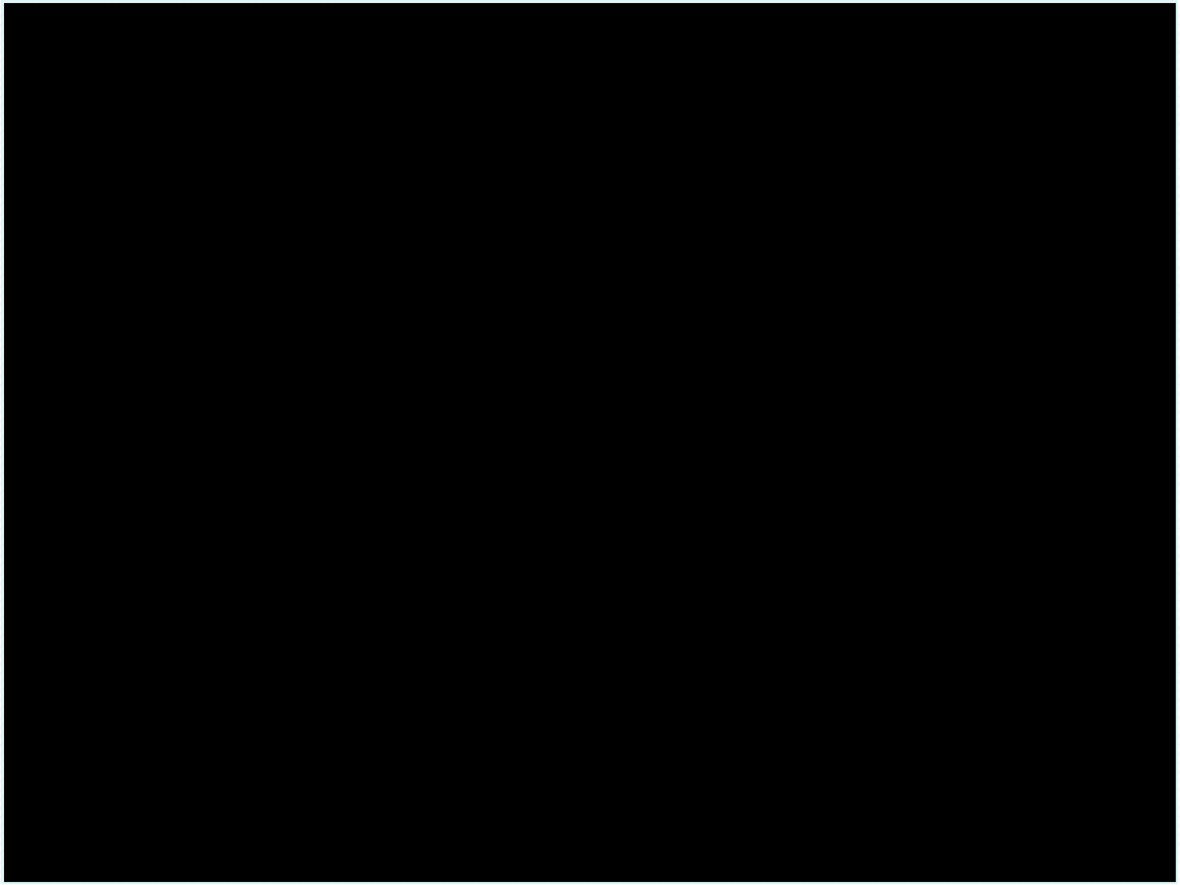
Tray hydraulics on sieve tray - TFM

Examples – heterogeneous nature of vapor-liquid flow

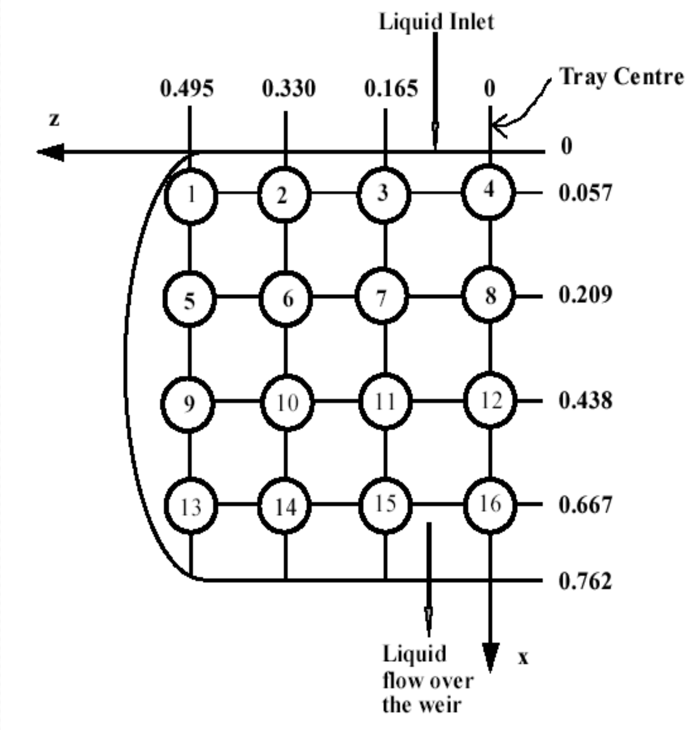


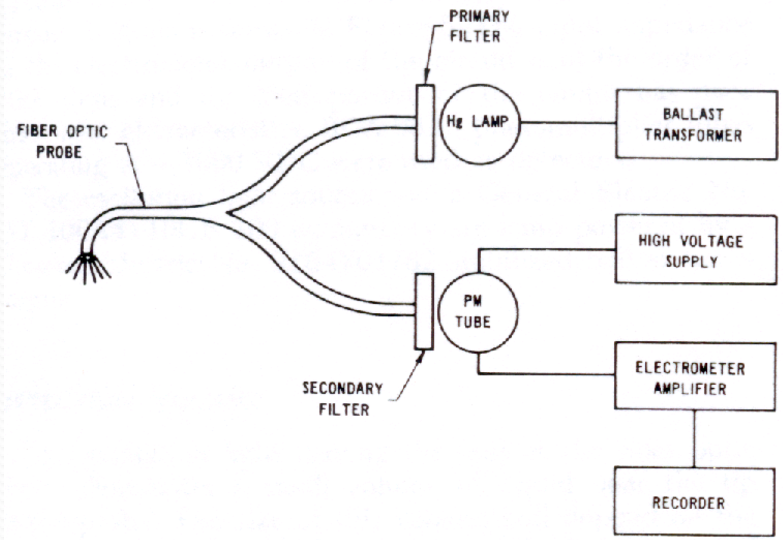
(a) $Q_L = 17.8\times10^{-3} m^3/s$, $F_S = 0.462$ (40,000 nodes with 45 holes)
(b) $Q_L = 6.94\times10^{-3} m^3/s$, $F_S = 0.462$ (40,000 nodes with 45 holes)
(c) $Q_L = 17.8\times10^{-3} m^3/s$, $F_S = 0.462$ (90,000 nodes with actual number of holes)
(d) $Q_L = 6.94\times10^{-3} m^3/s$, $F_S = 1.464$ (40,000 nodes with 45 holes)

CFD simulation of Tray hydraulics - TFM



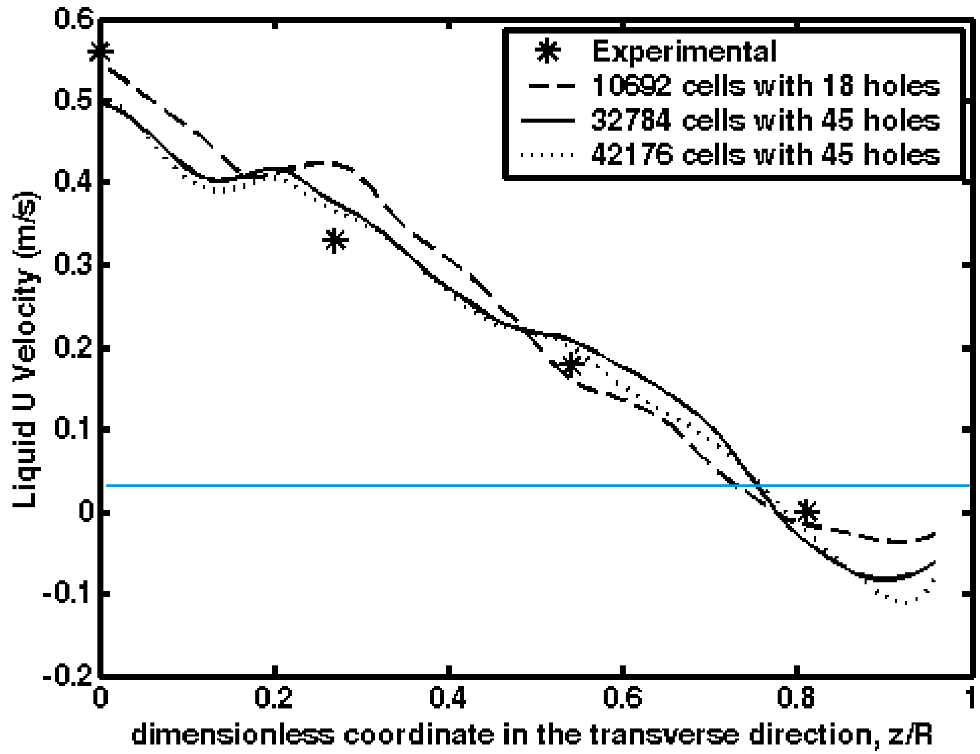
Tray hydraulics on sieve tray - EXP





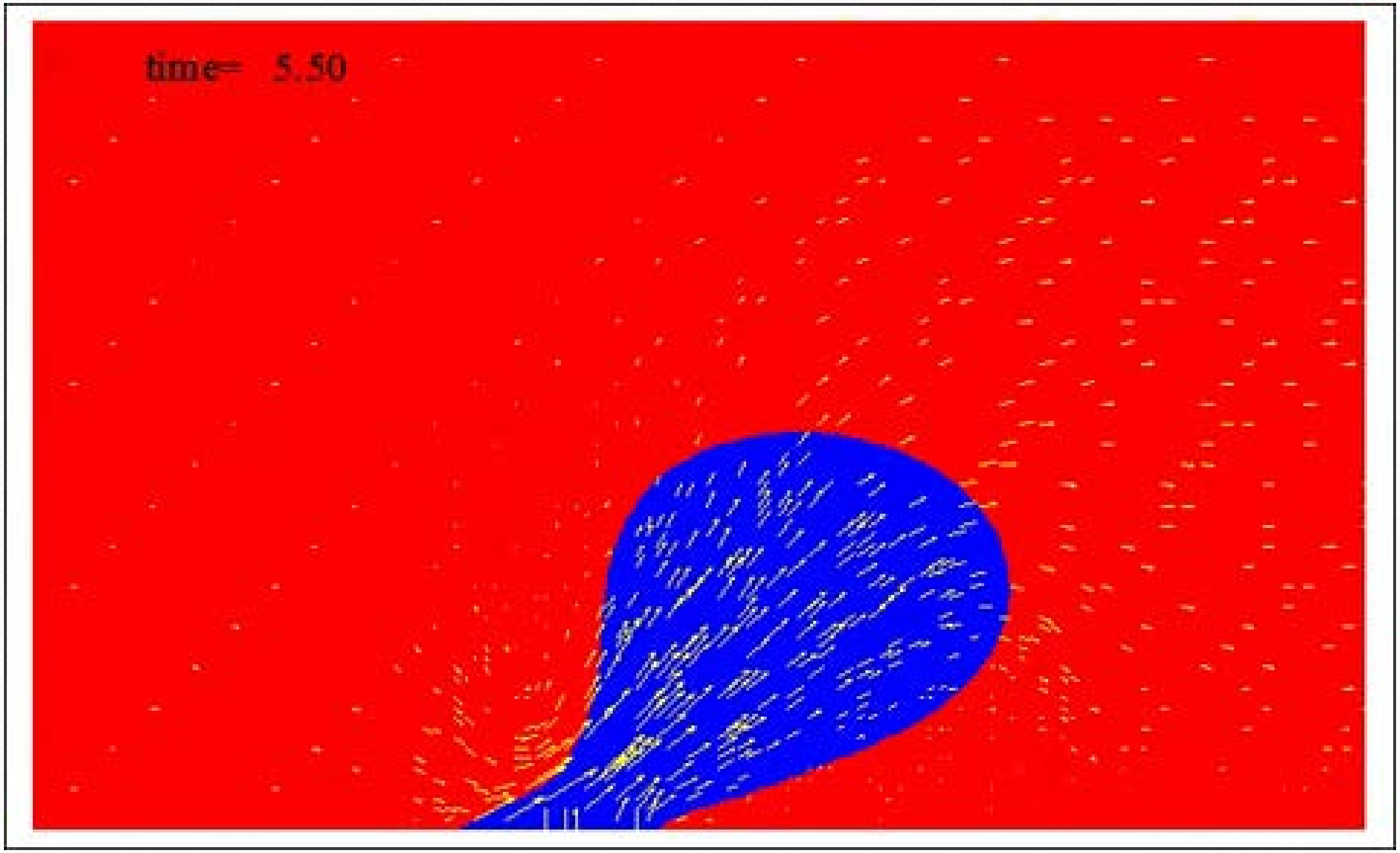
Experimental probe positions of Solari and Bell (1986).
The plane of the probes is at an elevation of 0.038m above the tray floor

Tray hydraulics on sieve tray - TFM



Sensitivity of the liquid velocity profile prediction to grid spacing, and hole number and size (CFX4.4), Q_L = 17.8x10-3m^3/s, F_S = 0.462.

Injection of a bubble through an orifice with cross flow (Distillation) – DNS-LS



Packed column models

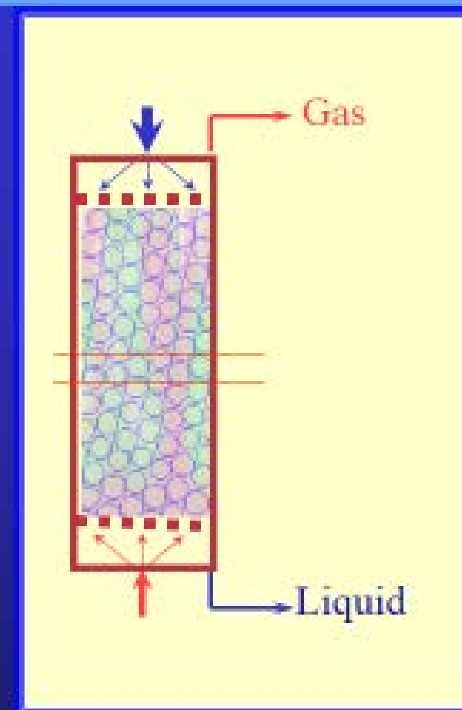
Current Status

One-dimensional Models/empirical equations/limitations

- Assume plug flow in both phases
- No radial/circumferential variation in porosity, flow & concentration profiles
- Negligible dispersion
- Mass transfer coefficient is constant

$$Z = \frac{G}{K_G a P}\int_{y_1}^{y_2}\frac{dy}{y - y^*} = HTU \times NTU$$

Such a model is *not* scale invariant.
Hence scale up is a problem.



Packed column models

Current Status

One-dimensional Models/empirical equations/limitations

Leva equation for pressure drop:

$$\frac{\Delta p}{z} = C_1 G_f^{2} 10^{C_2 L_f} + 0.774 \left(\frac{L_f}{20000} \right)^{0.1} \left(C_1 G_f^{2} 10^{C_2 L_f} \right)^{4}$$

$$G_f = \begin{cases} G\left[\dfrac{1.2}{\rho_G}\right]^{-0.5}\left[\dfrac{F_{pd}}{65.62}\right]^{0.5} & \text{for } p \le 1\,atm \\ G\left[\dfrac{1.2}{\rho_G}\right]^{-0.5}\left[\dfrac{F_{pd}}{65.62}\right]^{0.5} 10^{0.0187\rho_G} & \text{for } p > 1\,atm \end{cases}$$

$$L_f = \begin{cases} L\left[\dfrac{1000}{\rho_L}\right]\left[\dfrac{F_{pd}}{65.62}\right]^{-0.5} \mu_L^{0.1} & \text{for } F_{pd} \ge 15 \\ L\left[\dfrac{1000}{\rho_L}\right]\left[\dfrac{65.62}{F_{pd}}\right]^{-0.5} \mu_L^{0.1} & \text{for } F_{pd} < 15 \end{cases}$$

Onda's mass transfer correlation:

$$k_L = 0.0051 \left(\frac{\mu_L g}{\rho_L} \right)^{\frac{1}{3}} \left(\frac{L}{a_w \mu_L} \right)^{\frac{2}{3}} \left(\frac{\mu_L}{\rho_L D_L} \right)^{-\frac{1}{2}} \left(a_p d_p \right)^{\frac{2}{5}}$$

$$k_G = k_p \left(a_p D_G \right) \left(\frac{G}{a_p \mu_G} \right)^{\frac{7}{10}} \left(\frac{\mu_G}{\rho_G D_G} \right)^{\frac{1}{3}} \left(a_p d_p \right)^{-2.0}$$

Input as closure model to CFD

Packed column models

Current Status

One-dimensional Models/empirical Approach/limitations

$$\frac{a_w}{a_p} = 1 - \exp\left[-1.45\left(\frac{\sigma_c}{\sigma}\right)^{\frac{3}{4}}\left(\frac{L}{a_p\mu_L}\right)^{\frac{1}{10}}\left(\frac{L^2 a_p}{\rho_L{}^2 g}\right)^{-\frac{1}{20}}\left(\frac{L^2}{\rho_L\sigma a_p}\right)^{\frac{1}{5}}\right]$$

Mass dispersion correlation:

$$Pe_L = 5.337\times10^{-4}\left(\frac{d_e L}{\mu_L}\right)^{0.472}\left(\frac{d_e G}{\mu_G}\right)^{0.293}\left(\frac{d_e}{D}\right)^{-0.867}$$

Porosity variation

$$\varepsilon = 1-(1-\varepsilon_b)\left\{1-\exp\left[-2\left(\frac{R-r}{d_p}\right)^2\right]\right\}$$

Input as closure model to CFD

Packed column models

Current Status

One-dimensional Models/empirical Approach/limitations

HETP correlation Wagner et al I&ECR (1997):

$$HETP = C_{pk}\frac{Z^{0.5}}{a_p}\left(\frac{\pi(\varepsilon - h)u_V}{4D_V}\right)^{0.5}\left[1+\left(\frac{hD_V M_L \rho_V}{(\varepsilon-h)D_L M_L \rho_L}\frac{V}{L}\right)^{0.5}\right]\left[\left(\frac{1-\varepsilon+h}{1-\varepsilon}\right)^{2/3}-1\right]^{-1}$$

Billet's holdup correlation:

$$h_L = \left(12\frac{1}{g}\frac{\mu_L}{\rho_L}u_L a^2\right)^{1/3}\left(\frac{a_h}{a}\right)^{2/3}$$

$$Re_L = \frac{u_L\rho_L}{a\mu_L} < 5: \quad \frac{a_h}{a} = C_h\left(\frac{u_L\rho_L}{a\mu_L}\right)^{0.15}\left(\frac{u_L^2 a}{g}\right)^{0.1}$$

$$Re_L = \frac{u_L\rho_L}{a\mu_L} \geq 5: \quad \frac{a_h}{a} = 0.85C_h\left(\frac{u_L\rho_L}{a\mu_L}\right)^{0.25}\left(\frac{u_L^2 a}{g}\right)^{0.1}$$

NOTE: HETP depends on height, Z!

Packed column models

Relation to traditional one-D models

Species conservation

$$\cancel{\frac{\partial}{\partial t}}\left(\gamma_\alpha \rho_\alpha Y_{i\alpha}\right)+\nabla\cdot\left[\gamma_\alpha\left(\rho_\alpha \mathbf{U}_\alpha Y_{i\alpha}-\cancel{\Gamma\nabla Y_{i\alpha}}\right)\right]=\sum_{\beta=1,\ \beta\neq\alpha}^{N} \dot{m}^{i}_{\alpha\beta} \qquad \alpha = L, G \qquad i=1,\cdots\cdots,N_C$$

Assume steady conditions

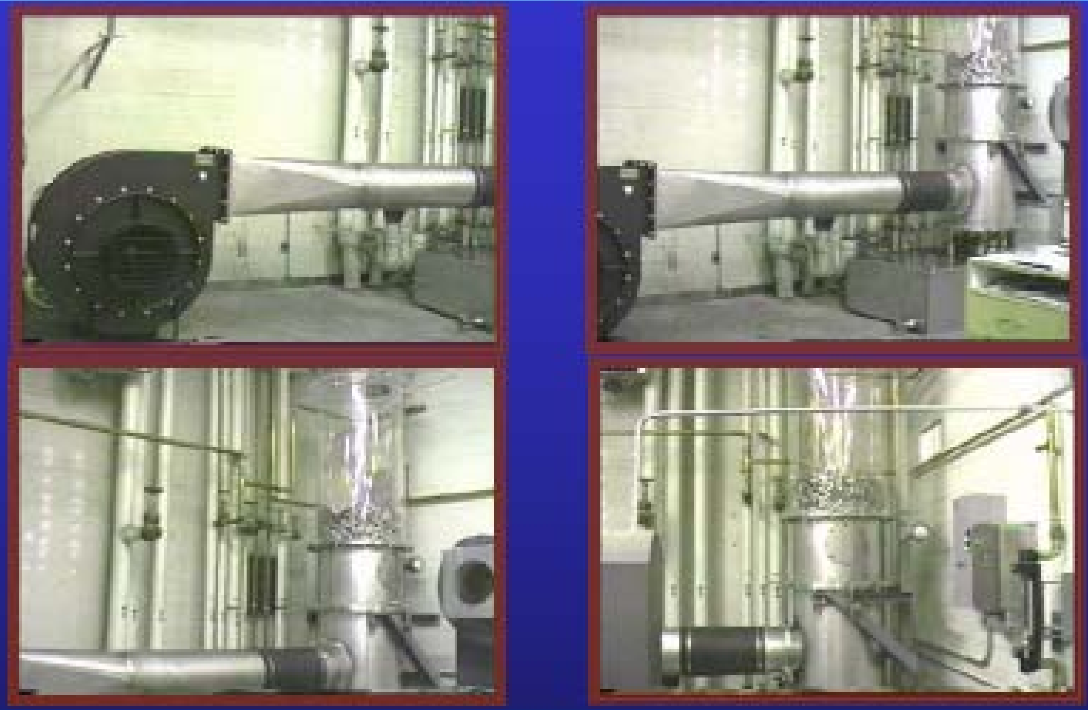
No dispersion in any direction

Plug flow (U is constant) & one-dimensional flow (z-dn only)

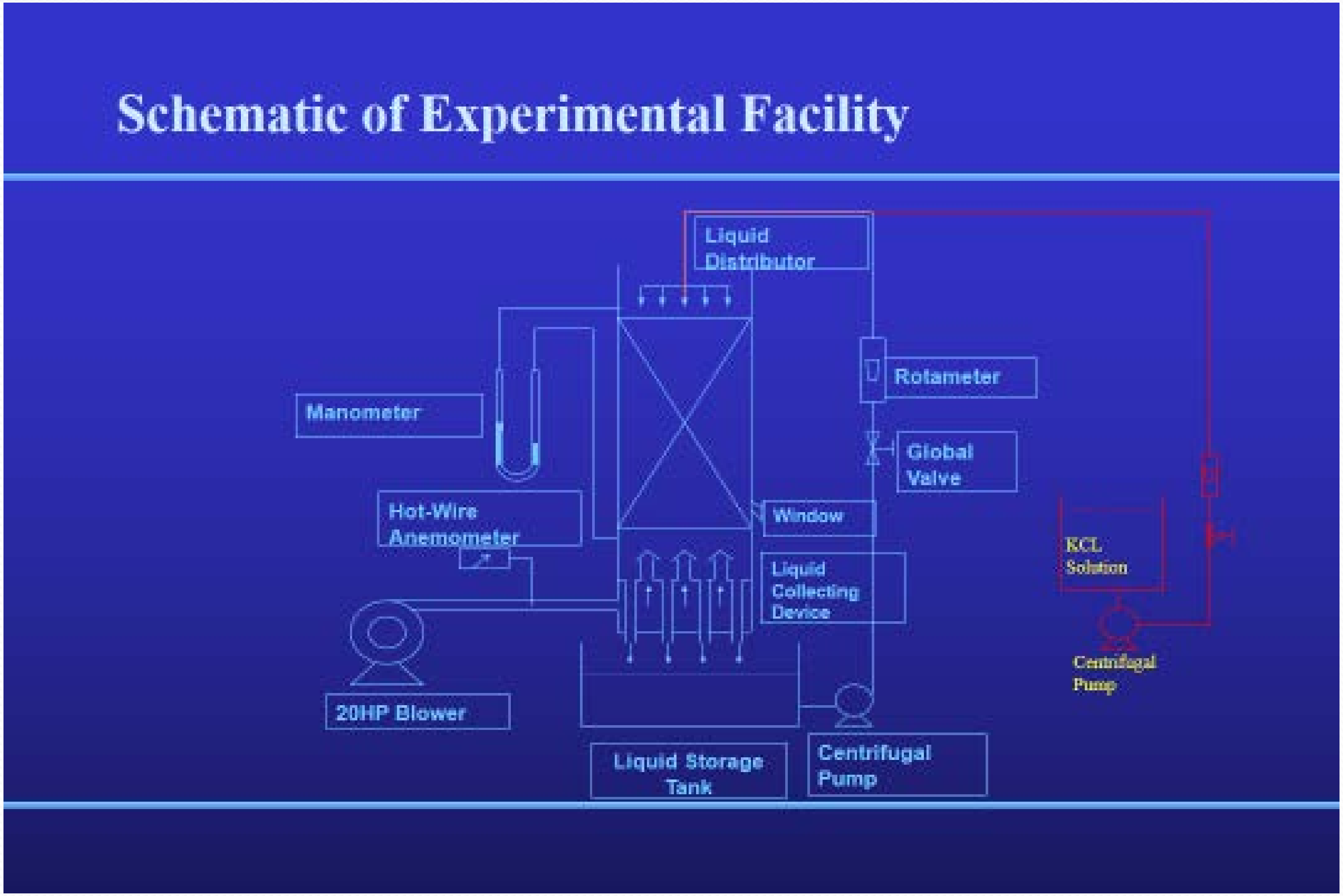
$$\boxed{\gamma_G\left(\rho_G \mathbf{U}_G\right)\frac{dY_{iG}}{dz}=\dot{m}^{i}_{LG}=K_G a_e M_A\left(Y^{*}_{iL}-Y_{iG}\right)}$$

Packed column models

Two feet air-water column

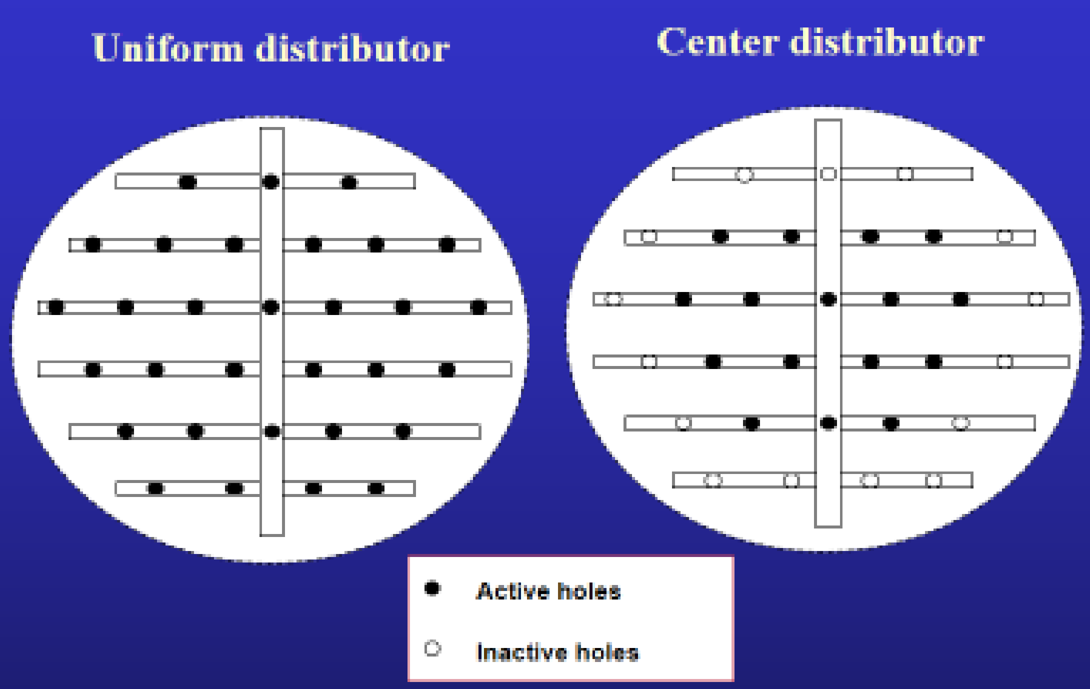


Packed column models



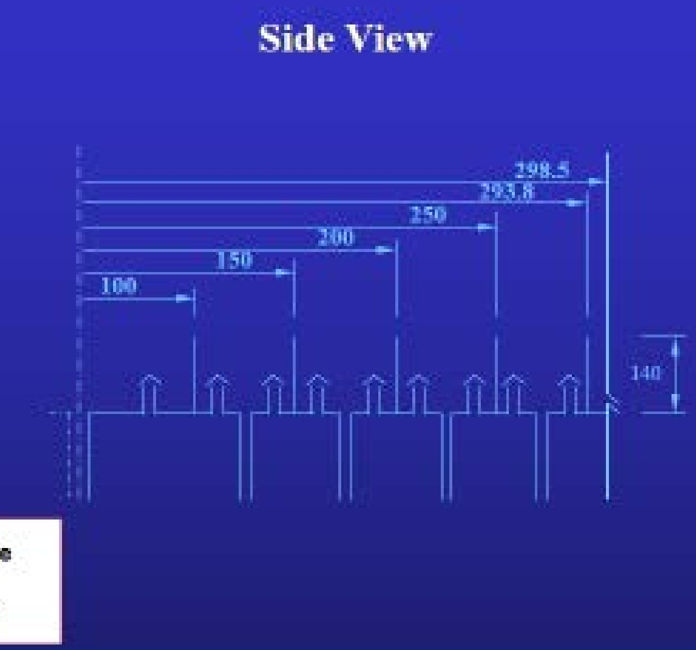
Packed column models

Schematic of Liquid Distributor



Packed column models

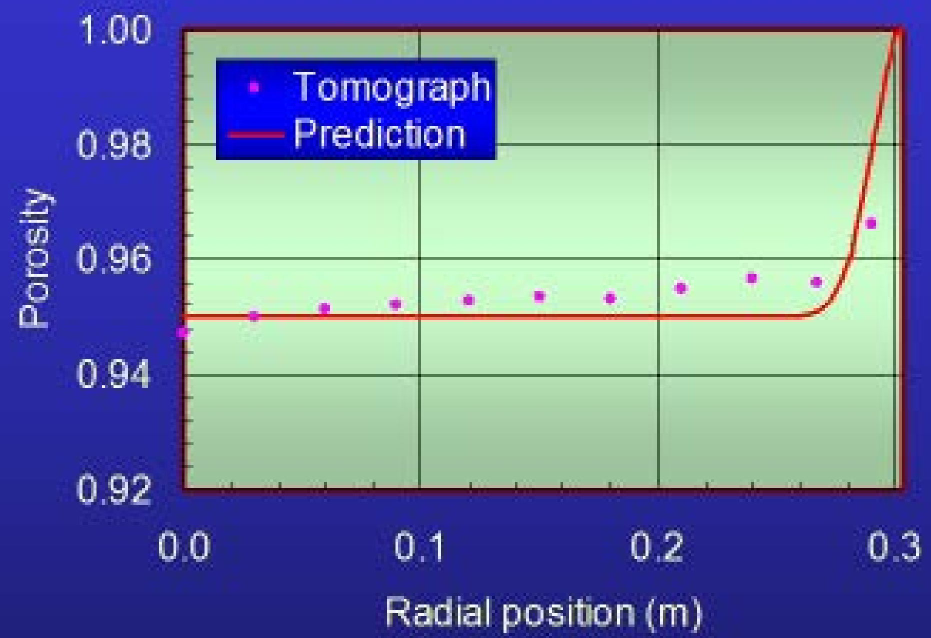
Schematic of Liquid Collector



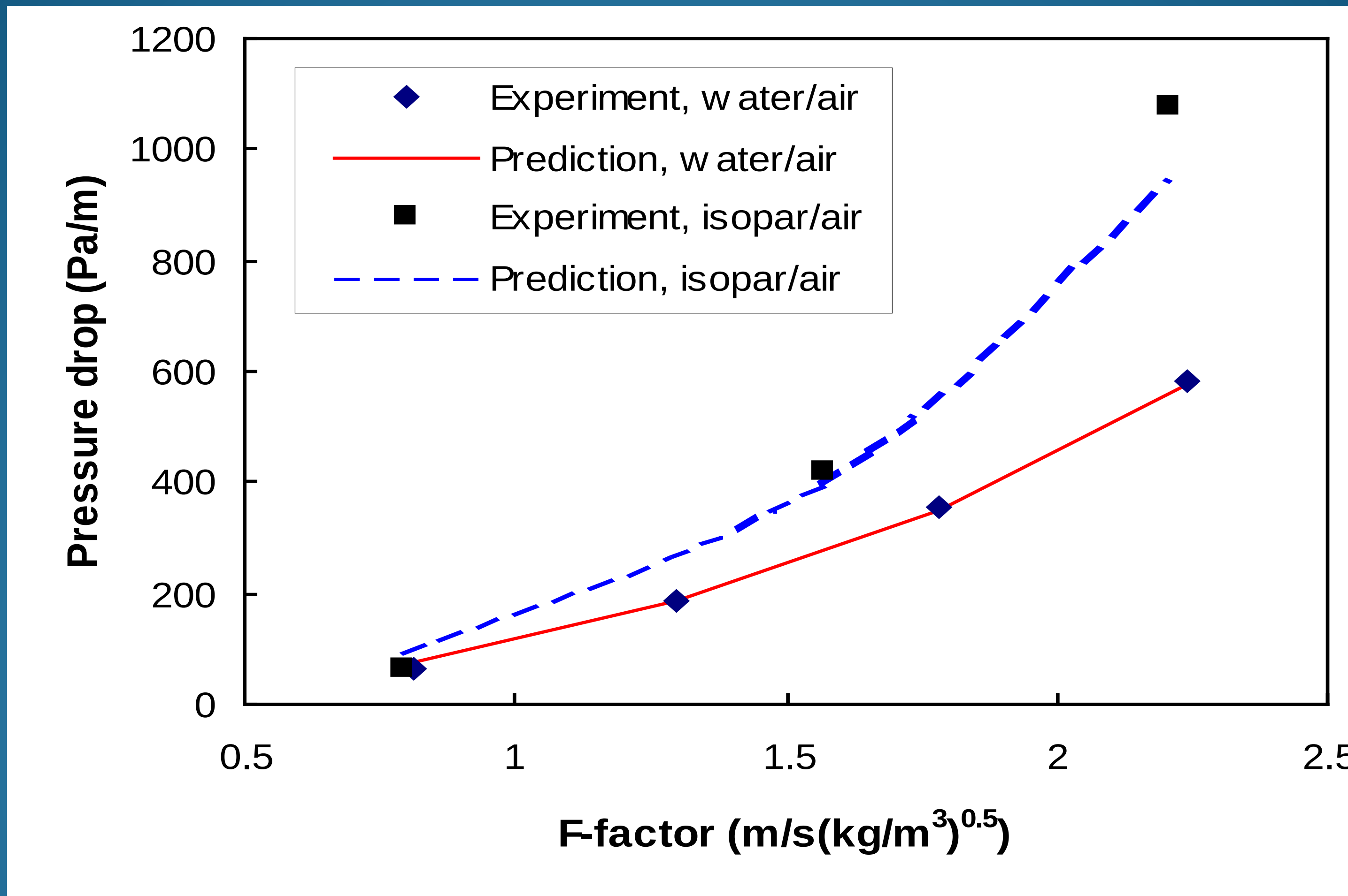
Packed column models

(A) Radial Variation of Porosity

25 mm metal Pall Ring



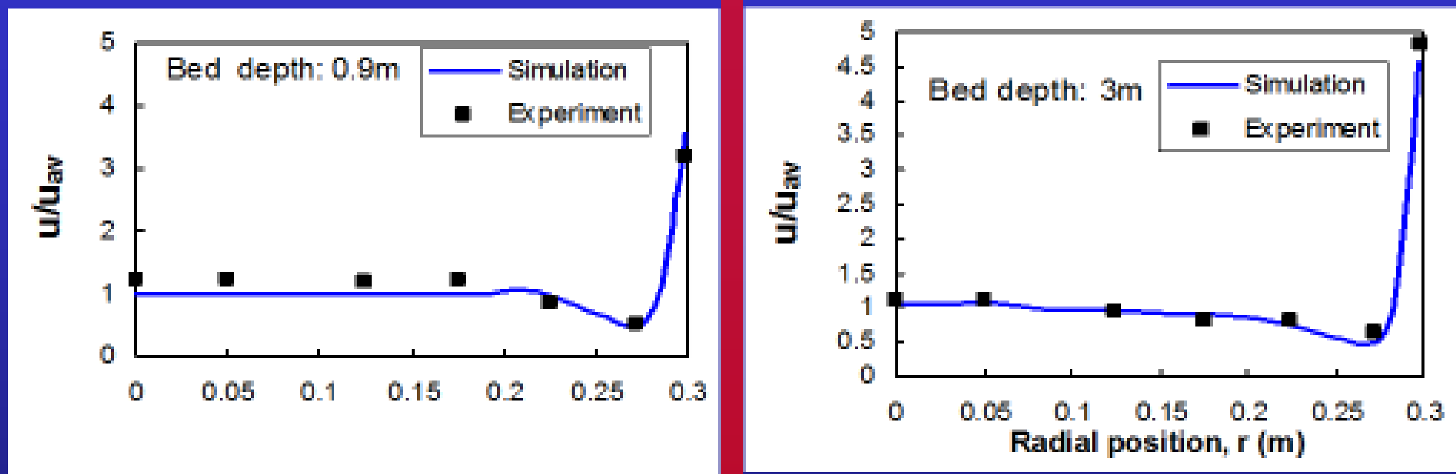
Packed column models



Packed column models

(a) Validation of flow profile from CFD

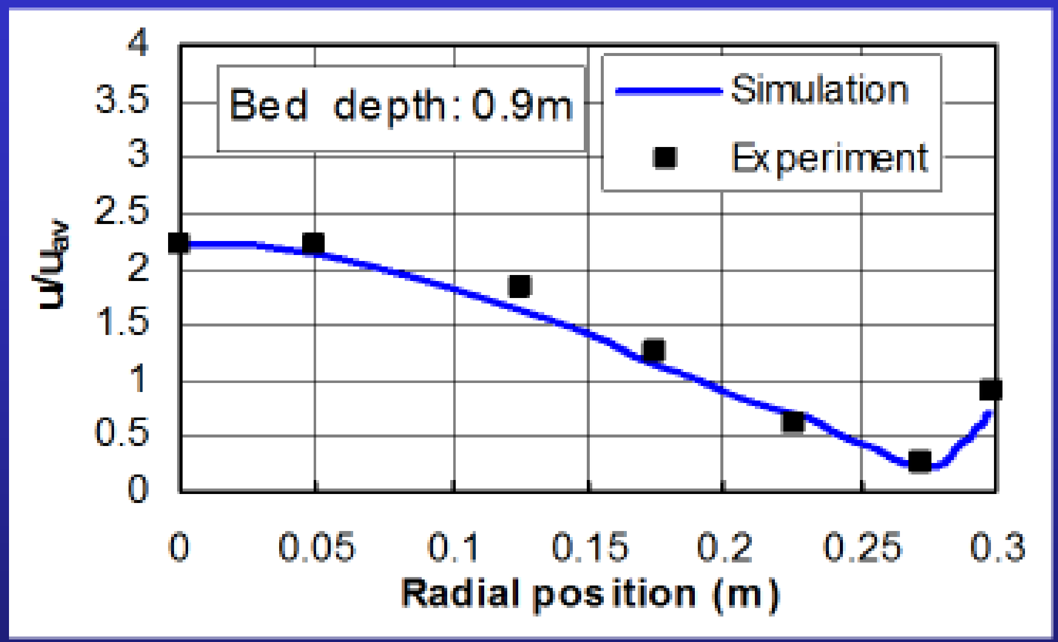
uniform inlet distribution, water/air, $L=4.78\ kg\ m^{-2}\ s^{-1}$, $G=0.75\ kg\ m^{-2}\ s^{-1}$



Packed column models

(a) Validation of flow profile from CFD

43% inlet distribution, water/air, $L=4.78\ kg\ m^{-2}\ s^{-1}$, $G=0.75\ kg\ m^{-2}\ s^{-1}$



Packed column models

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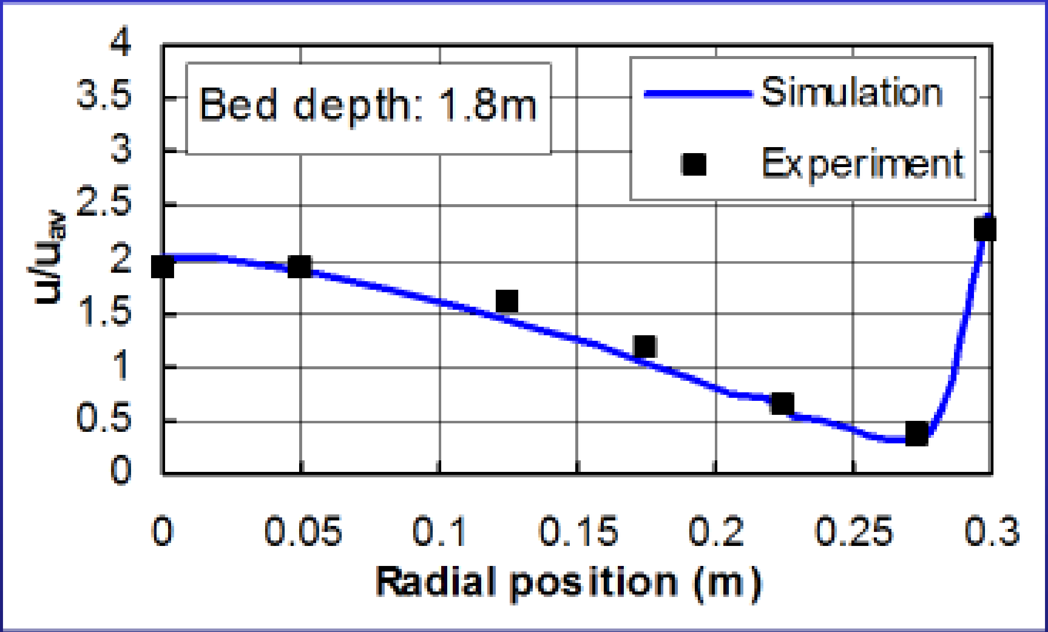

Packed column models

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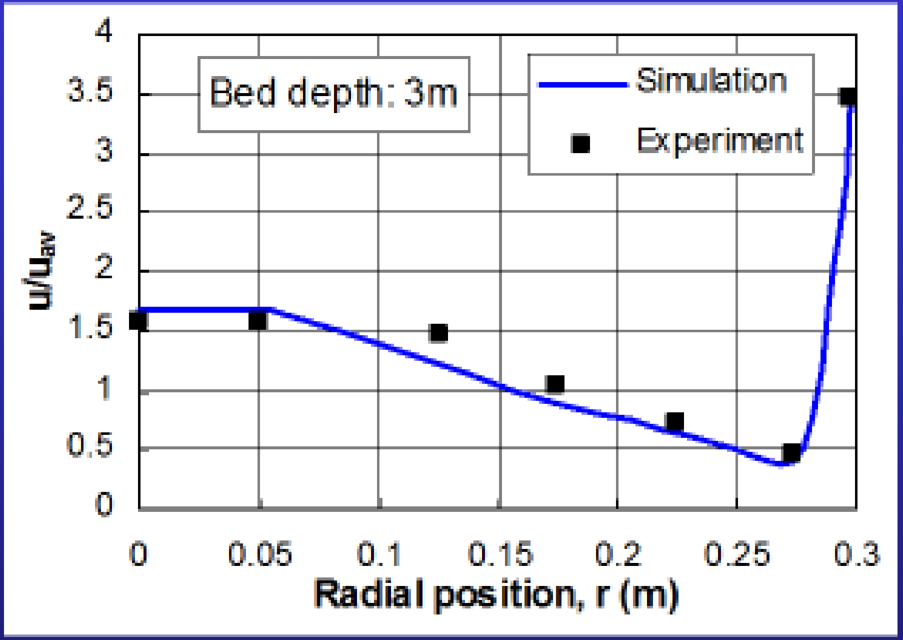


Packed column models

(c) Closure models for *mass transfer* in CFD

$$\frac{\partial}{\partial t}(\gamma_\alpha \rho_\alpha Y_{i\alpha}) + \nabla \cdot \left[\gamma_\alpha \left(\rho_\alpha \mathbf{U}_\alpha Y_{i\alpha} - \Gamma_{i\alpha} \nabla Y_{i\alpha}\right)\right] = \sum_{\beta=1,\, \beta\neq\alpha}^{N} \dot{m}^{i}_{\alpha\beta} \qquad \alpha = L,\, G \qquad i = 1, \cdots\cdots, N_C$$

$$\dot{m}^{A}_{LG} = k_L a_e M_A \left(x_A - x^I_A\right)$$

$$\dot{m}^{A}_{LG} = k_G a_e M_A \left(y^I_A - y_A\right)$$

$$y^I_A = \frac{\alpha x^I_A}{1+(\alpha-1)x^I_A}$$

$$k_L = 0.0051\left(\frac{\mu_L g}{\rho_L}\right)^{\frac{1}{3}}\left(\frac{L}{a_w \mu_L}\right)^{\frac{2}{3}}\left(\frac{\mu_L}{\rho_L D_L}\right)^{-\frac{1}{2}}(a_p d_p)^{\frac{2}{5}}$$

$$k_G = k_p (a_p D_G)\left(\frac{G}{a_p \mu_G}\right)^{\frac{7}{10}}\left(\frac{\mu_G}{\rho_G D_G}\right)^{\frac{1}{3}}(a_p d_p)^{-2.0}$$

$$\frac{a_w}{a_p} = 1 - \exp\left[-1.45\left(\frac{\sigma_c}{\sigma}\right)^{\frac{3}{4}}\left(\frac{L}{a_p \mu_L}\right)^{\frac{1}{10}}\left(\frac{L^2 a_p}{\rho_L^2 g}\right)^{-\frac{1}{20}}\left(\frac{L^2}{\rho_L \sigma a_p}\right)^{\frac{1}{5}}\right]$$

$$Pe_L = 5.337 \times 10^{-4}\left(\frac{d_e L}{\mu_L}\right)^{0.472}\left(\frac{d_e G}{\mu_G}\right)^{0.293}\left(\frac{d_e}{D}\right)^{-0.867}$$

Packed column models

(c) Validation of *mass transfer* from CFD

Simulation Conditions (FRI data)

- **System: cyclohexane/n-heptane at total reflux**
- **Operating Pressures: 33.3 and 165.5 kPa**
- **Column Diameter: 1.22 m**
- **Packed Bed Height: 3.66 m**
- **Packings: 15.9, 25.4, 50.8 mm metal Pall rings**

Local HETP is calculated as follows:

$$N_{OGl} = \int_{y_{AZ}}^{y_{AZ+\Delta Z}} \frac{dy}{y_A^* - y_A}$$

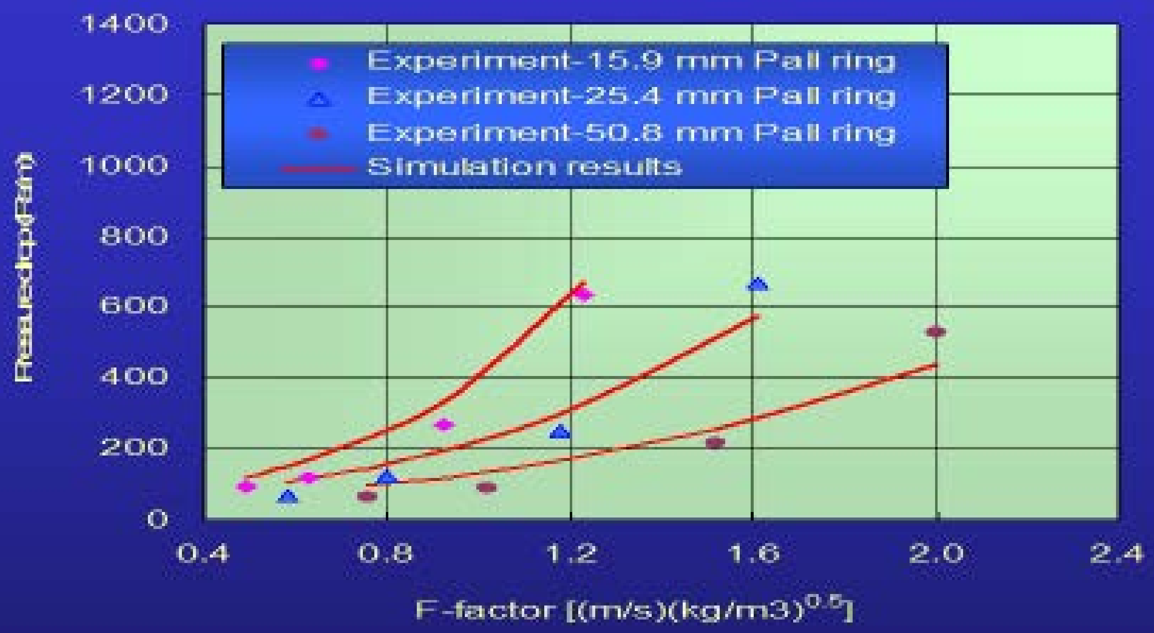
$$H_{OGl} = \frac{\Delta Z}{N_{OGl}}$$

$$HETP_l = H_{OGl} \frac{\ln\left(m_l \frac{G_l}{L_l}\right)}{m_l \frac{G_l}{L_l} - 1}$$

Packed column models

(c) Validation of *mass transfer* from CFD

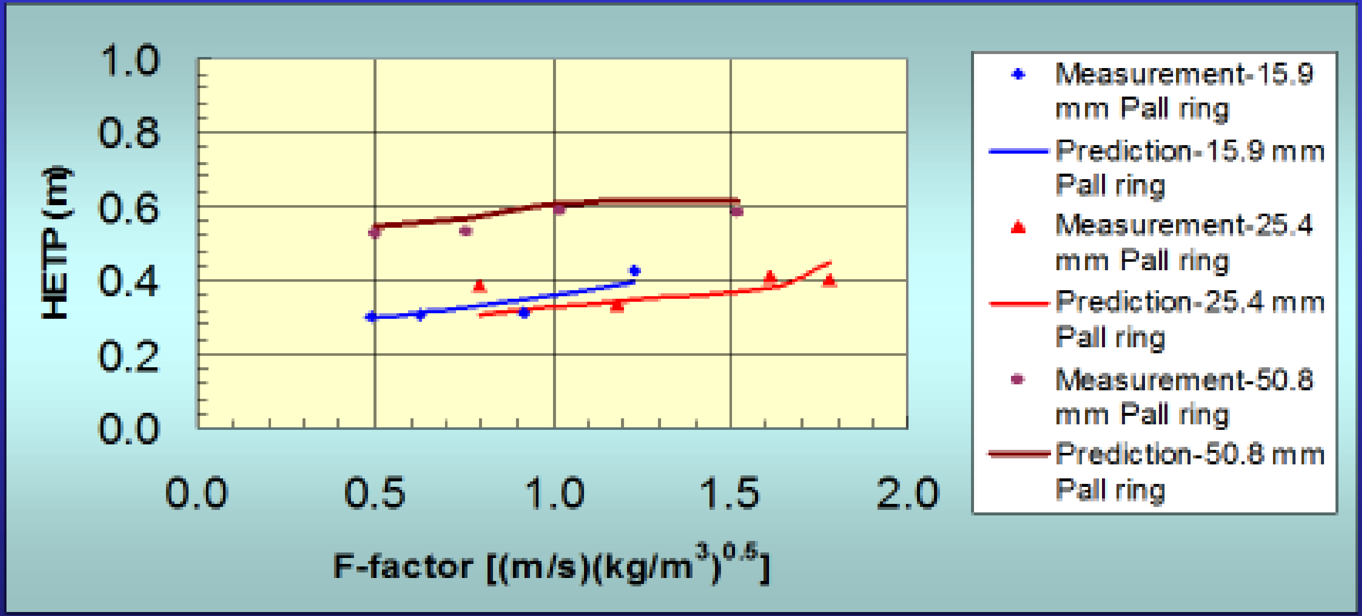
FRI data on pressure drop System: C_6/C_7,
uniform inlet, Diameter of column: 1.22 m, 165.5 kPa



Packed column models

(c)Validation of *mass transfer* from CFD

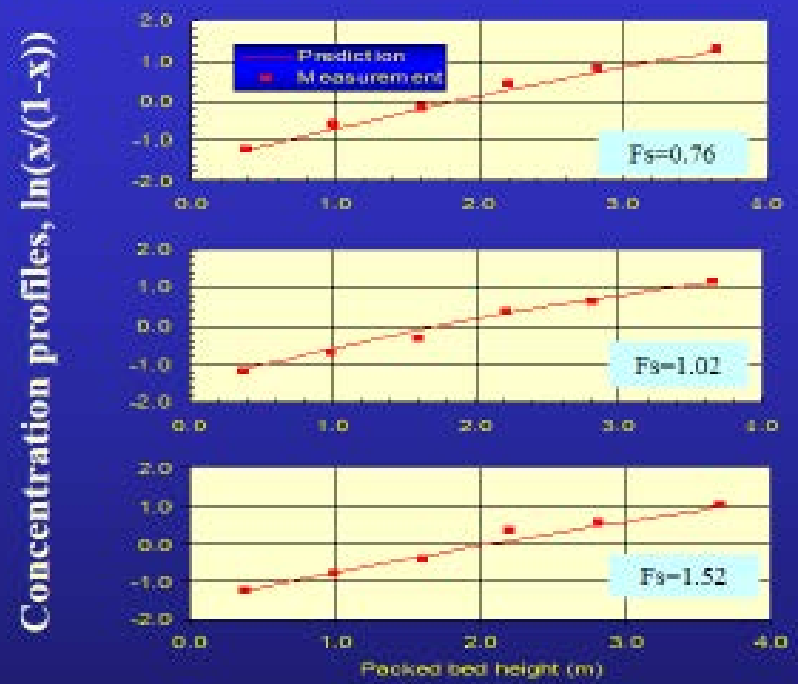
FRI data on HETP System: C_6/C_7,
uniform inlet, P=165.5 kPa



Packed column models

(c) Validation of *mass transfer* from CFD

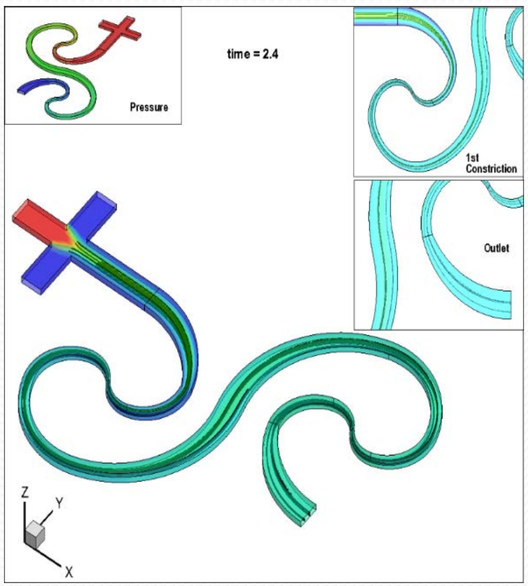
FRI data on concentration: System-C_6/C_7,
50.8mm Pall rings, uniform inlet, 165.5 kPa



Multiphase flows – challenges

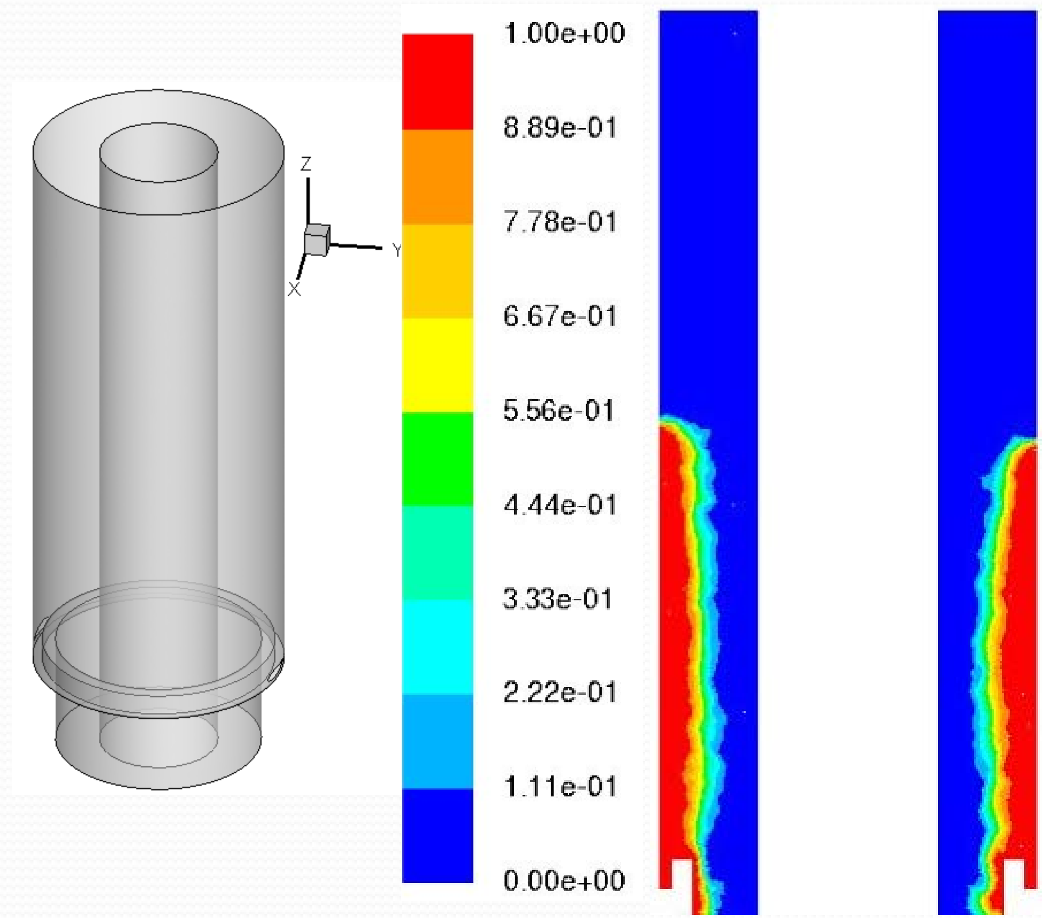
- Multiphase flows are ubiquitous in chemical, petroleum, mineral, food processing industries.
    - Gulf of Mexico Oil Spill,
    - Heavy-oil with sand and water,
    - progressive cavity pumps,
    - Gravity separation vessels,
    - Hydro transport in pipelines,
    - Crude distillation towers,
    - packed towers, tray columns,
    - Fuel cells
    - Polymer processing – mixing
    - Microfluidic devices
    - Erosion problems and many more.
- *Fluid mechanics is often ignored by assuming well mixed, spatially homogeneous conditions and using effective properties.*
- But large scale flow pattern can change with changing operating conditions or scale up of devices.
- *Will the measured tray efficiency or RTD remain the scale invariant?*
  Can Multiphase CFD aid in scaling up equipment without the need for expensive pilot scale experiments?
- *Can we understand and manage the spatial heterogeneities inside vessels to improve performance of separation or reaction systems.*

Examples of novel designs



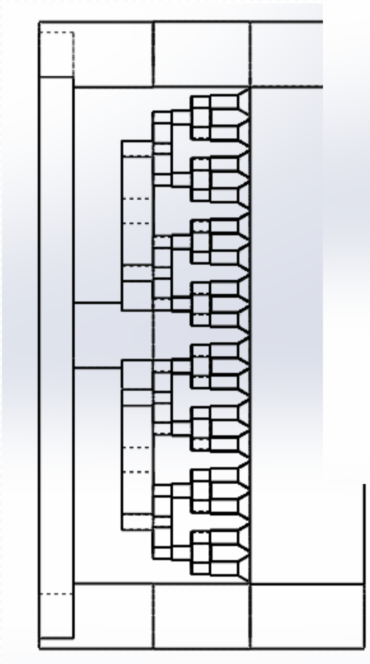
Micro mixer for cryopreserved sperm cell activation

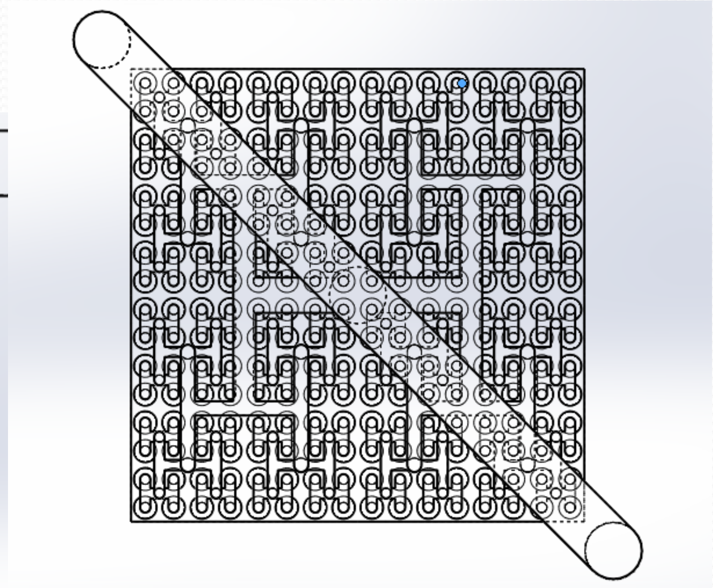
Small Company Hydroflame

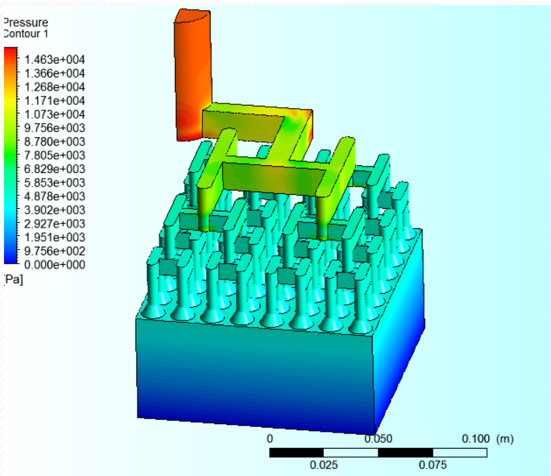


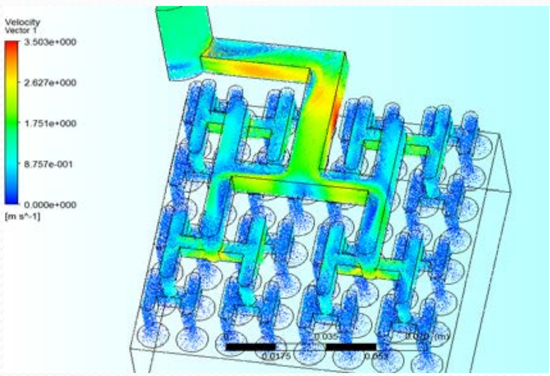
Examples of novel designs

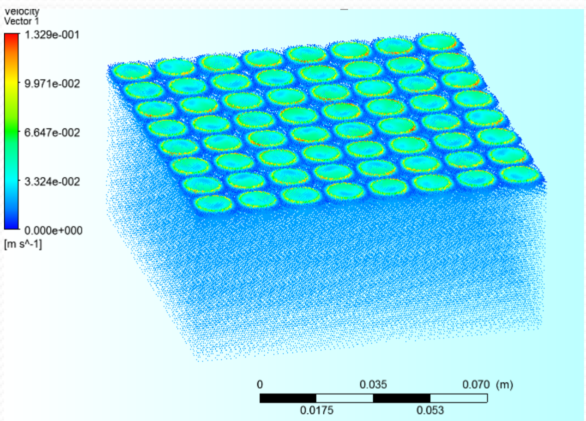
Fractal based distributors – medium sized ARi





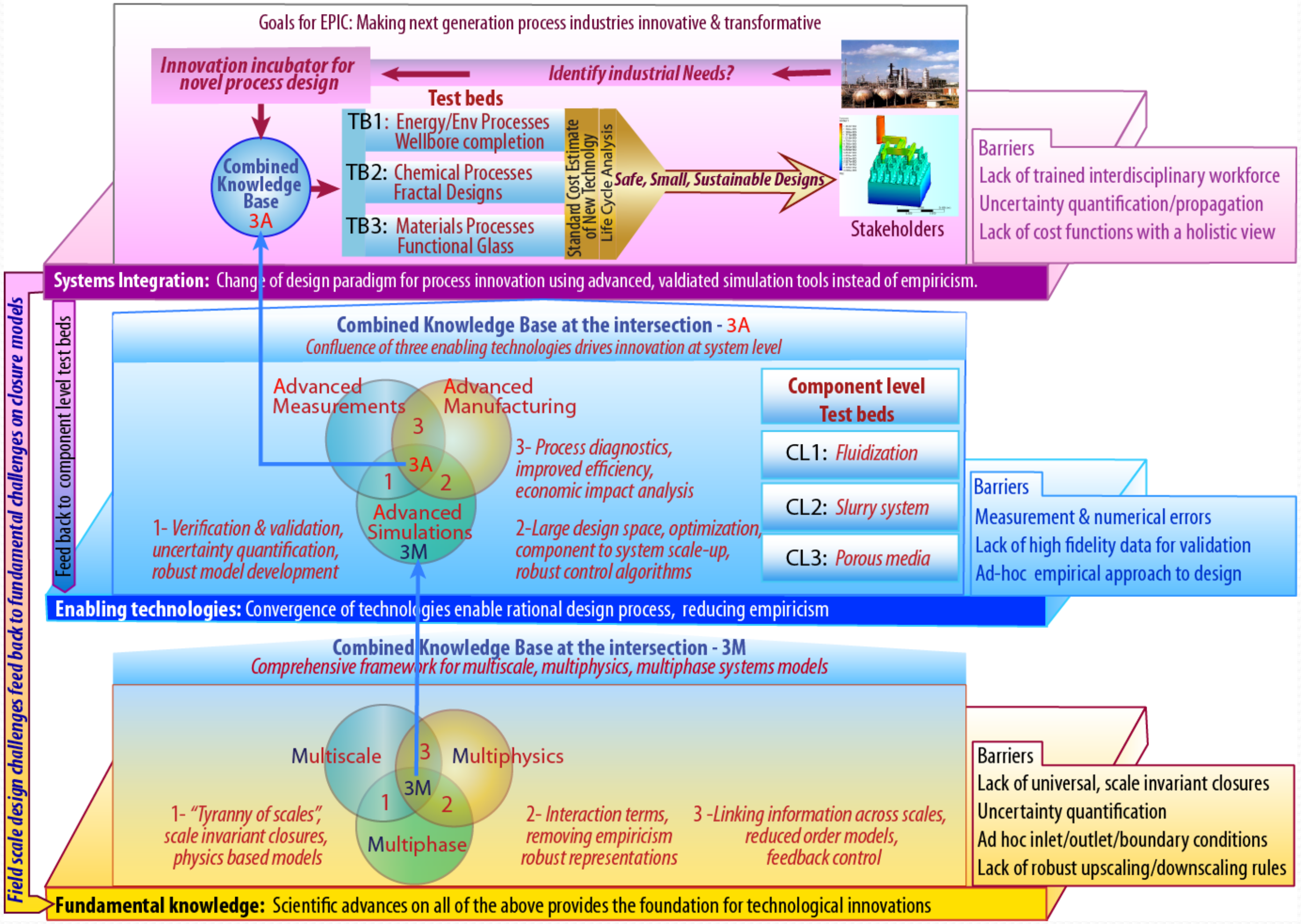




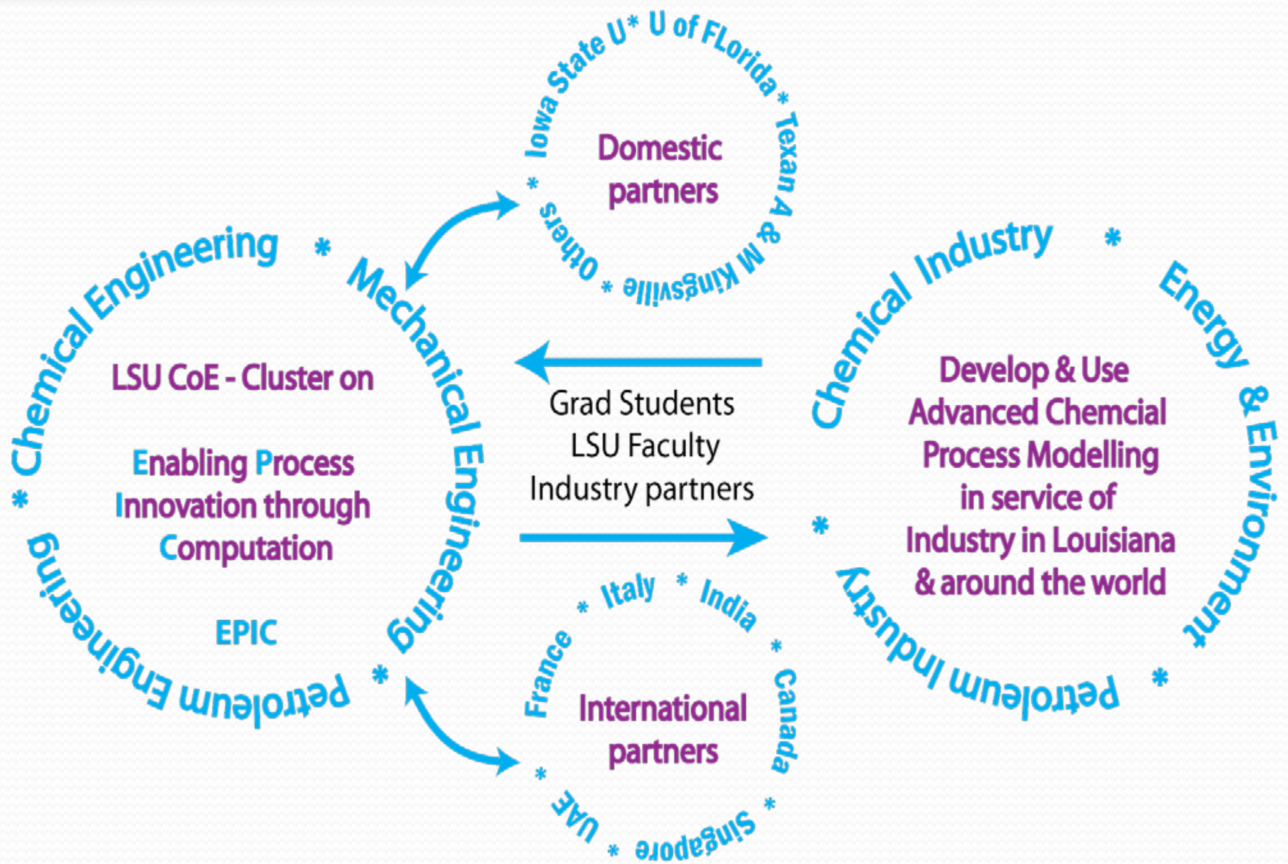


Design innovation cycle for process industries

L02435109, Nandakumar, NSF ERC- Enabling Process Innovation through Computation - EPIC, Louisiana State University



Internationally interlinked clusters on multiphase flow problems



Joint Doctoral program between US Universities and the PI

Joint Annual Technical Conference for ADNOC group of companies and LCA in Baton Rouge

Some concluding observations and quotes

"*Essentially, all* ***models*** *are wrong, but some are useful* " – - George Box.

- let us not wait for that perfect model before we start using the models to innovate process systems.

"*For the* ***theory-practice iteration to work****, the scientist must be, as it were, mentally ambidextrous; fascinated equally on the one hand by possible meanings, theories, and tentative models to be induced from data and the practical reality of the real world, and on the other with the factual implications deducible from tentative theories, models and hypotheses*" - – George Box.

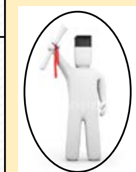
- Although none of us were trained to be ambidextrous, let us train the next generation of graduate students to be so.

Enabling Process Innovation through Computation

Road map for integrated graduate training in Chemical Processes

Look at that.
A model T to Porche
That is what
I call transformative!
I feel neglected!

Industrial problems
+
Raw doctoral candidates



Well, don't despair
I will be the transformative agent for you.
I am going to LSU to learn the tricks!

Process Diagnostics
Use data mining, process knowledge to identify troubled units
(Triantaphyllou, Romagnoli)

Process Modeling
Use ASPEN, to reconcile plant data with design spec. to understand deviation from expected performance
(Nandakumar, Flake, Knopf)

(a) Supporting multiscale & molecular dynamic simulations
(b) Algorithm development for nonlinear PDE
(Hung, Tyagi, Zhang, Brenner)

Supporting experimental program for detailed examination of interfacial and other processes
(e.g. AFM, Surface Tension etc)
(Valsaraj, Dooley, Knopf, Griffin, Flake)

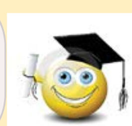
Advanced Multiphase Modeling
Detailed multiphase flow modelling of process vessel. Identify causes of poor performance
(Nandakumar, Acharya, Tyagi, Thompson, Sundaresan)

Advanced Multiphase Experiments
Use small scale experiments to measure parameters needed in the multiphase model valdiaton.
(Knopf, Acharya, Rao, Kochergin)

Process Improvement & Intensificaton
Using detailed models examine process intensificaton, alternate design/operating conditions.
(Nandakumar, Tyagi, Wen)

Process Optimizaton & Co ntrol
Develop reduced order models
(eg Proper Orthogonal Decomposition)
for nonlinear model predictive control
(Romagnoli, Gu, Zhang, Brenner)

The degree is nice.
Nicer still is to see that my findings have transformed you!



Improved solutions
+
IGERT trained Fellows

Thank you.
Now I feel energized and efficient. I will be less threatening to the environment too!