

CFD Simulations of a Large-Scale Aerated Reactor with Multiple Impellers

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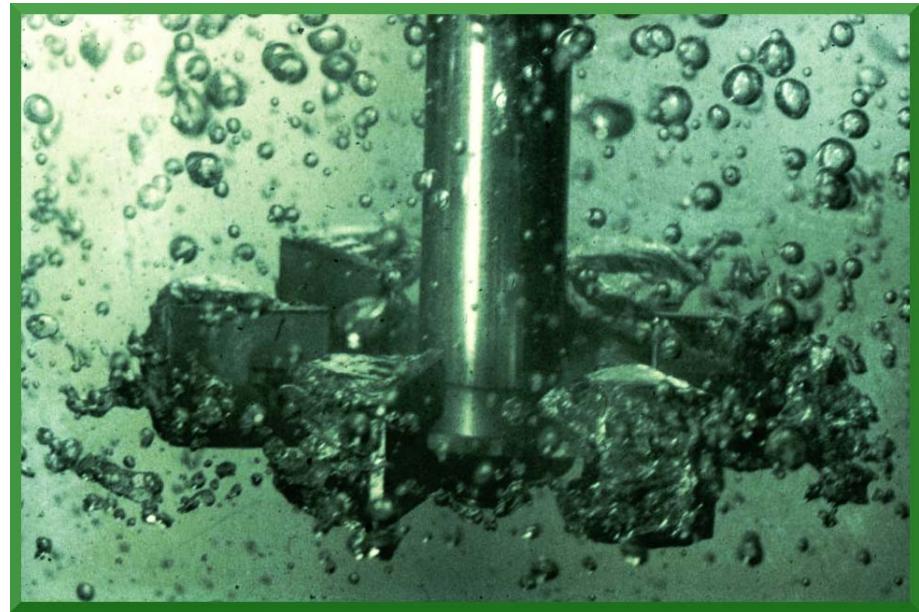
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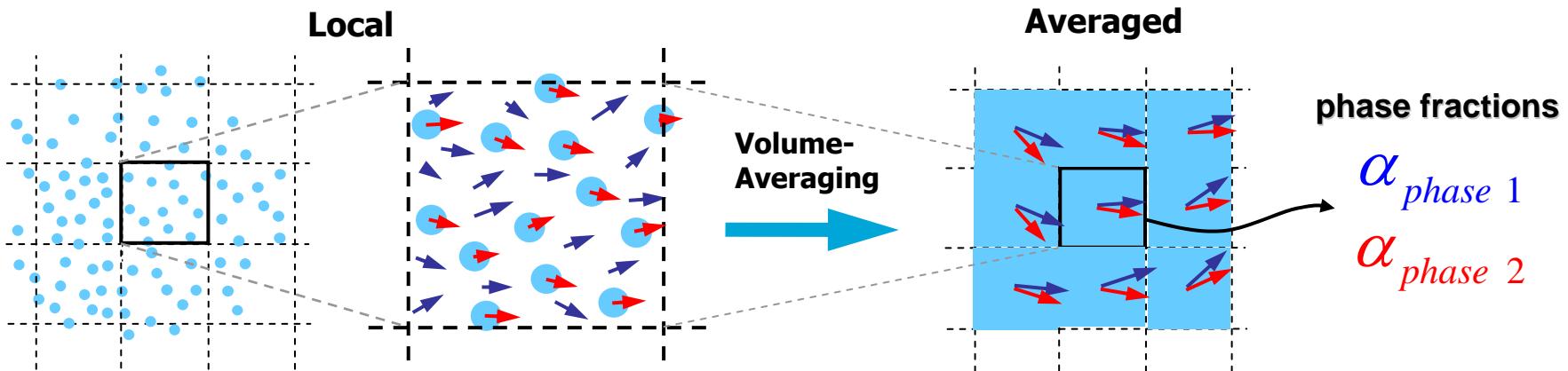
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Outline

- CFD model
 - Multiphase modeling
 - Euler-Euler (Two-fluid) approach
 - Modeling of the moving parts
- Fermenter geometry
- Computational set-up
- Results: single- and two-phase
- Conclusions



Multiphase Modeling - Euler-Euler (2-fluid) Approach



Local instantaneous mass & mom. eqs.



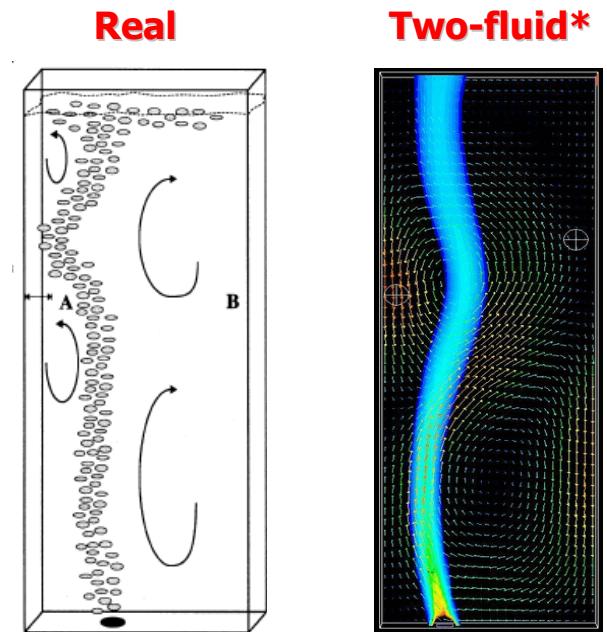
Averaging (e.g. time, volume, ensemble)



Averaged conservation eqs. (per phase)

- Interpenetrating continua concept:

$$\alpha = f(x, y, z, t), \quad \alpha_{\text{phase 1}} + \alpha_{\text{phase 2}} = 1$$



* Runo Mijnarends

Continuity (phase 1)

$$\frac{\partial}{\partial t}(\alpha_1 \rho_1) + \nabla \cdot (\alpha_1 \rho_1 \vec{v}_1) = 0 ; \quad \vec{v} : \text{mean velocity vector}$$

Momentum (phase 1)

$$\frac{\partial}{\partial t}(\alpha_1 \rho_1 \vec{v}_1) + \nabla \cdot (\alpha_1 \rho_1 \vec{v}_1 \vec{v}_1) = -\alpha_1 \nabla p + \nabla \cdot [\alpha_1 (\bar{\tau}_1 + \bar{\tau}_1^t)] + \alpha_1 \rho_1 \vec{g} + \vec{F}_{body,1}$$

+ 

averaged interfacial forces

shared pressure field

Reynolds stress tensors
(turbulence model needed)

Coriolis & centrifugal forces
in rotating r.f. (for MRF)

Turbulence Modeling

→ RANS Approach (closure via k-ε model)

Continuous phase quantities:

→ standard k-ε model + production terms for interphase turbulent momentum transfer

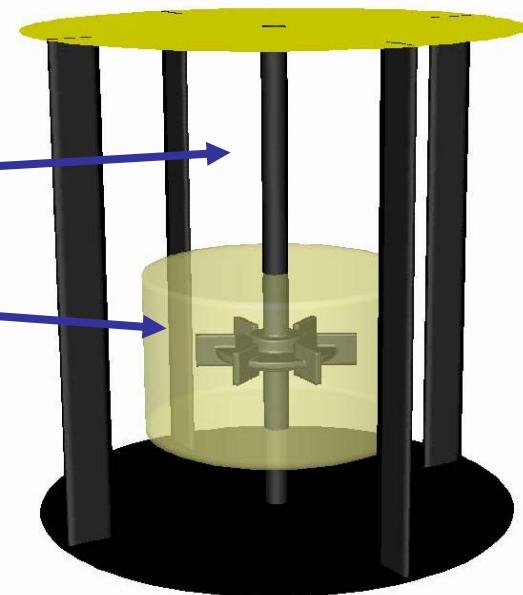
Dispersed phase quantities:

→ from cont. phase quantities, using ratio (eddy-particle interaction time) / (particle relaxation time) and Tchen-theory correlations (Simonin 1990, Tchen 1947)

Modeling of moving parts

Multiple Reference Frame Model (MRF)

- 2 fluid zones defined
 - **Bulk of the tank:** normal inertial r.f.
 - **Impeller zone:** rotating r.f.
 - centrifugal & Coriolis forces in momentum eq.
- Solves **steady** flow field in corresponding r.f.'s
 - **Assumption:** steady flow field at the interface !
 - Holds for weak impeller-baffle interactions (**D/T small !**)
 - **fixed impeller position !!** (frozen rotor approach)



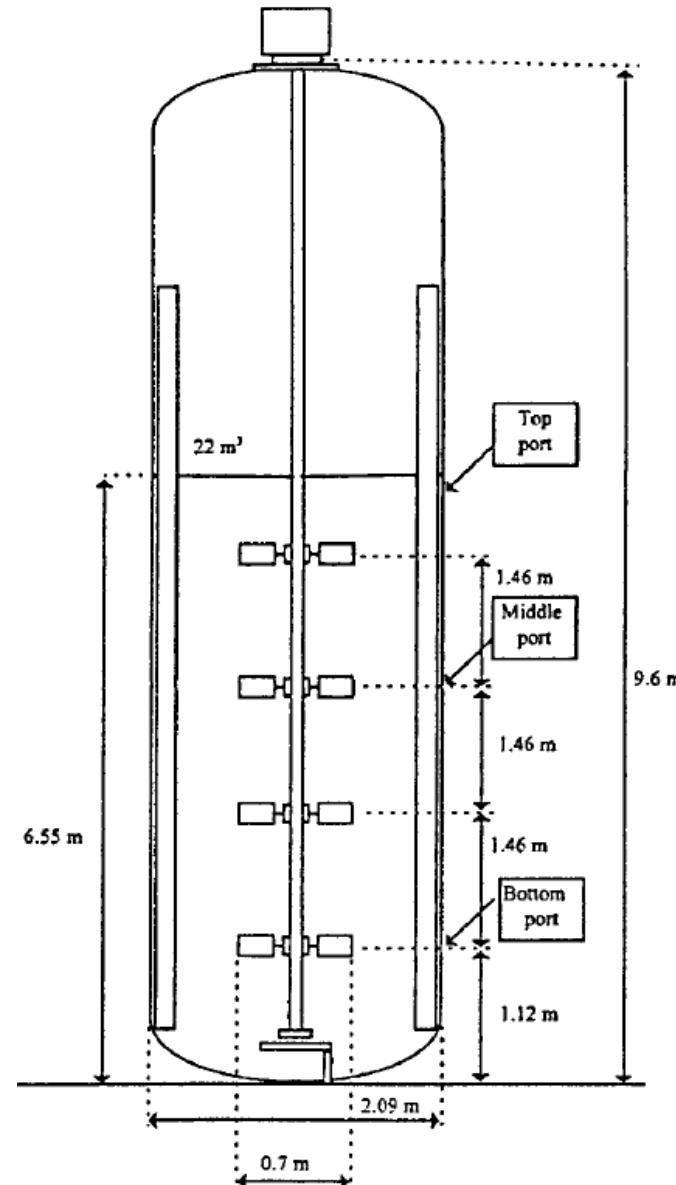
Good agreement with Sliding Mesh Model (Lane 2005, Luo et al. 1994)

→ computational time $\approx \underline{x10 \text{ less}}$!!!

Multi-impeller 30 m³ fermenter

- Tank diameter **T = 2.09 m**
- Impeller diameter **D = 0.70 m ($D/T = 1/3$)**
- Liquid volume: **22 m³** (liquid level: **6.55 m**)
- Total height = **9.6 m**

- **4** vertical baffles (baffle width **0.167 m**)
 - **4** Rushton disc turbines with **6** blades
 - Blade height: **0.14 m**, length: **0.170 m**
 - Bottom & mutual impeller clearance:
 - $C_B=1.12 \text{ m}$, $C_I=1.45 \text{ m}$
- **$C_I/D > 2$**



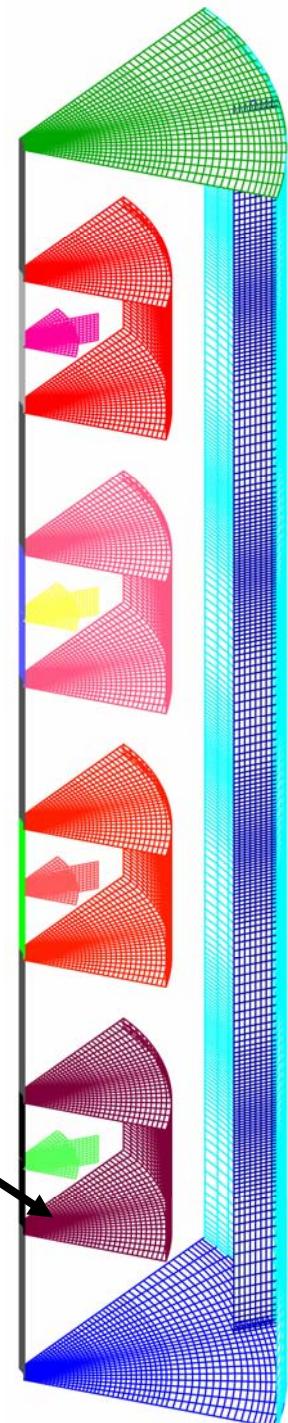
Vrabel et al., 1999

Computational set-up (single-phase)

- Mesh generator: **Gambit 2.3** ; Solver: **Fluent 6.3**
- Domain: **60°** of tank
 - symmetry → 6 baffles
 - extra baffling has negligible effect (Lane 2005)
- Working fluid: **water**
- **324 448** structured cells ($260 \times 52 \times 24$)
- Walls: zero-thickness, no-slip, standard wall functions
- Impeller modeling: **MRF (steady-state)**
 - 4 x moving zone
- Turbulence model: **k- ϵ**
- Discretization scheme: **2nd order upwind, QUICK**

→ Serves as an initial solution for two-phase simulations

MRF grid interface



Single-phase simulations cases

Impeller speed (rpm)	Tip speed (m/s)	$Re = \rho_l N D^2 / \mu_l$
70	2.55	$\sim 570\,000$
115	4.19	$\sim 940\,000$
133	4.85	$\sim 1\,090\,000$

- Convergence after ~ 5100 iterations (residuals $< 10^{-5}$)
- Simulation time ~ 18 h (single CPU)

Basic fluid dynamic parameters – Power Number (N_P)

$$N_P = \frac{P}{\rho_i N^3 D^5}$$

P = Impeller power draw (via dissipation ε or torque Γ)

N = stirring frequency [s^{-1}],

D = impeller diameter ($= T/3$)

fully turbulent ($Re > 2 \times 10^4$), single impeller:

$N_P \approx 5.5$ (Nienow, 1998)

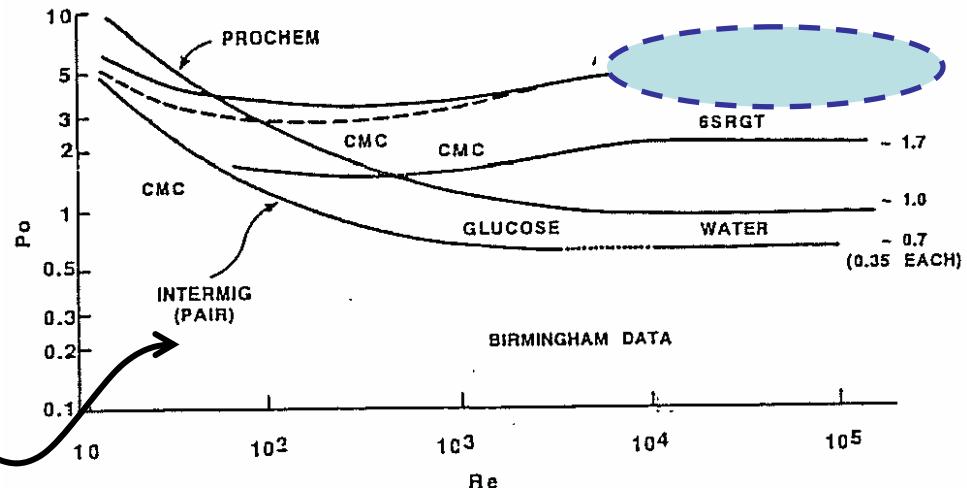


Fig 17. Some typical Po v Re data

Power Draw (P) can be calculated from:

→ Turbulent energy dissipation (ε):

$$P = \int_{V_{\text{tank}}} \rho_i \varepsilon dV$$

→ Torque (Γ) on rotating parts:

$$\Gamma = \left(\int_S \vec{r} \times (\bar{\sigma} \cdot \vec{n}) dS \right) \cdot \vec{a}, \quad P = 2\pi N \Gamma$$

S : surface of rotating parts, \vec{r} : position vector,
 $\bar{\sigma}$: total stress tensor, \vec{n} : unit normal,
 \vec{a} : unit vector parallel to rotation axis

Convergence profiles – Power Number (N_p)

Multi-impeller systems:

when $\Delta C/D > 1.5$:

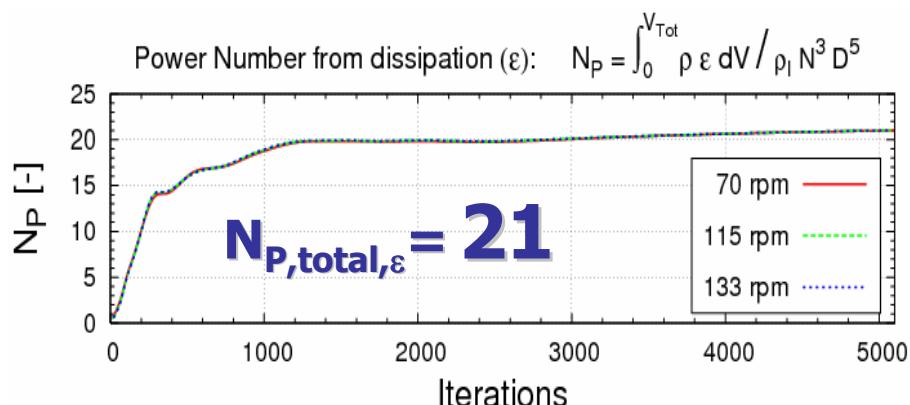
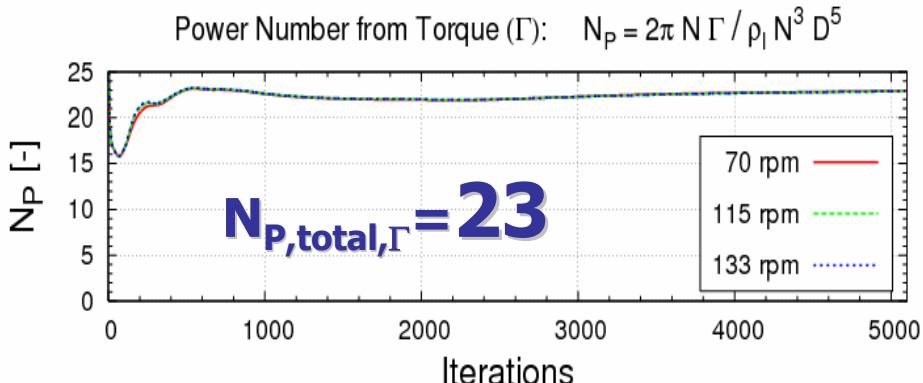
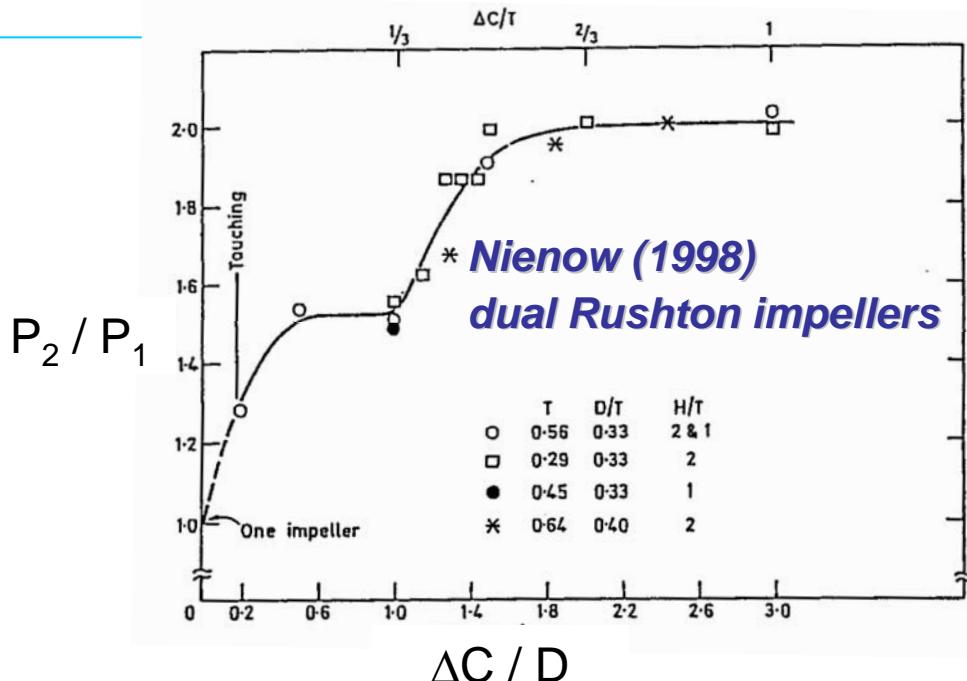
$$(N_p)_n = n(N_p)_{n=1}$$

(for Rushton turbines, ungassed)

our case $\rightarrow \Delta C/D > 2$

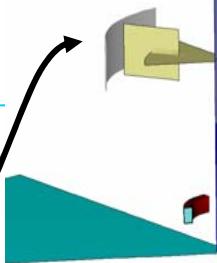
So, ideally we expect:

$$N_{p,\text{total}} = 4 \times N_{p,\text{single}} \approx 22$$



Convergence profiles – Flow Number (N_Q)

Flow Number $N_Q = \frac{Q_I}{ND^3}$ Q_I = Liquid flow through impeller swept area

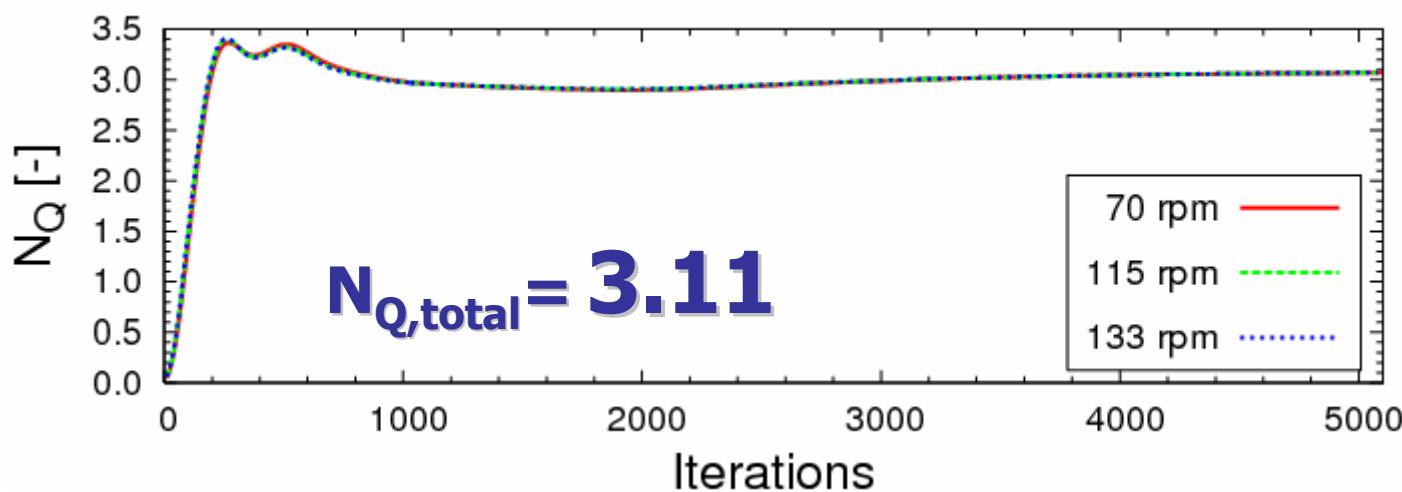
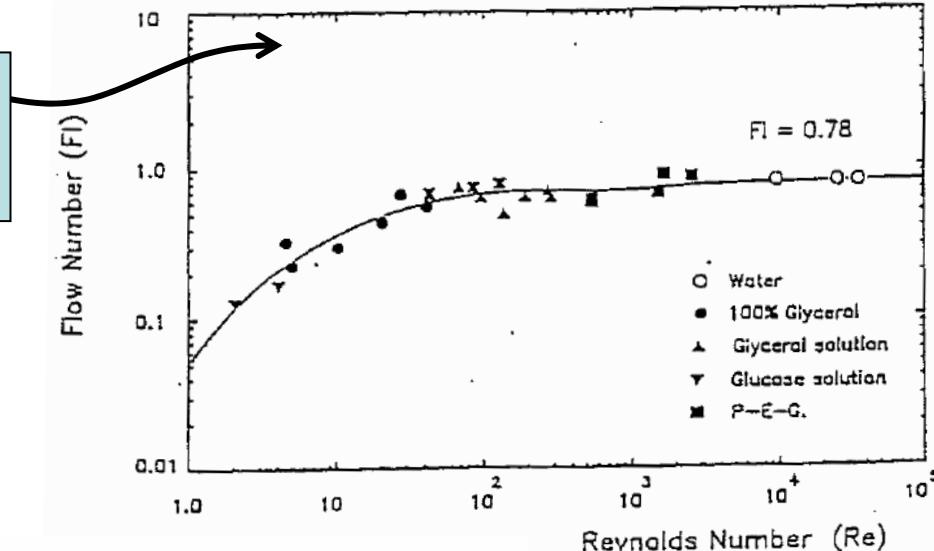


fully turbulent ($Re > 2 \times 10^4$), single impeller:

$N_Q \approx 0.78$ (Nienow, 1998)

So, ideally we expect:

$$N_{Q,\text{total}} = 4 \times N_{Q,\text{single}} \approx 3.12$$



$$N_{Q,\text{total}} = 3.11$$

Mixing time calculations

Scalar transport eq. solved for tracer species

- same properties with bulk fluid
- transient simulation on frozen flow field

Local mass-fraction of species Y_i calculated via **convection-diffusion equation**:

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho \vec{v} Y_i) = -\nabla \cdot \vec{J}_i$$

Diffusion flux for species i
due to concentration
gradients

$$\vec{J}_i = - \left(\rho D_{i,m} + \frac{\mu_t}{Sc_t} \right) \nabla Y_i$$

$D_{i,m}$: Diffusion coefficient for species i in
the mixture (**laminar flow**)

Turbulent Schmidt

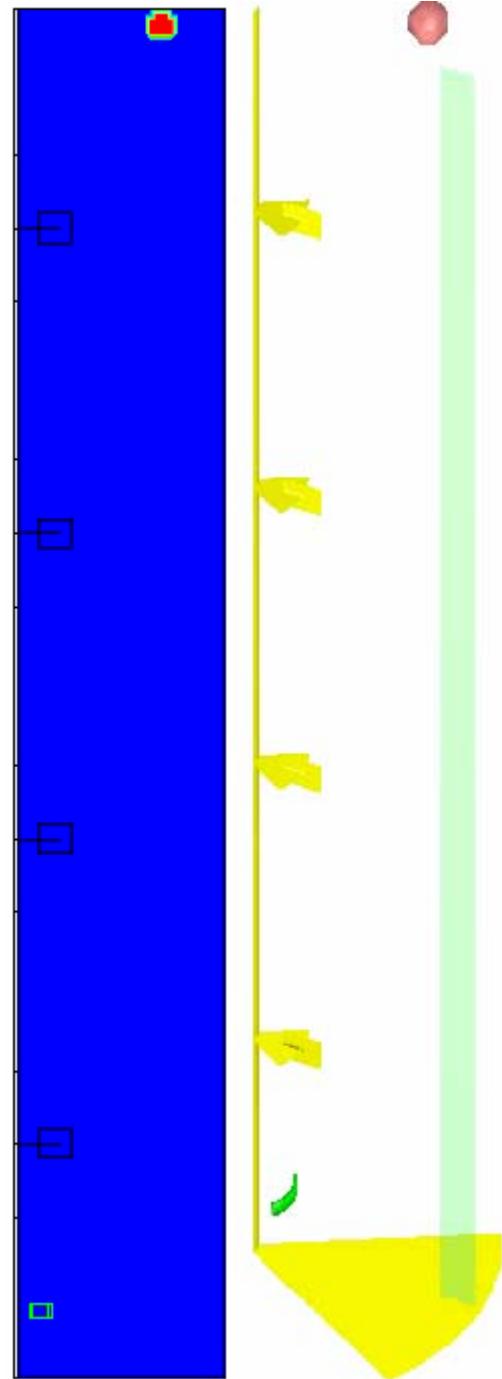
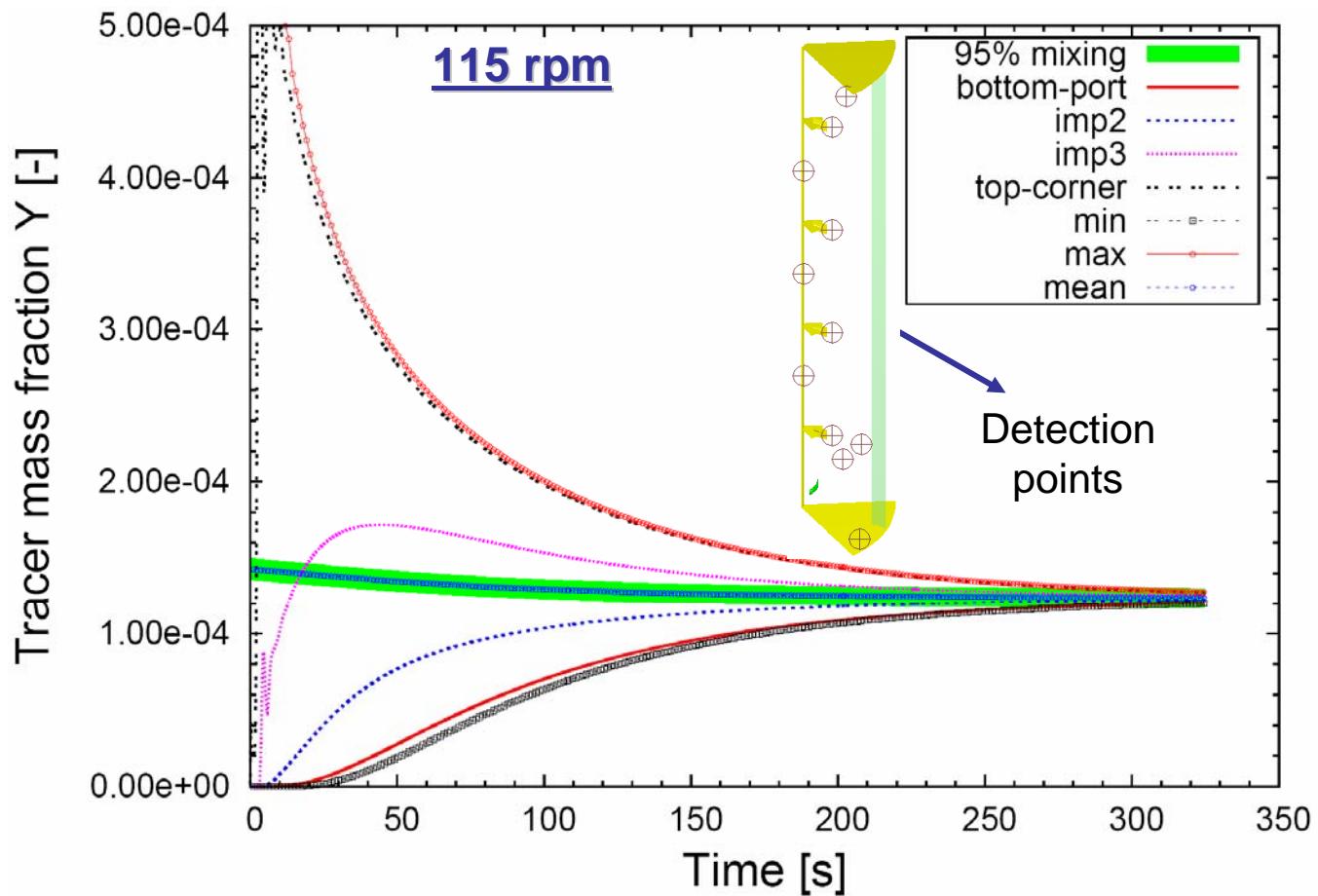
number Sc_t : $\frac{\mu_t}{\rho D_t}$

μ_t : Turbulent viscosity

D_t : Turbulent diffusivity

Point injection close to free surface

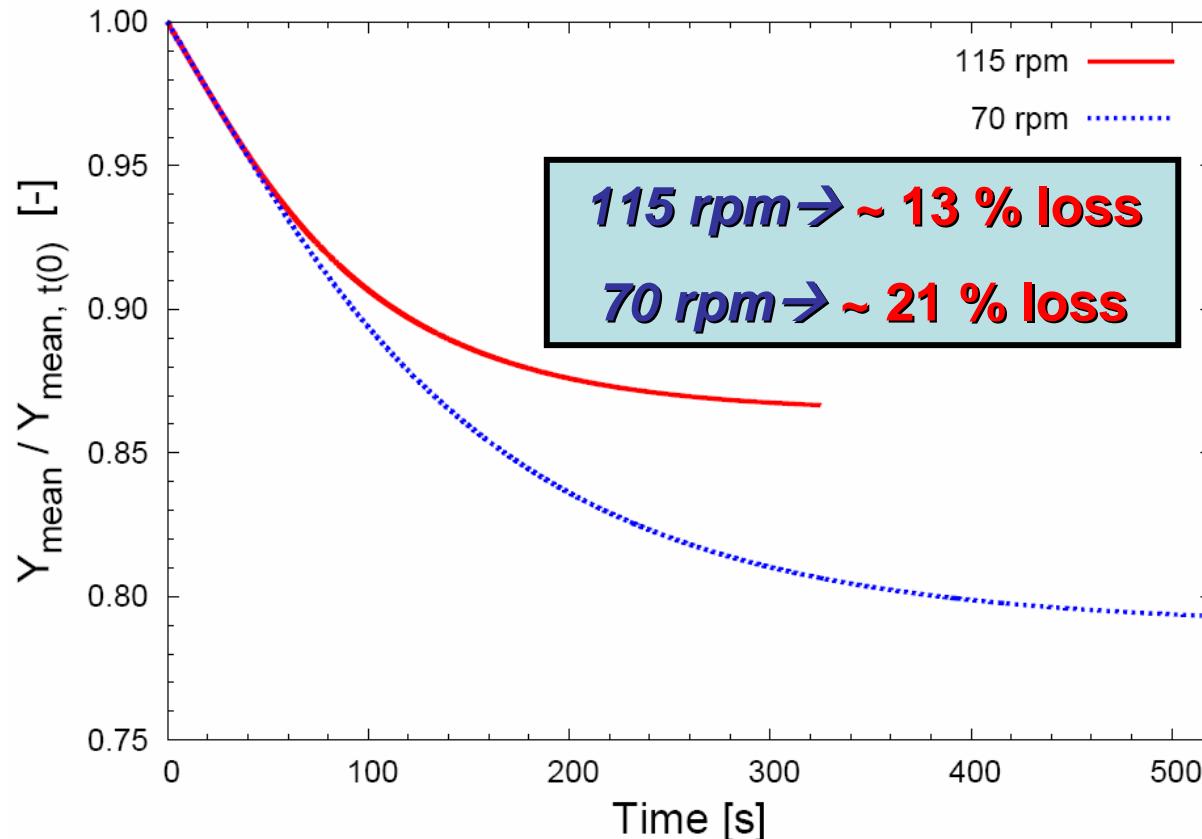
- Injection fluid: tracer species of mass fraction **1.0**
- Overall tracer mass fraction Y_{mean} : **$1.43 \cdot 10^{-4}$**



Tracer mass conservation

Tracer mass not conserved !

- *Indicates a problem in solving tracer transport equation under MRF formulation*
- *Further investigation needed (reported to FLUENT Support)*



Comparison with experiments

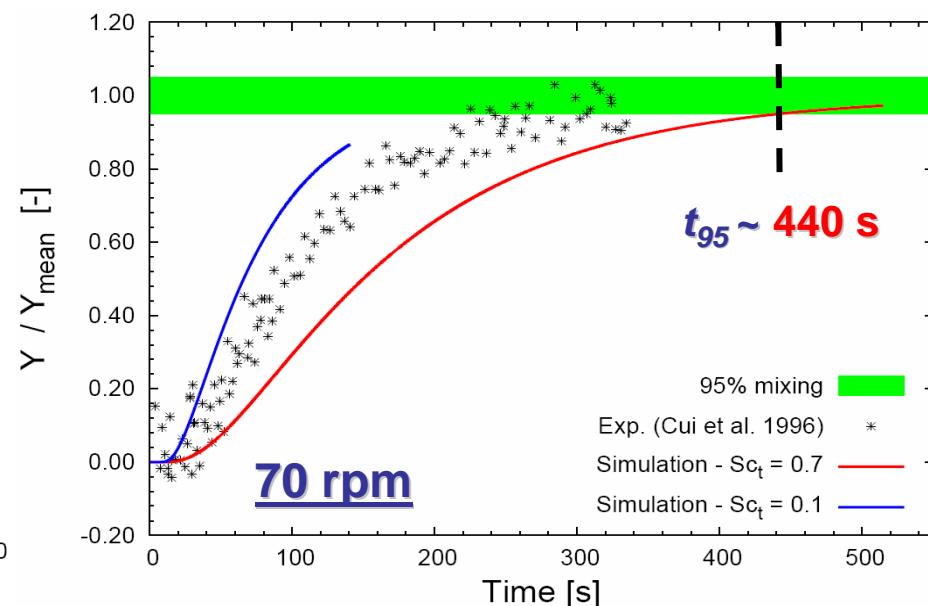
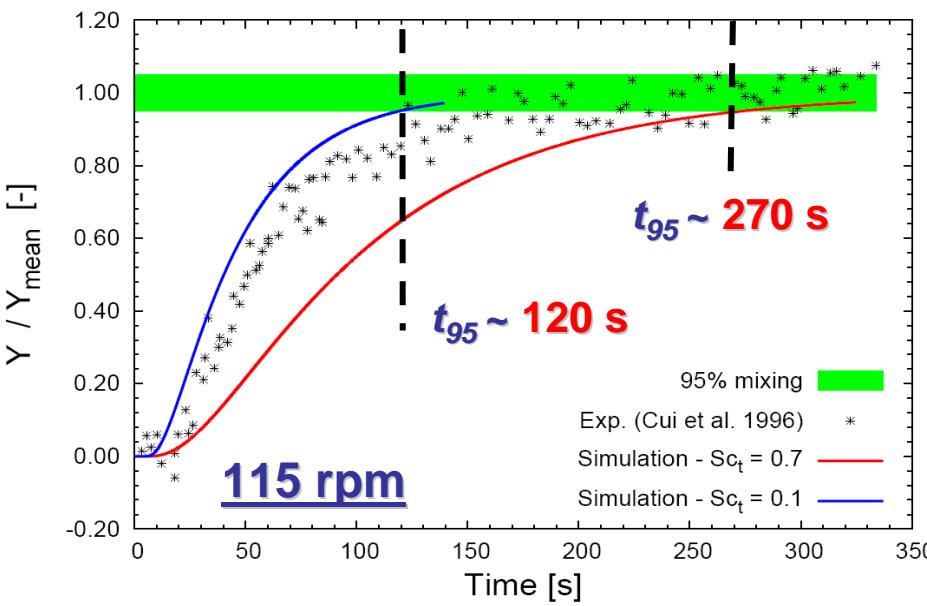
Fluorescent tracer pulse-response experiments from Cui et al. (1996):
(Injection at top, detection at bottom impeller outflow)

$$t_{95} \text{ (115 rpm)} \sim 150 \text{ s} ; t_{95} \text{ (70 rpm)} \sim 280 \text{ s}$$

Montante and Magelli (2004):

$Sc_t = 0.7 \rightarrow$ overestimation of t_{95} by **140 %** !

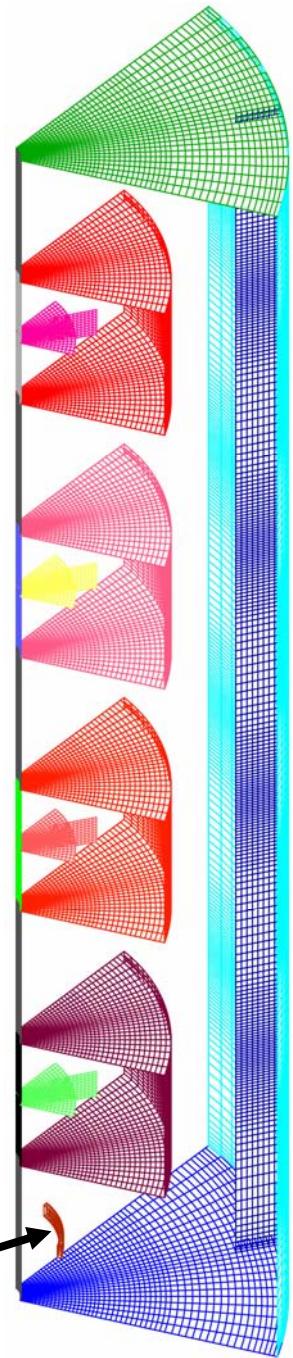
$Sc_t = 0.1 \rightarrow$ good agreement with experimental data (for Rushton & PBT)



Computational set-up (two-phase)

- Working fluid: **air-water**
- Impeller modeling: **MRF (steady-state)**
- Multiphase model: **Euler-Euler (2-fluid) Model**
- Turbulence model: **$k-\varepsilon$**
- De-gassing BC at free surface
- **Ring sparger** via mass & momentum source terms
- Discretization scheme: **1st/2nd order upwind, QUICK**
- **Fixed bubble diameter $\rightarrow d_b = 1, 2, 3 \text{ mm}$**
- Interface forces:
 - **Drag:** Schiller & Naumann (1935)
 - **Virtual Mass (VM)**

***Ring
sparger***



Two-phase simulations cases

	Impeller speed [rpm]	Aeration rate [m^3/s]	Sup. gas vel. [cm/s] $V_{Gs}=Q_g/\pi/4T^2$	Gas flow nr. [-] $Fl_g=Q_g/ND^3$	Froude nr. [-] $Fr=N^2D/g$
Case 1:	115	0.0263	0.77	0.040	0.261
Case 2:	115	0.0526	1.53	0.080	0.261
Case 3:	70	0.0263	0.77	0.067	0.097
Case 4:	70	0.0526	1.53	0.133	0.097

Some experimental data (gas holdup, P_g/P) available for these conditions (Vrabel et al. 1998, 2000)

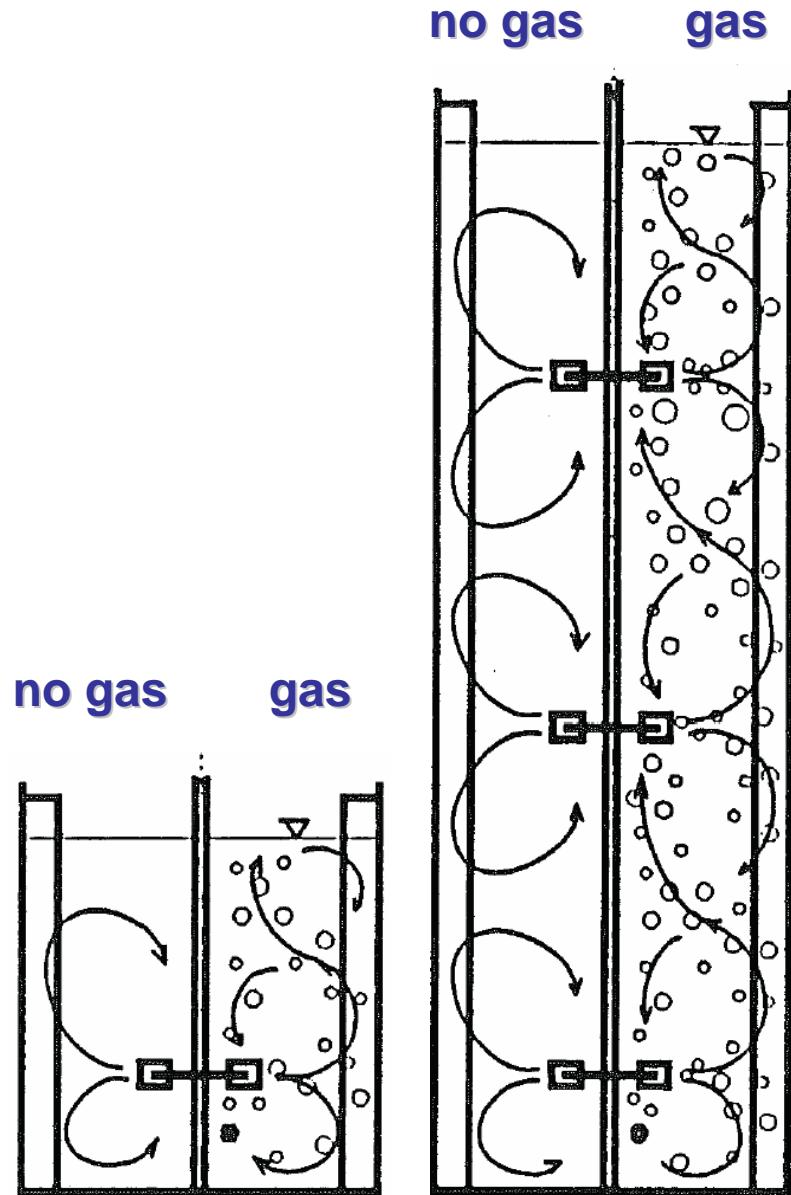
Global flow patterns - (*Rushton turbines*)

Non-Aerated

- If $C_I/D > 1.2-1.5$, parallel independent flow patterns similar to single-impellers (*Nienow 1998*)
- Secondary vortex at the top (*Schafer et al. 1997*)

Aerated

- Additional liquid stream connects adjacent impeller zones
- Secondary circulatory liquid cell forms at the top (*Rousar & van den Akker, 1994*)

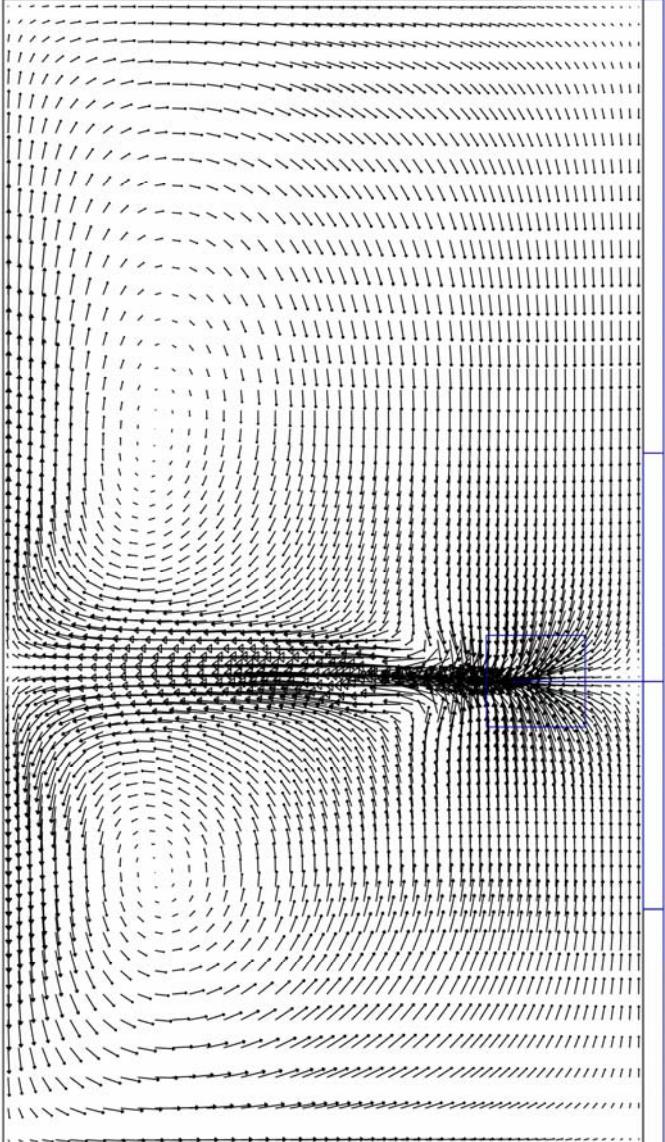


(*Rousar & van den Akker, 1994*)

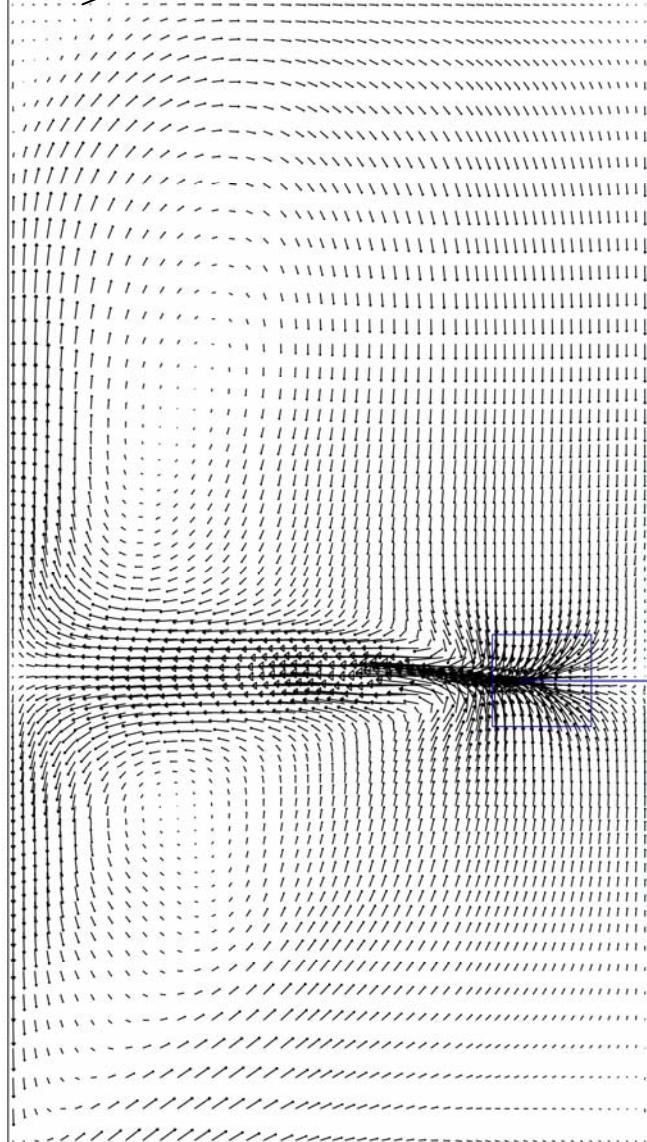
Global flow patterns – liquid velocity field

115 rpm - 0.0526 m³/s (3 mm, 2nd upw, VM)

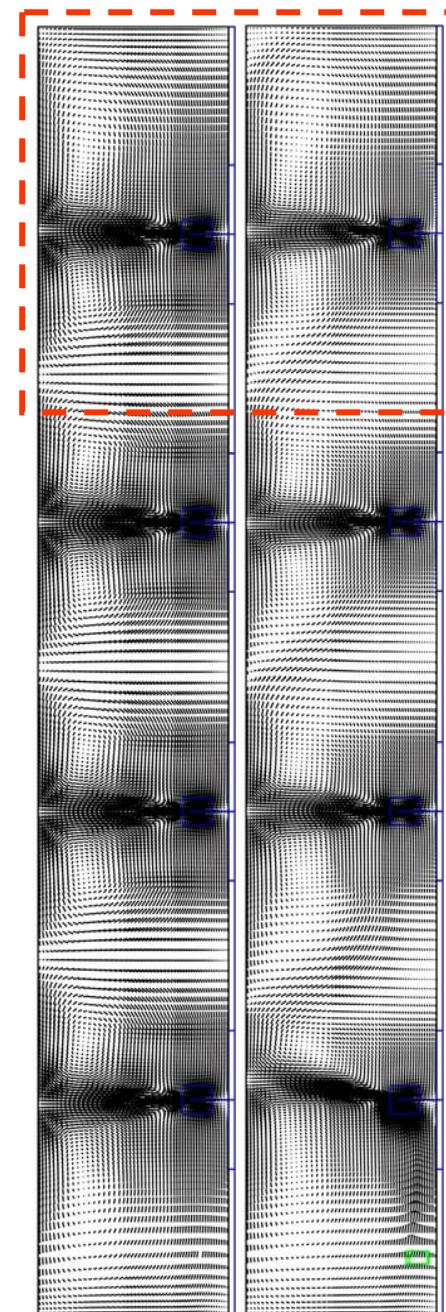
no gas



circulation
gas

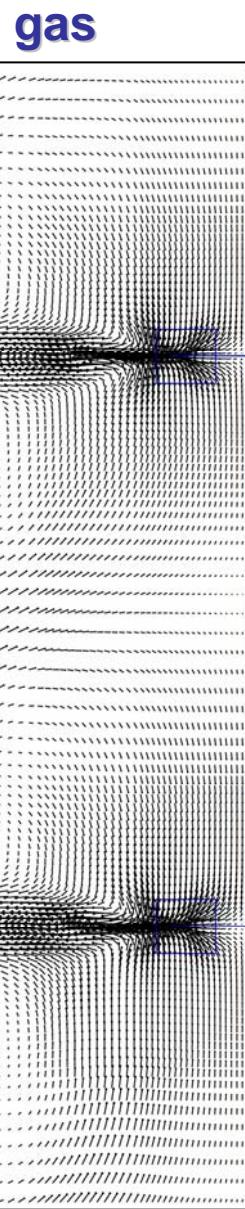
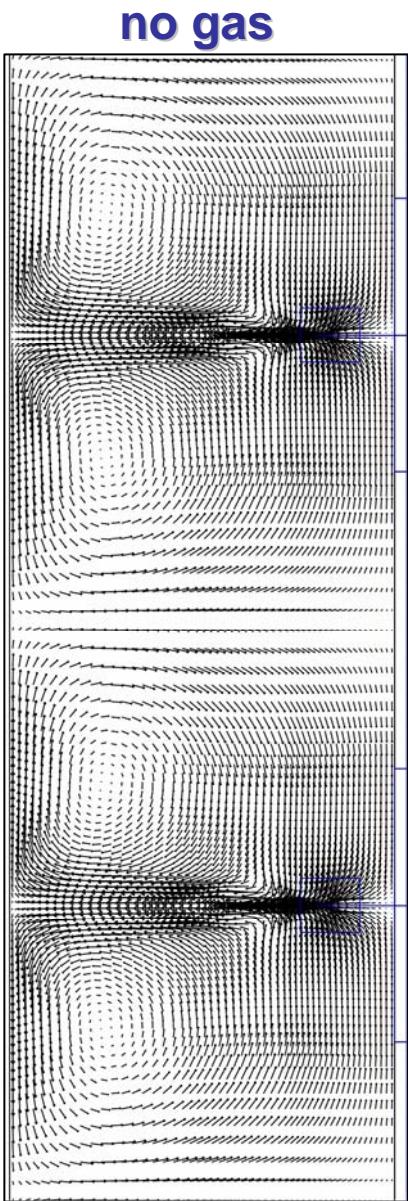


no gas gas

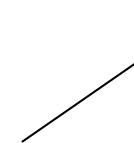


Global flow patterns – liquid velocity field

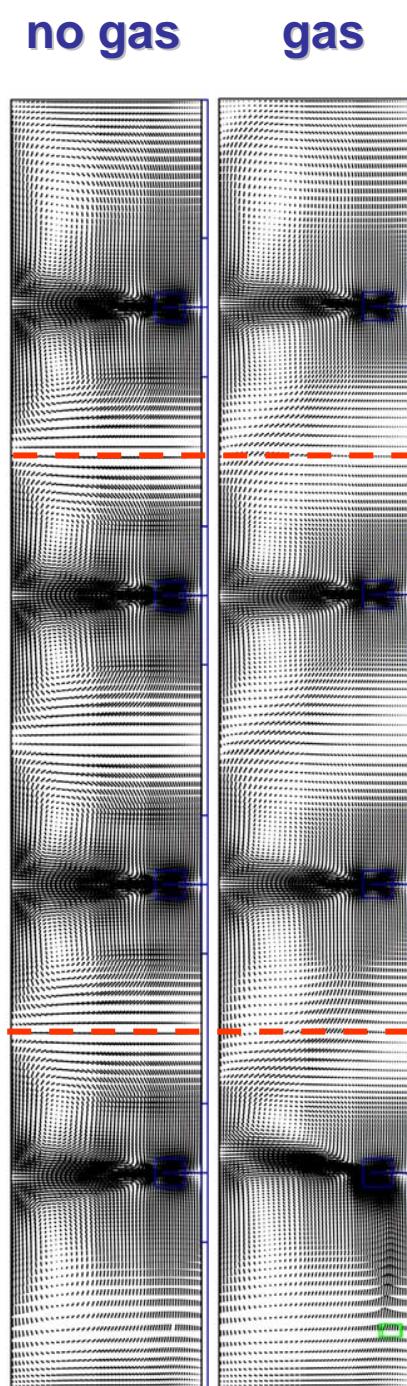
115 rpm - 0.0526 m³/s (3 mm, 2nd upw, VM)



Liquid stream
connecting
adjacent zones



A red arrow points from the text 'Liquid stream connecting adjacent zones' to a specific feature in the 'gas' flow pattern, indicating a vertical stream of liquid that links different flow regions.



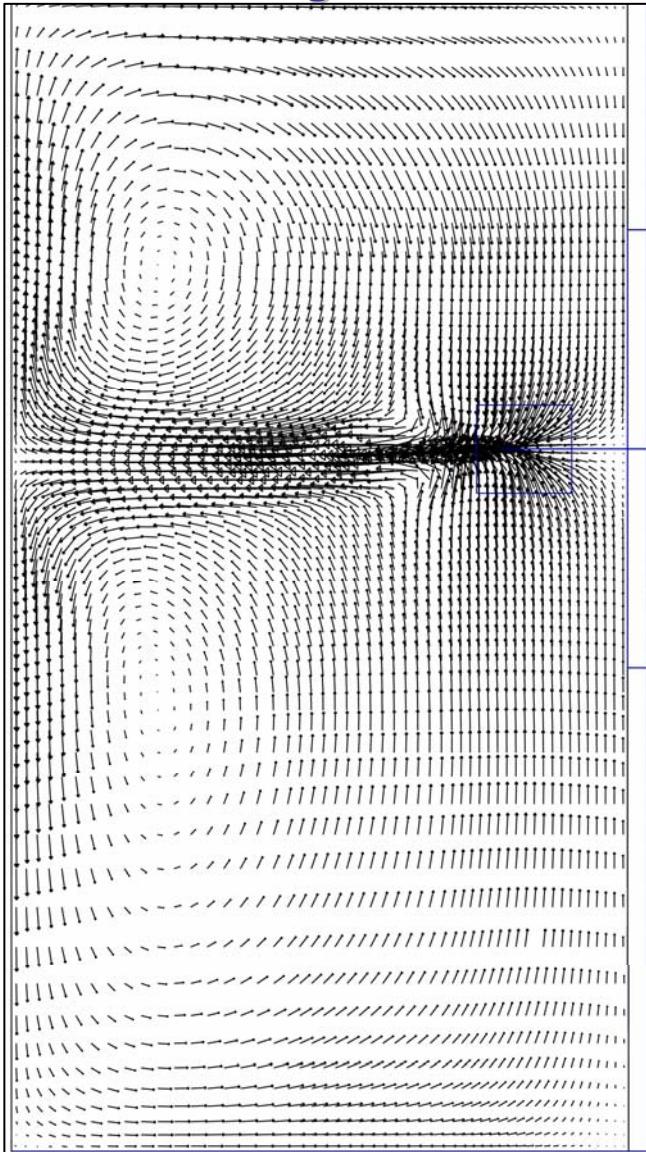
Global flow patterns – liquid velocity field

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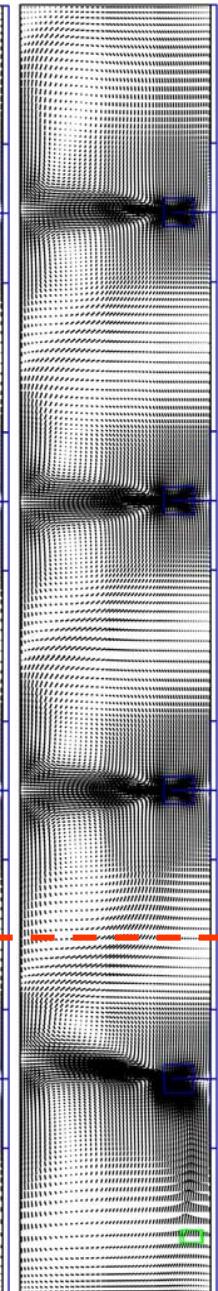
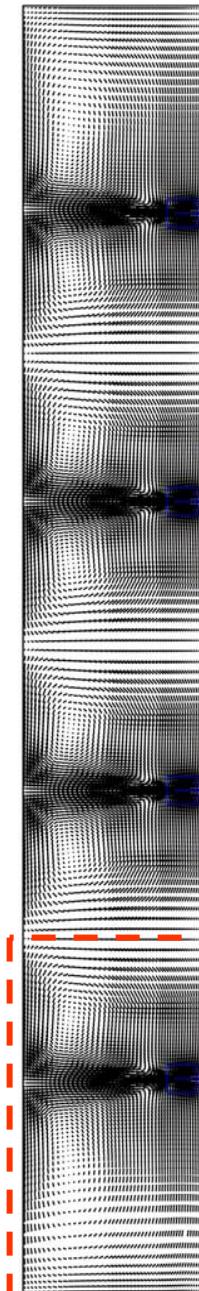
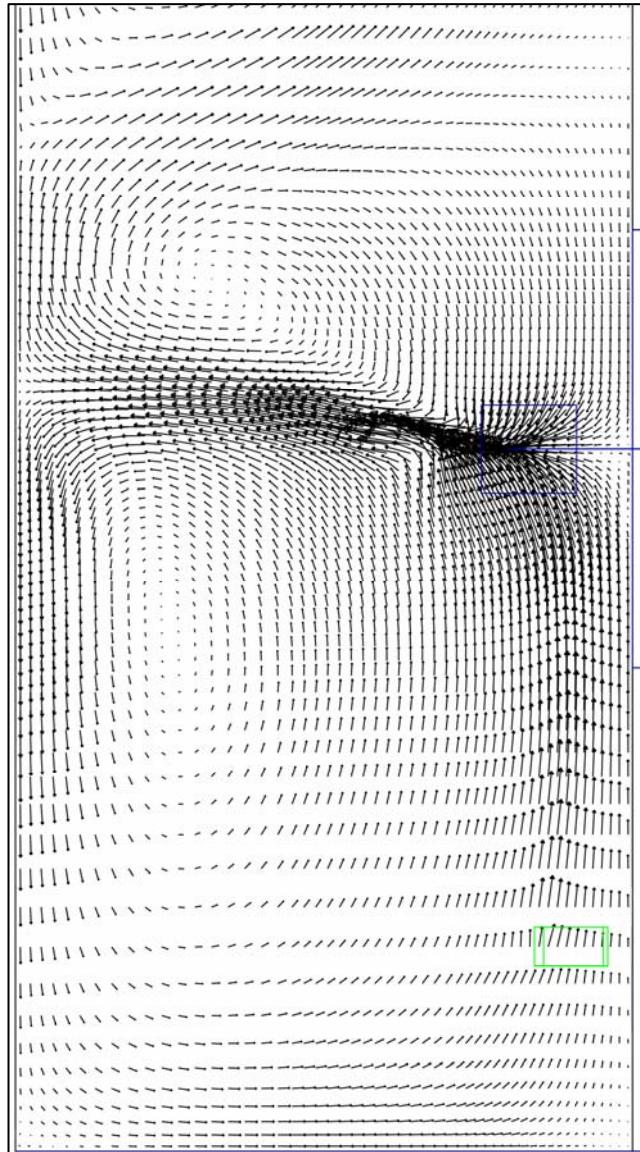
no gas

gas

no gas



gas



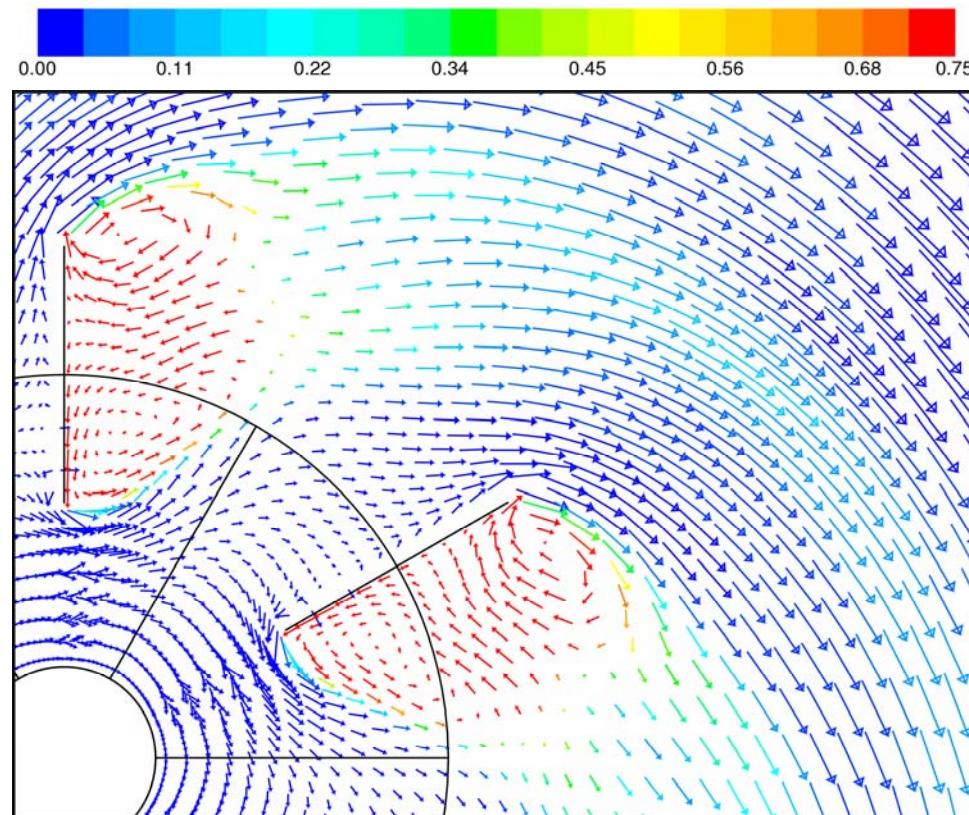
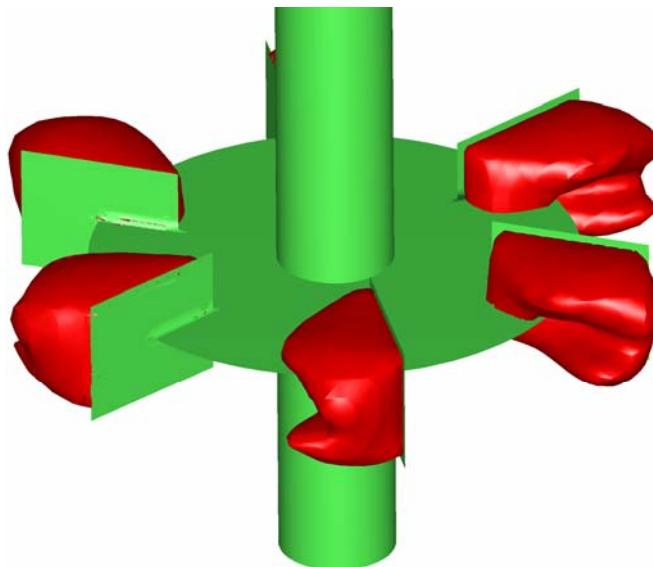
Cavity formation behind blades – bottom impeller

115 rpm - 0.0526 m³/s

Gas velocity field

- w.r.t. rotating reference frame at y=1.17 m (above impeller centerline)
- coloured by gas volume fraction

- Clinging cavities formed
- Highest gas at bottom impeller
- 2 circulation zones evident



Iso-surface of $\alpha=0.75$

Flow regime map (bottom impeller)

Transition loading-flooding*:

$$(Fl_g)_F = 30 \left(\frac{D}{T} \right)^{3.5} (Fr)_F$$

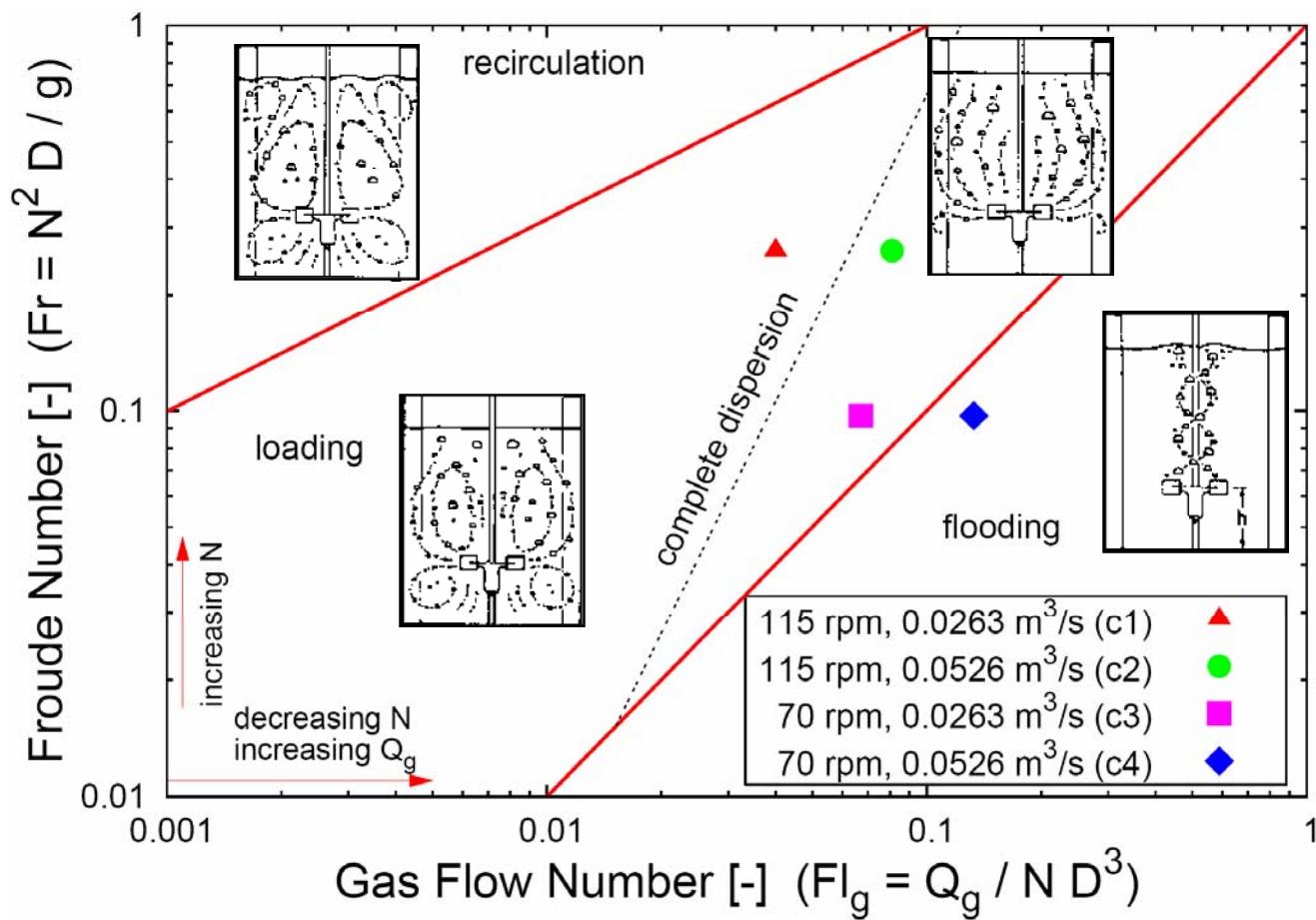
Complete dispersion condition*:

$$(Fl_g)_{CD} = 0.2 \left(\frac{D}{T} \right)^{0.5} (Fr)_{CD}^{0.5}$$

Transition loading-complete recirculation*:

$$(Fl_g)_R = 13 \left(\frac{D}{T} \right)^5 (Fr)_R^2$$

* Nienow et al. 1978, 1989 (coalescing systems, $H = T < 1.8$ m, $C = T/4$)



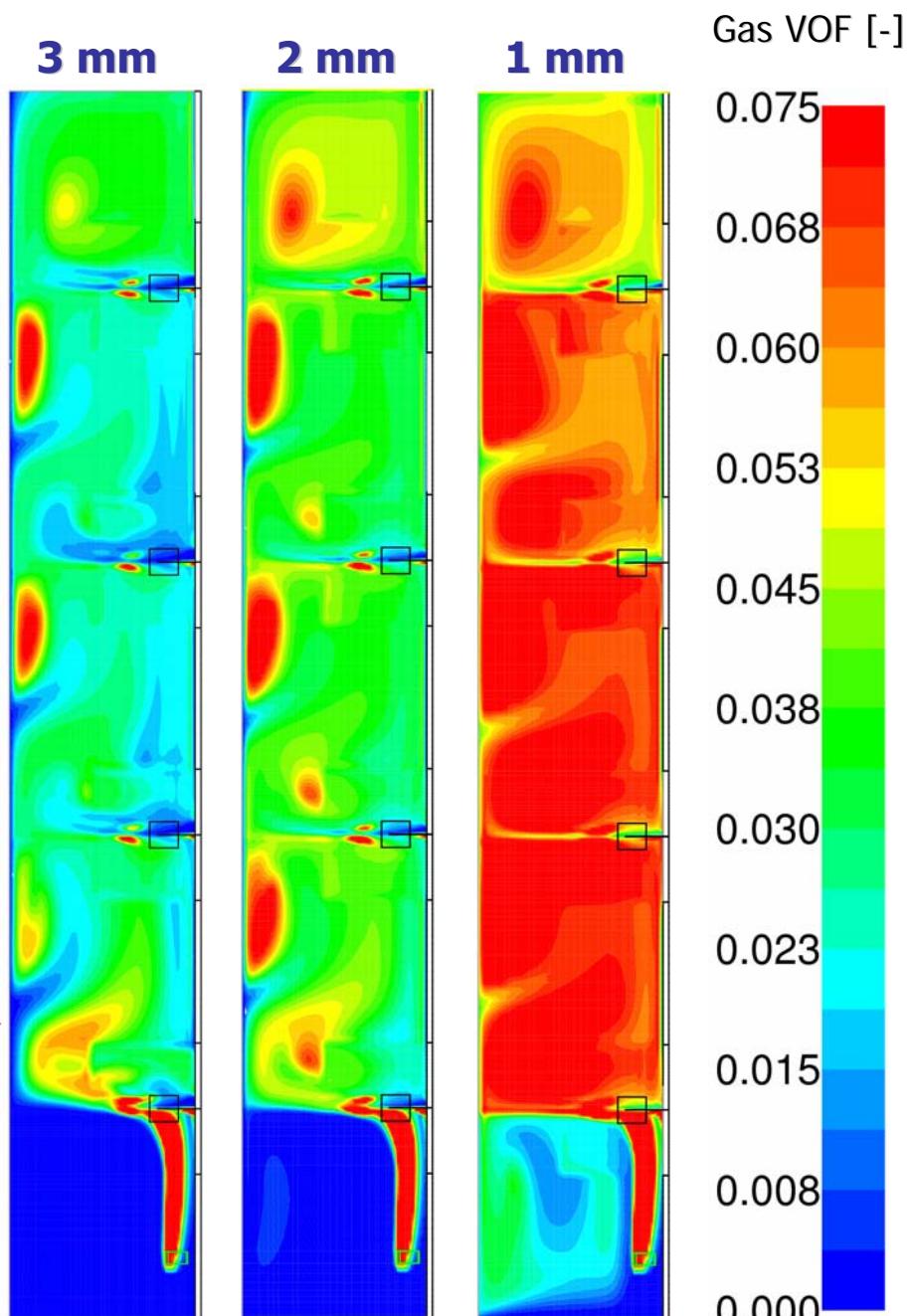
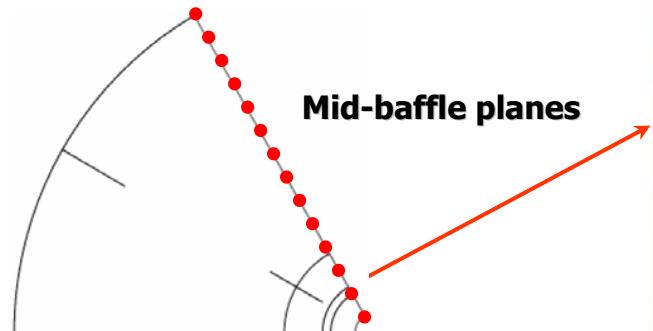
Bubble sizes

115 rpm - 0.0263 m³/s

- Drag only, 1st upwind

Case 1	Exp. ¹	3 mm	2 mm	1 mm
Holdup [%]	4.7	2.6	3.7	6.8
$P_g/P^*[-]$	0.65	0.80	0.80	0.82

(* P and P_g calculated from torque Γ)



¹Experimental (Vrabel et al. 1999, 2000)

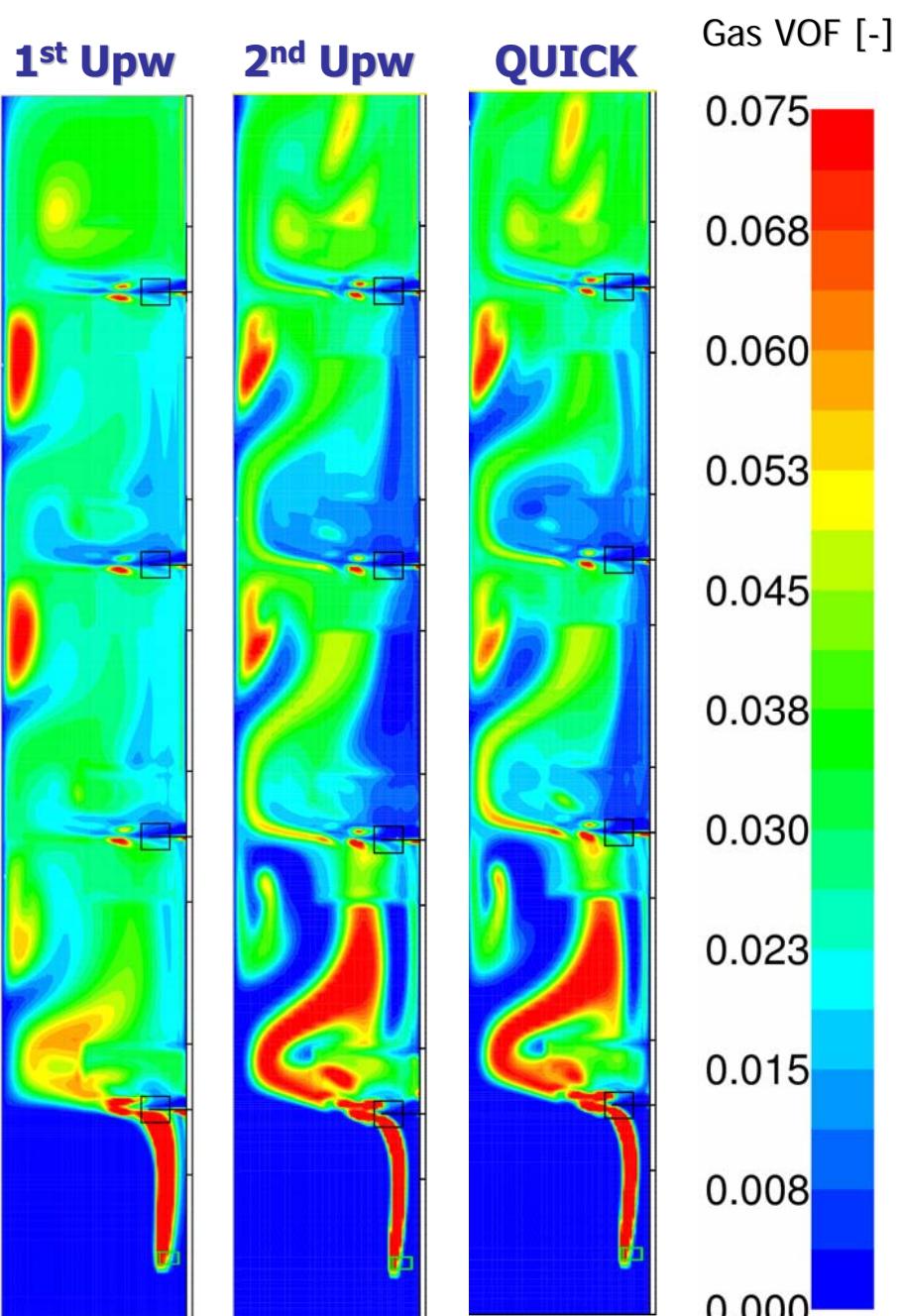
Discretization schemes

115 rpm - 0.0263 m³/s

- Drag only, 3 mm
- **QUICK:** weighted avg. of 2nd upw. and 2nd central interp.

Case 1	Exp. ¹	1 st upw	2 nd upw	QUICK
Holdup [%]	4.7	2.6	2.5	2.5
P _g /P [-]	0.65	0.80	0.63	0.63

- 1st upw. diffusive
 → 2nd upw. & QUICK very similar



¹Experimental (Vrabel et al. 1999, 2000)

Interfacial forces – Virtual Mass

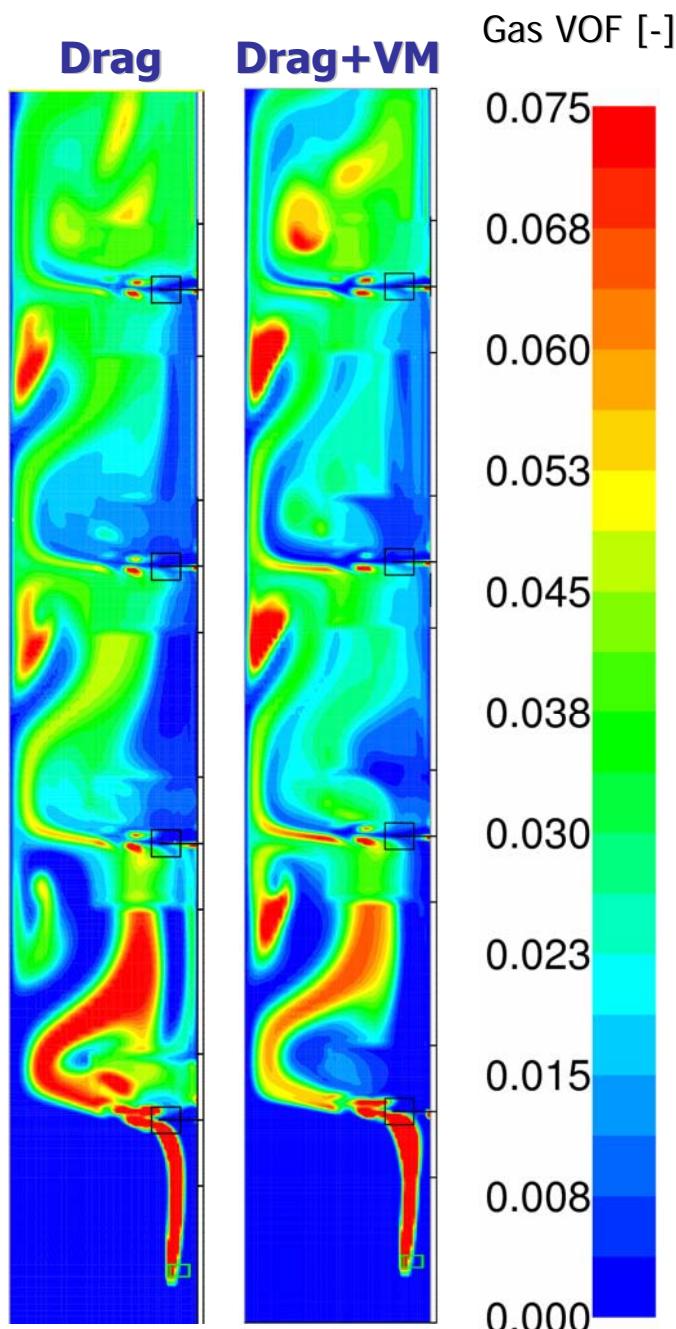
115 rpm - 0.0263 m³/s

- 3 mm, 2nd upwind

Case 1	Exp. ¹	Drag	Drag+VM
Holdup [%]	4.7	2.5	2.5
P _g /P [-]	0.65	0.63	0.81

- Holdups same, BUT gas distribution changes
- More gas at recirculation regions

! Lift and turbulent dispersion forces not included (divergence)



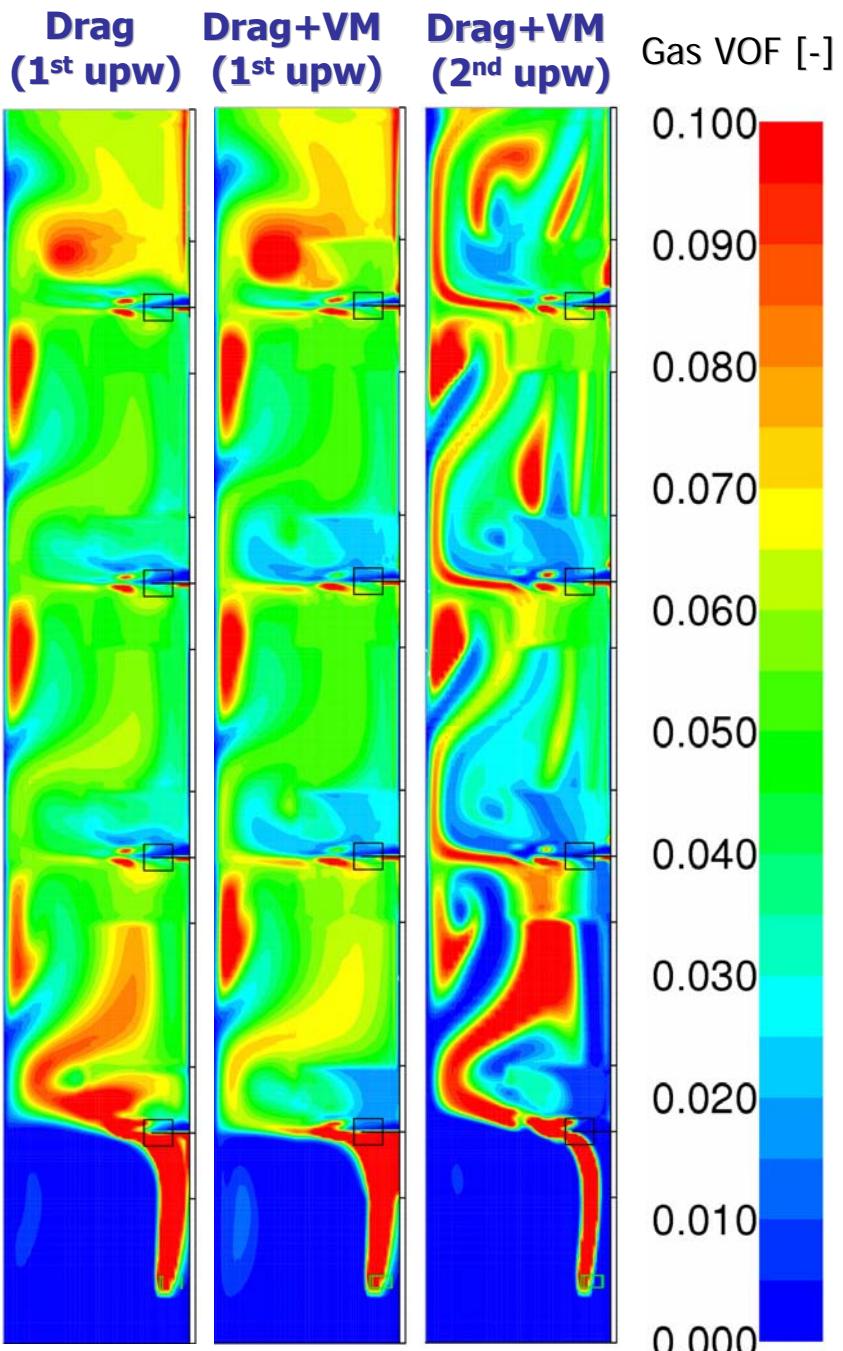
¹Experimental (Vrabel et al. 1999, 2000)

Increasing aeration

115 rpm - 0.0526 m³/s

- 3 mm

Case 2	Exp. ¹	Drag (1 st upw)	Drag+VM (1 st upw)	Drag+VM (2 nd upw)
Holdup [%]	8.9	4.6	4.6	4.2
P _g /P [-]	0.54	0.70	0.81	0.70



→ Holdups lower than exp.

→ P_g overestimated

→ No convergence for Drag only
(2nd upw)

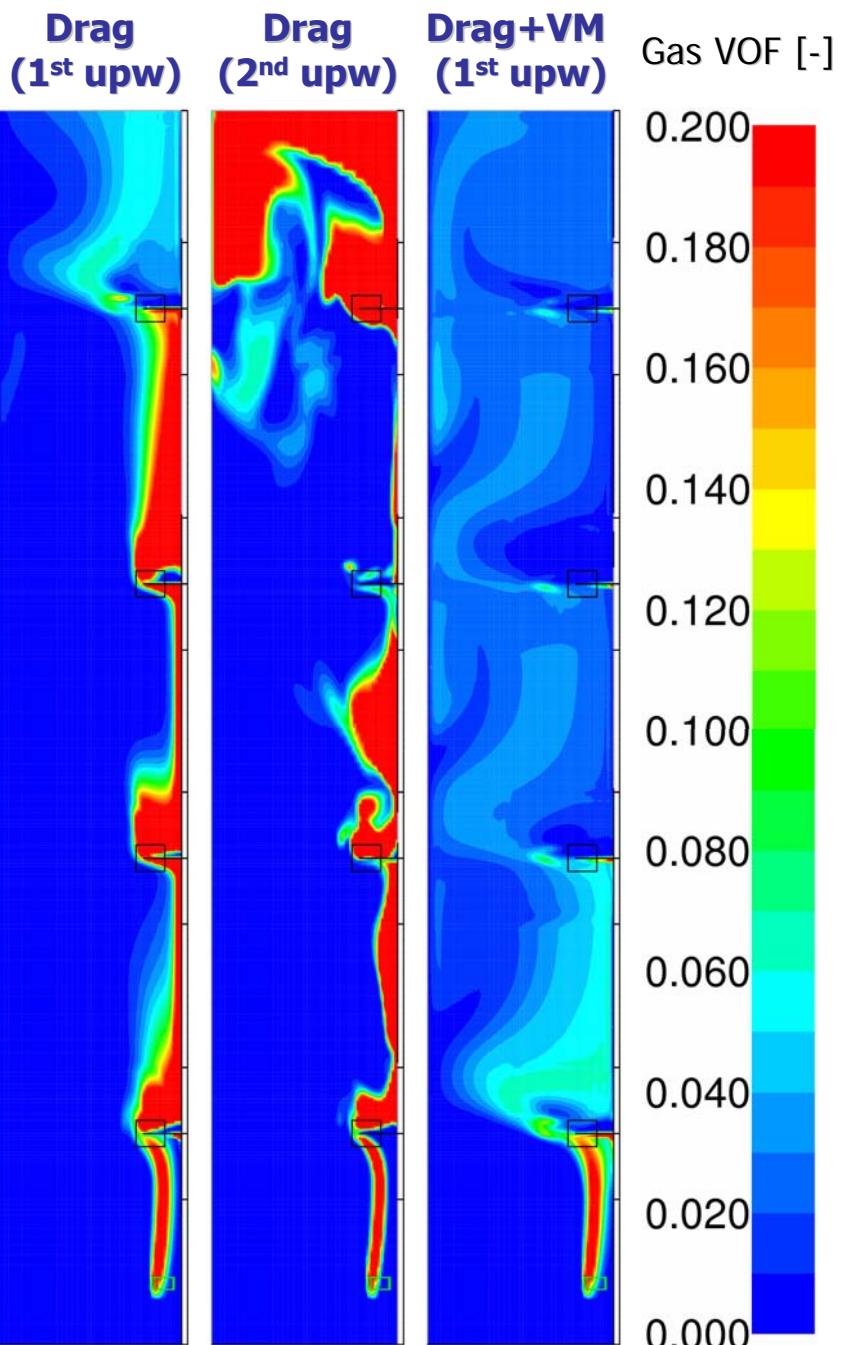
¹Experimental (Vrabel et al. 1999, 2000)

Decreasing stirring rate

70 rpm - 0.0263 m³/s

- 3 mm

Case 3	Exp. ¹	Drag (1 st upw)	Drag (2 nd upw)	Drag+VM (1 st upw)
Holdup [%]	4.0	1.4 ?	5.5 ?	2.2
P _g /P [-]	-	0.61 ?	0.65 ?	0.90



→ Convergence problems...

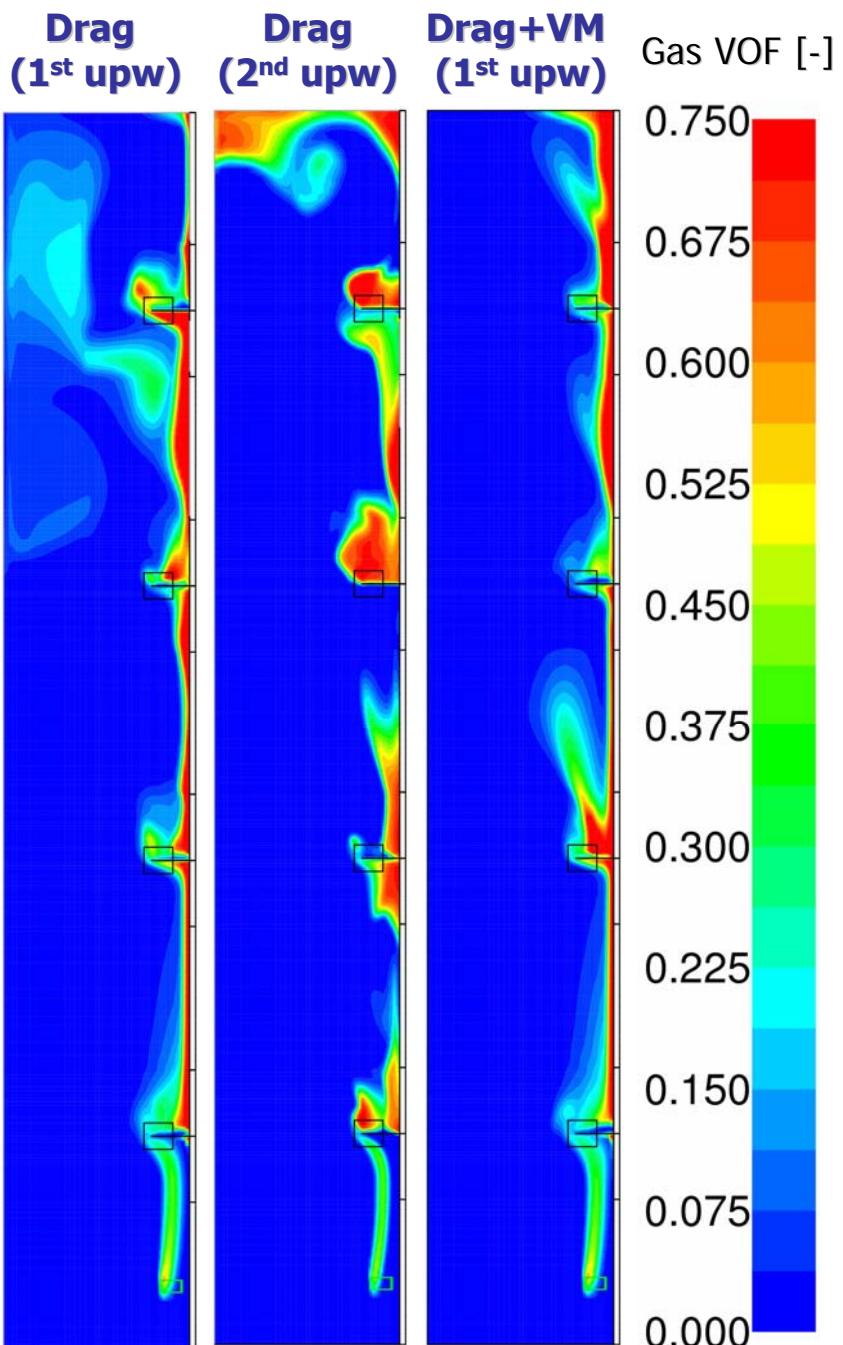
¹Experimental (Vrabel et al. 1999, 2000)

Increasing aeration

70 rpm - 0.0526 m³/s

- 3 mm

Case 4	Exp. ¹	Drag (1 st upw)	Drag (2 nd upw)	Drag+VM (1 st upw)
Holdup [%]	7.3	4.0 ?	4.9 ?	1.8 ?
P _g /P [-]	-	0.50 ?	0.70 ?	0.54 ?



→ Experimental: **FLOODING**

→ Convergence problems...

¹Experimental (Vrabel et al. 1999, 2000)

Conclusions

Single-phase results:

- Good prediction of relevant non-dimensional numbers, MRF promising
- Problems with mixing calculations – loss of tracer mass

Two-phase results:

- Global flow fields are captured; gas distributions show the expected tendencies
- Flow regime transition from loading to flooding captured
- Holdups underestimated
 - Due to single bubble class (3 mm) → ***Population balance modeling in progress***
 - Modifications to interfacial forces for high gas fractions and turbulence also needed
- Gassed power draws inconsistent
- Convergence problems (for cases with low Froude Nr. → gravity dominates!)
 - due to transient nature of flooding → ***Transient simulations in progress***