UNIVERSITEIT GENT

FACULTY OF ENGINEERING AND ARCHITECTURE

Modeling Fast Biomass Pyrolysis in a Gas/Solid Vortex Reactor

Robert W. Ashcraft, Jelena Kovacevic,

Geraldine J. Heynderickx, Guy B. Marin

Laboratory for Chemical Technology, Ghent University

http://www.lct.UGent.be

ISCRE-22, Maastricht, 04 Sept. 2012

European Research Institute of Catalysis

History and Description

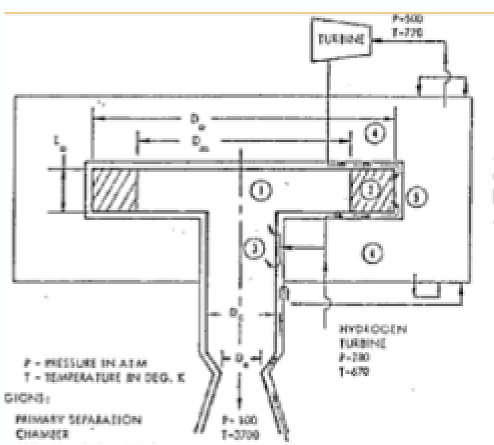
Vortex Reactor Development Timeline

1961 — 1969 — 1971 — 1974 — 1992 — 1993 — 1999 — 2005 — 2006 - present

Kerrebrock et al., 1961,
"Vortex containment for the gaseous-fission rocket"

Kochetov et al., 1969,
Vortex drying chambers

Anderson et al., 1971,
Colloid core nuclear rocket



Folsom, 1974,
Annular fluidized beds

Loftus et al., 1992,
Flue gas scrubbing

Volchkov et al., 1993,
Fluid dynamics in vortex chambers

Haldipure et al., 1999,
Liquid/solid vortex contactor

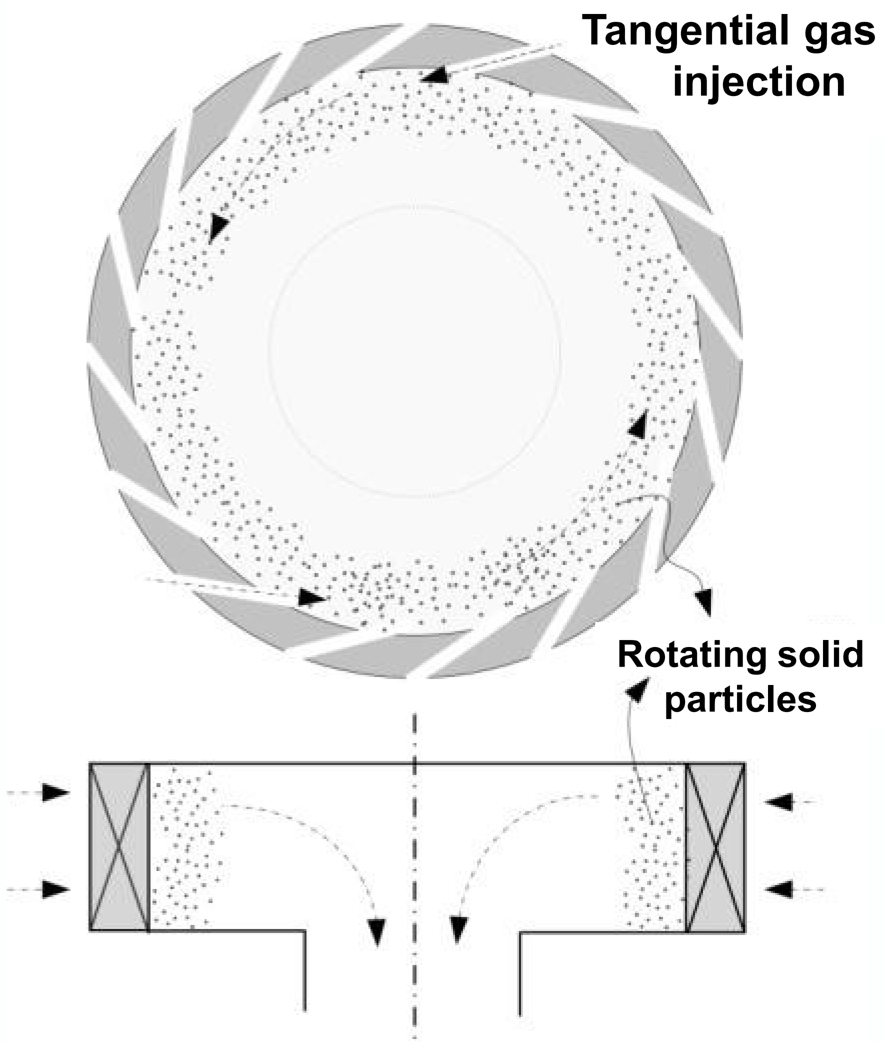
Kuzmin et al., 2005,
Vortex centrifugal bubbling reactor

Recent Work:

- De Broqueville
- De Wilde
- Kuzmin
- Marin
- Parmon
- Ryazantsev
- Trachuk

- ➢ Hydrodynamics
- ➢ Mass & Heat Transfer
- ➢ FCC
- ➢ Biomass gasification
- ➢ Adsorption

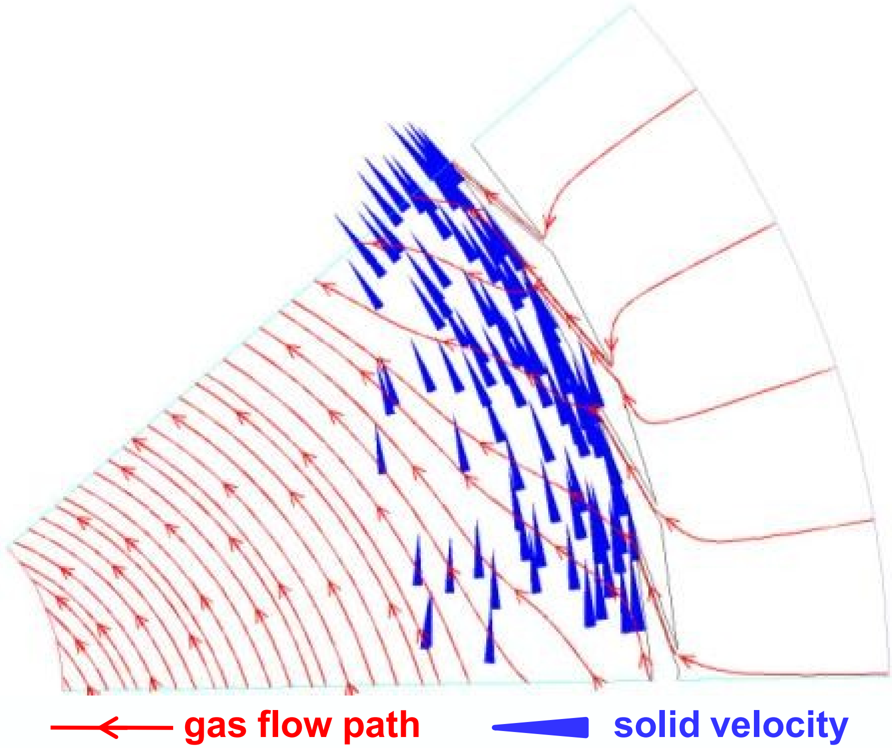
Gas/Solid Vortex Reactor (GSVR)



GSVR Characteristics:

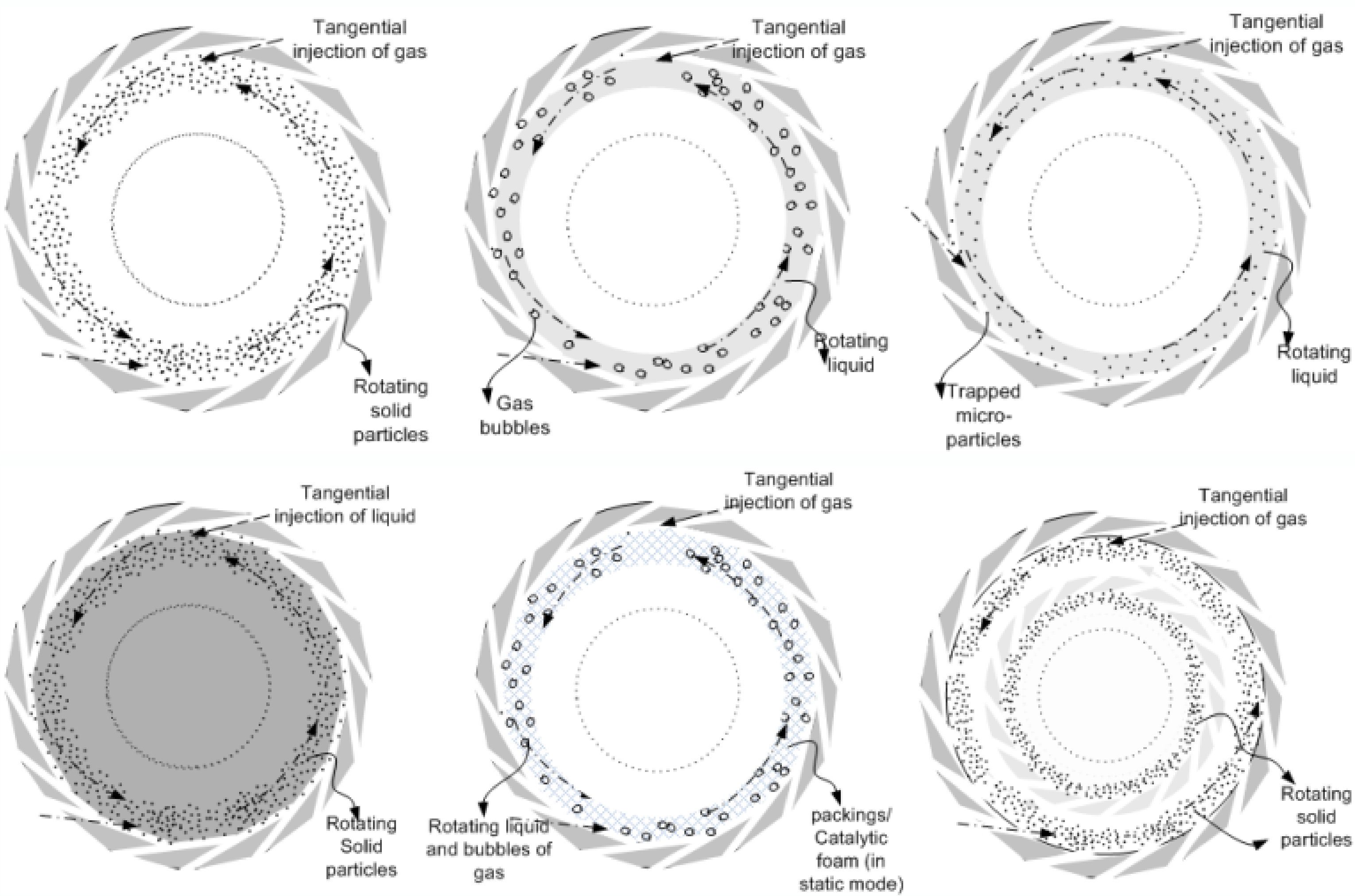
- Gas injection forces bed rotation & induces fluidization
- Centrifugal forces resist drag

➢ Dense bed
➢ High radial slip velocity



General Vortex Reactors

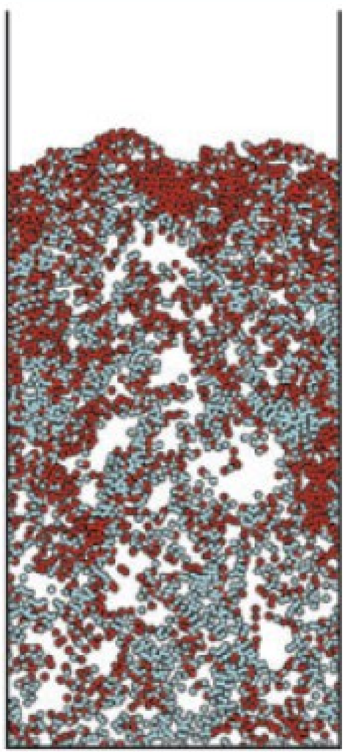
Rotating Bed Reactors in a Static Geometry (RBR-SG)



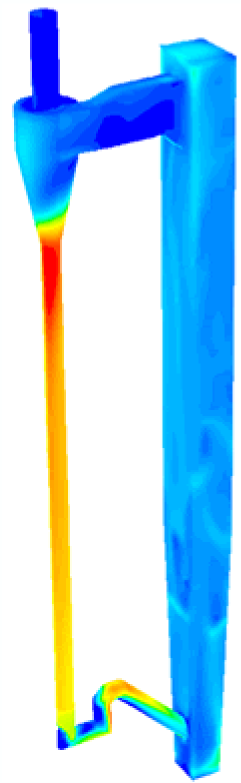
[Anderson et al, 1972], [Kuzmin et al, 2005], [Loftus et al, 1992, Fichman, et al, 2008], [Haldipur P, 1999], [Trachuk A. V., 2009], [Entoleter Inc, 1973]

Gas/Solid Fluidization Reactors

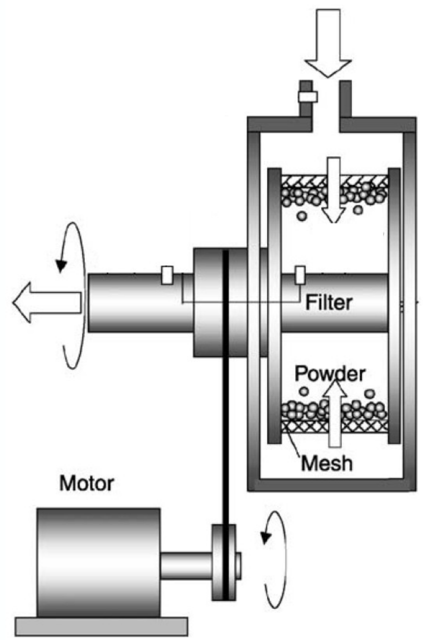
Conventional Fluidized Bed [1]



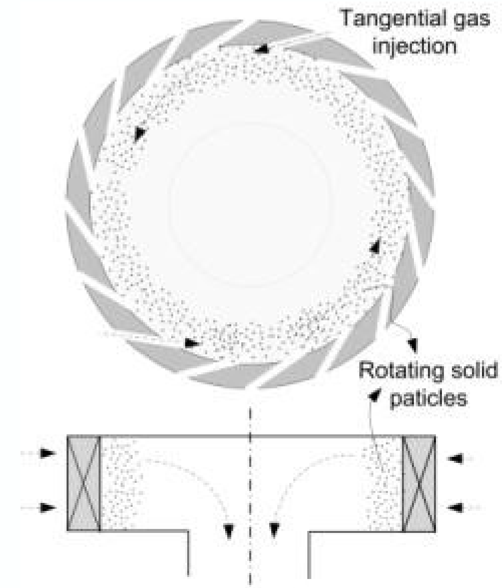
Riser/Circulating Fluidized Bed [2]



Conventional Rotating Fluidized Bed [3]



Gas/Solid Vortex Reactor



gravitational technologies

centrifugal technologies

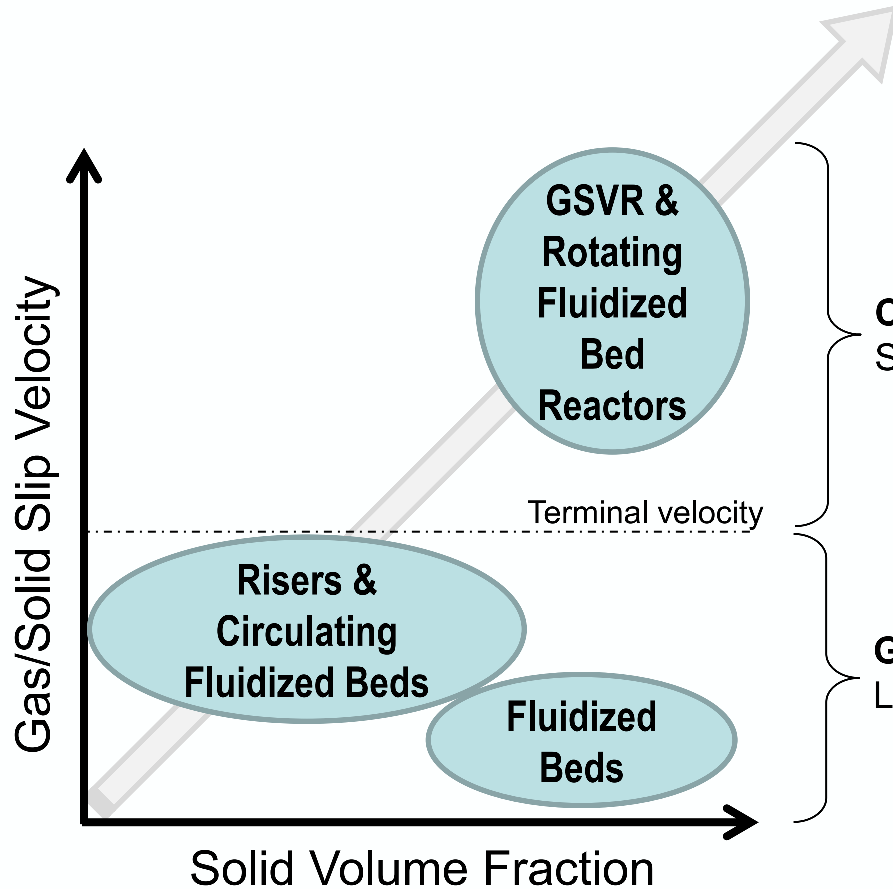
1. van Hoef et al., Ann. Rev. Fluid Mech. 40 (2008) 47-70
2. http://www.fluidcodes.co.uk/fbed.html
3. adapted from Watano et al., Powder Tech.131 (2003) 250-255

Gas/Solid Fluidization Reactors

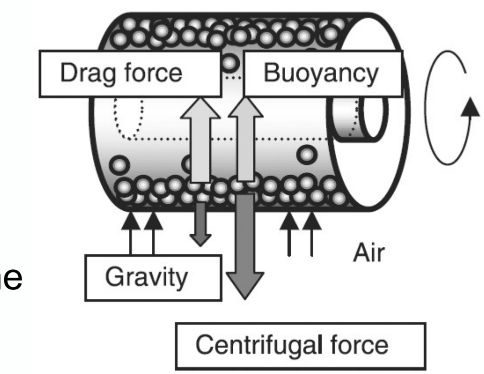
Improved gas/solid mass transfer

Larger surface area per reactor volume

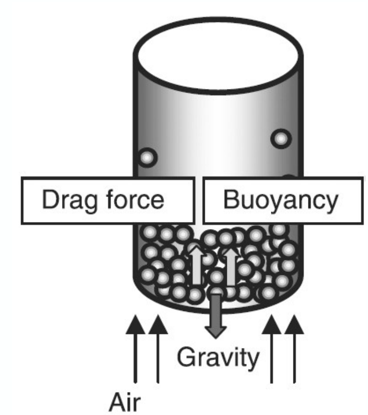
Larger potential for intensification



Centrifugal technologies
Shorter gas/solid contact time



Gravitational technologies
Longer gas/solid contact time

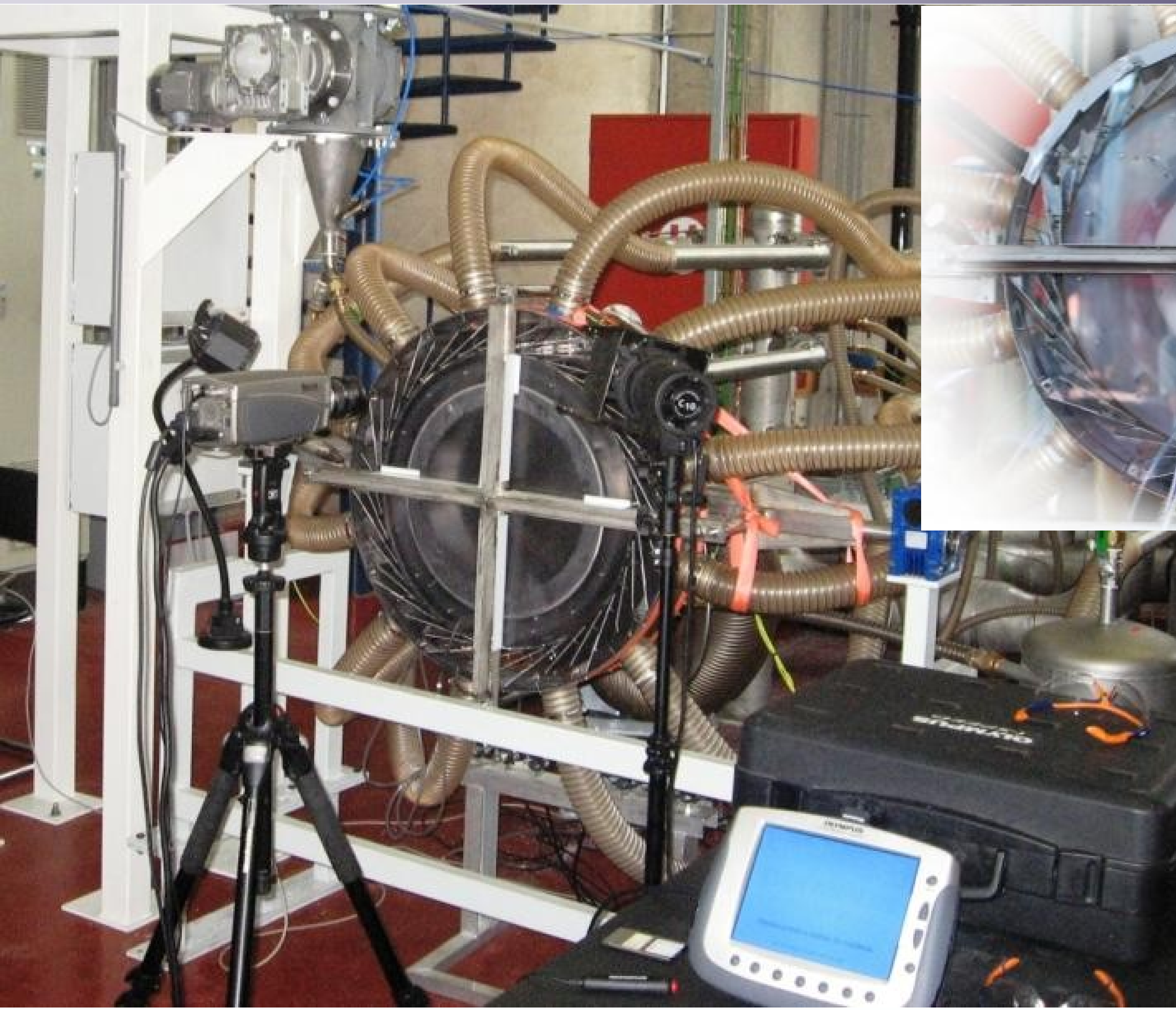


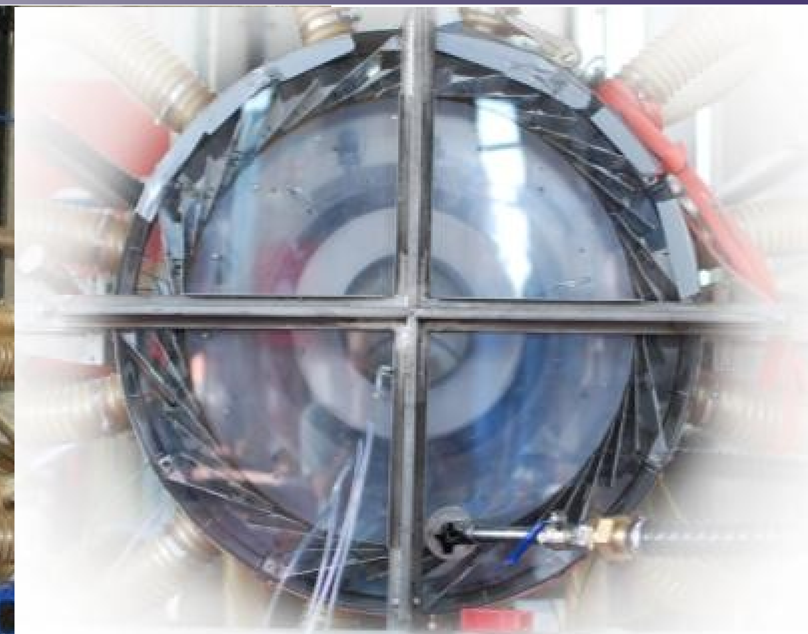
Images from: Watano et al., Powder Tech.131 (2003) 250-255

Experimental

with Jelena Kovacevic

Experimental GSVR Set-up



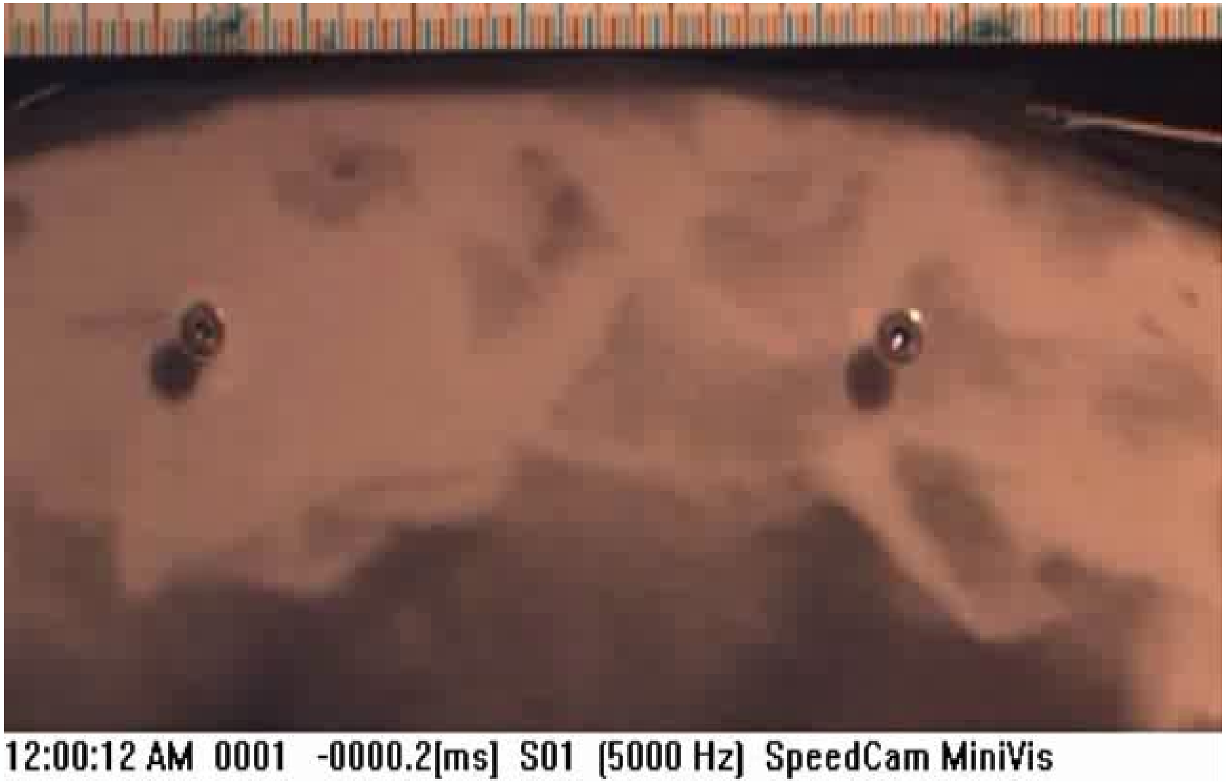


Real-time Video

0.9 mm polyvinylidene fluoride particles (ρ = 1800 kg/m^3)
~1 kg/s air flow
~5 kg bed mass

High-Speed Video – Small Particles

70 micron particles
(5000 FPS)



~1.6 mm particles
(10000 FPS)

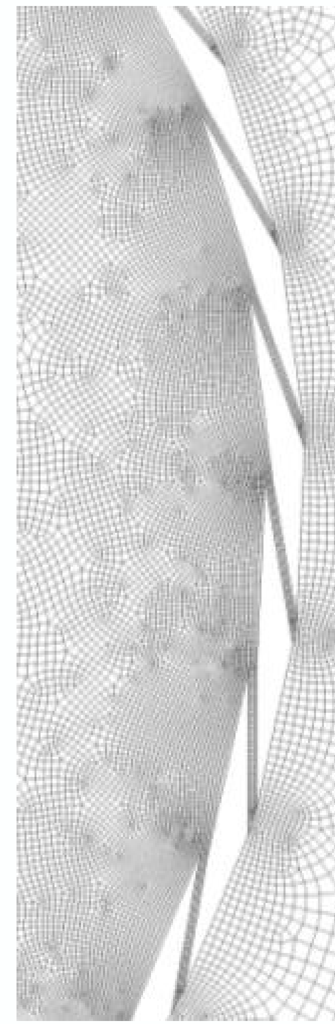
Non-reacting Flow Modeling

Computational Fluid Dynamics

- Computational fluid dynamics → Fluent 13.0
- Eulerian/Eulerian two-fluid model, granular solid phase
- Gidaspow drag model [1]

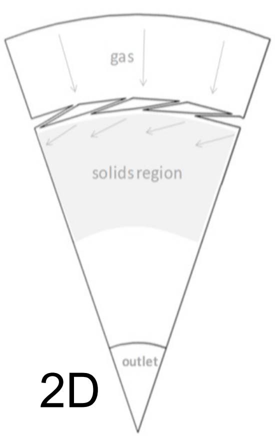
$$\begin{cases} \beta = 150\dfrac{\alpha_p(1-\alpha_g)\mu_g}{\alpha_g d_p^2} + 1.75\dfrac{\rho_g\alpha_p\left|\vec{u}_p-\vec{u}_g\right|}{d_p} & \text{for } \alpha_g \le 0.8 \\ \beta = \dfrac{3}{4}C_D\dfrac{\alpha_p\alpha_g\rho_g\left|\vec{u}_p-\vec{u}_g\right|}{d_p}\alpha_g^{-2.65} & \text{for } \alpha_g > 0.8 \end{cases}$$

$$C_D = \begin{cases} \dfrac{24}{Re_p}\left(1+0.15Re_p^{0.687}\right) & (Re_p \le 1000) \\ 0.44 & (Re_p > 1000) \end{cases}$$



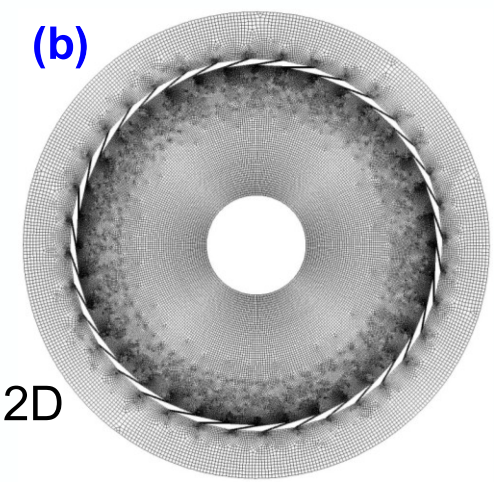
Model geometries tested:

(a)



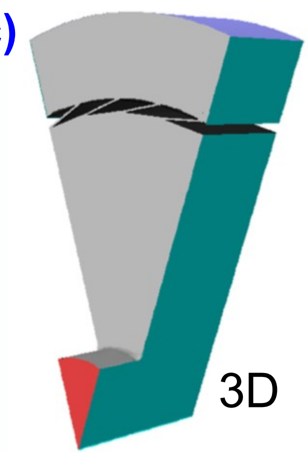
2D

(b)



2D

(c)



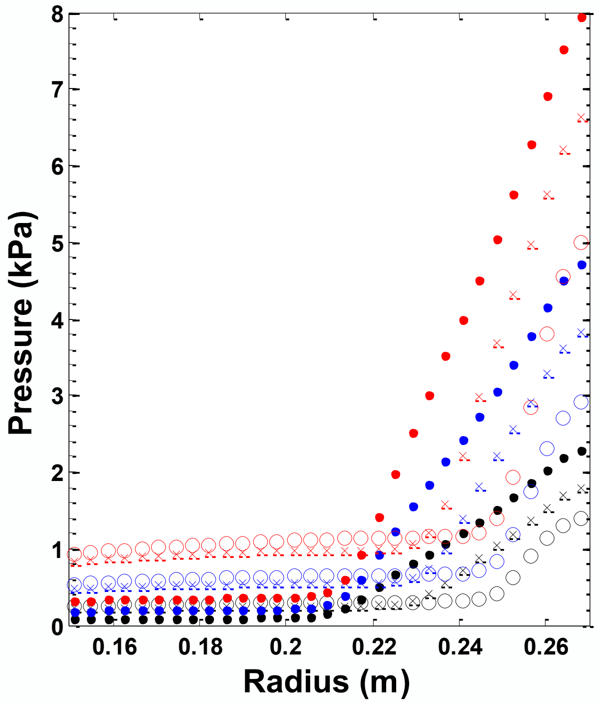
3D

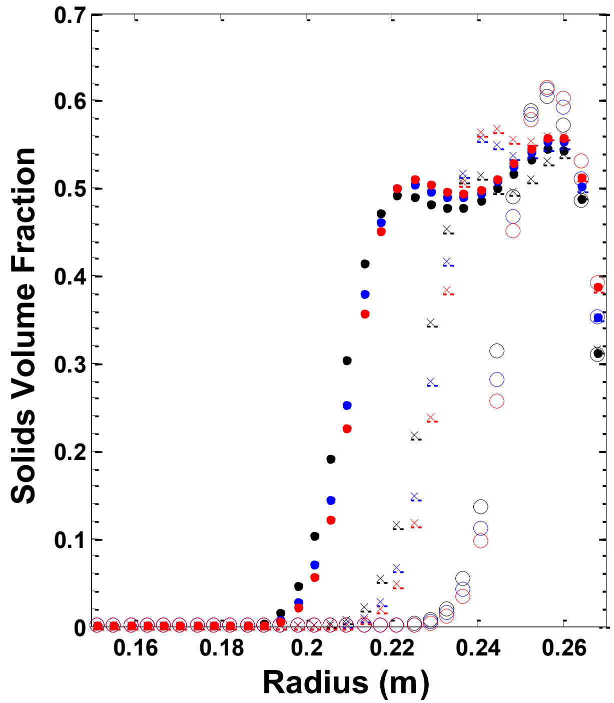
1. Gidaspow, D. (1994). *Multiphase flow and fluidization: Continuum and kinetic theory description. New York: Academic Press.*

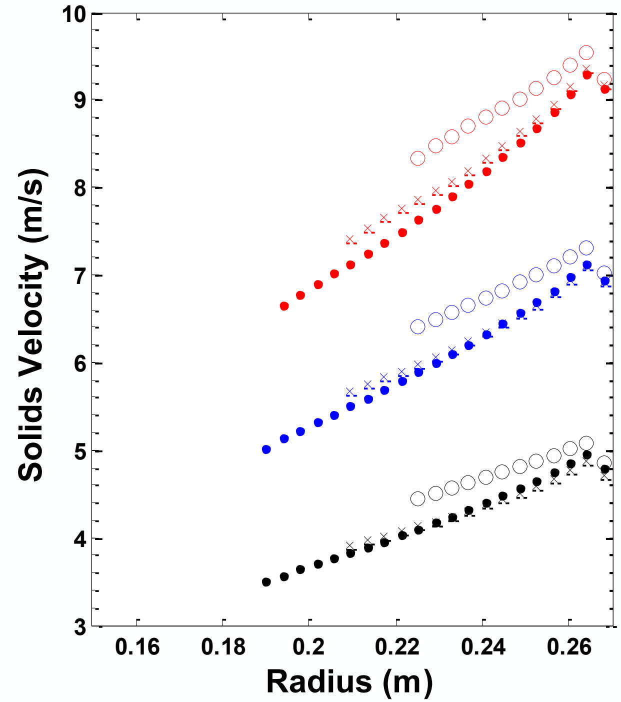
General Non-reacting Flow Results

Bed Mass: 2.1 kg – 4.4 kg

Air Flow Rate: 0.5 kg/s – 1.0 kg/s







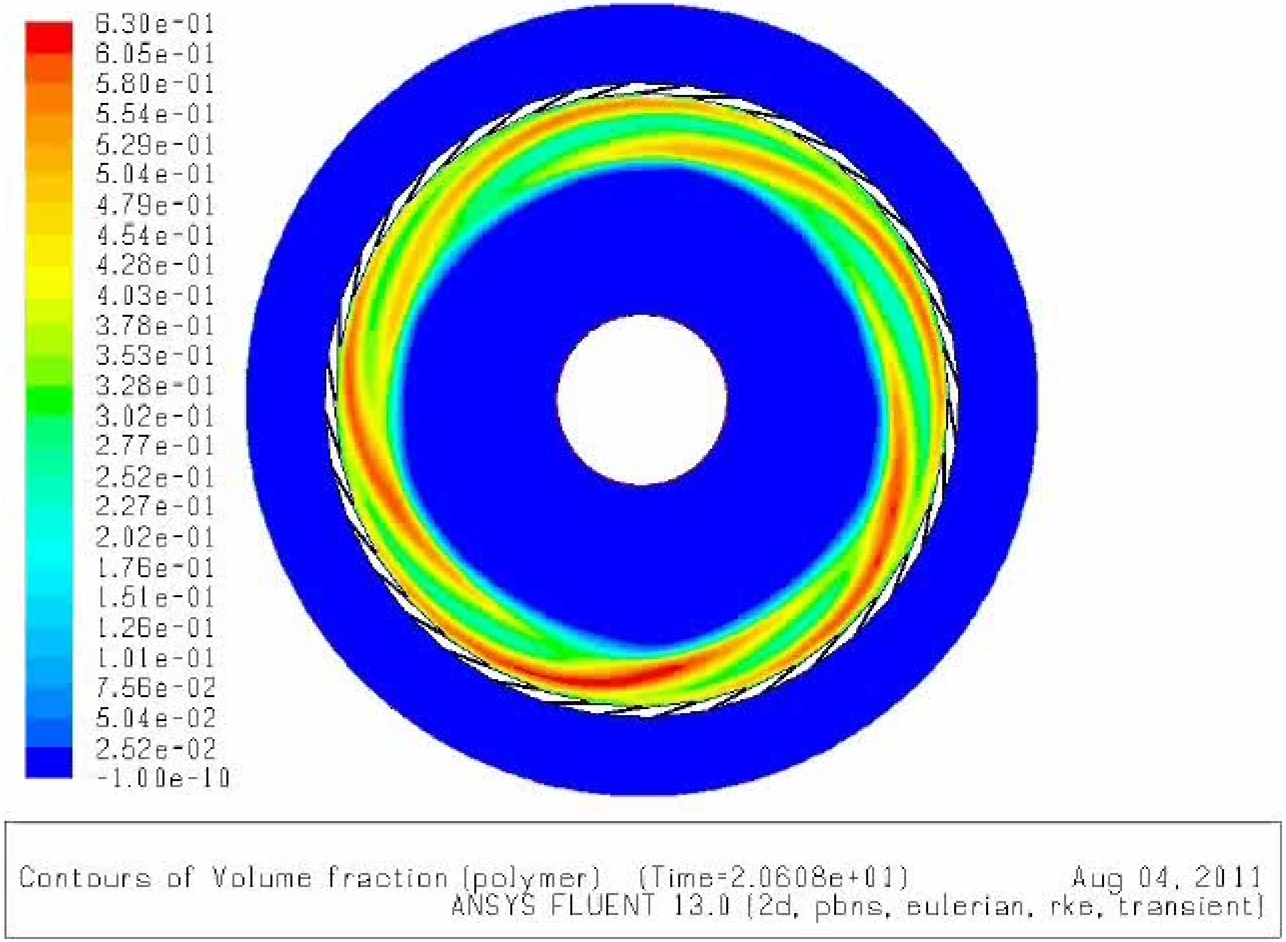
Bed ΔP: 2 kPa – 8 kPa

Solids VF: 0.4 – 0.6

Solids Velocity: 4 – 9 m/s

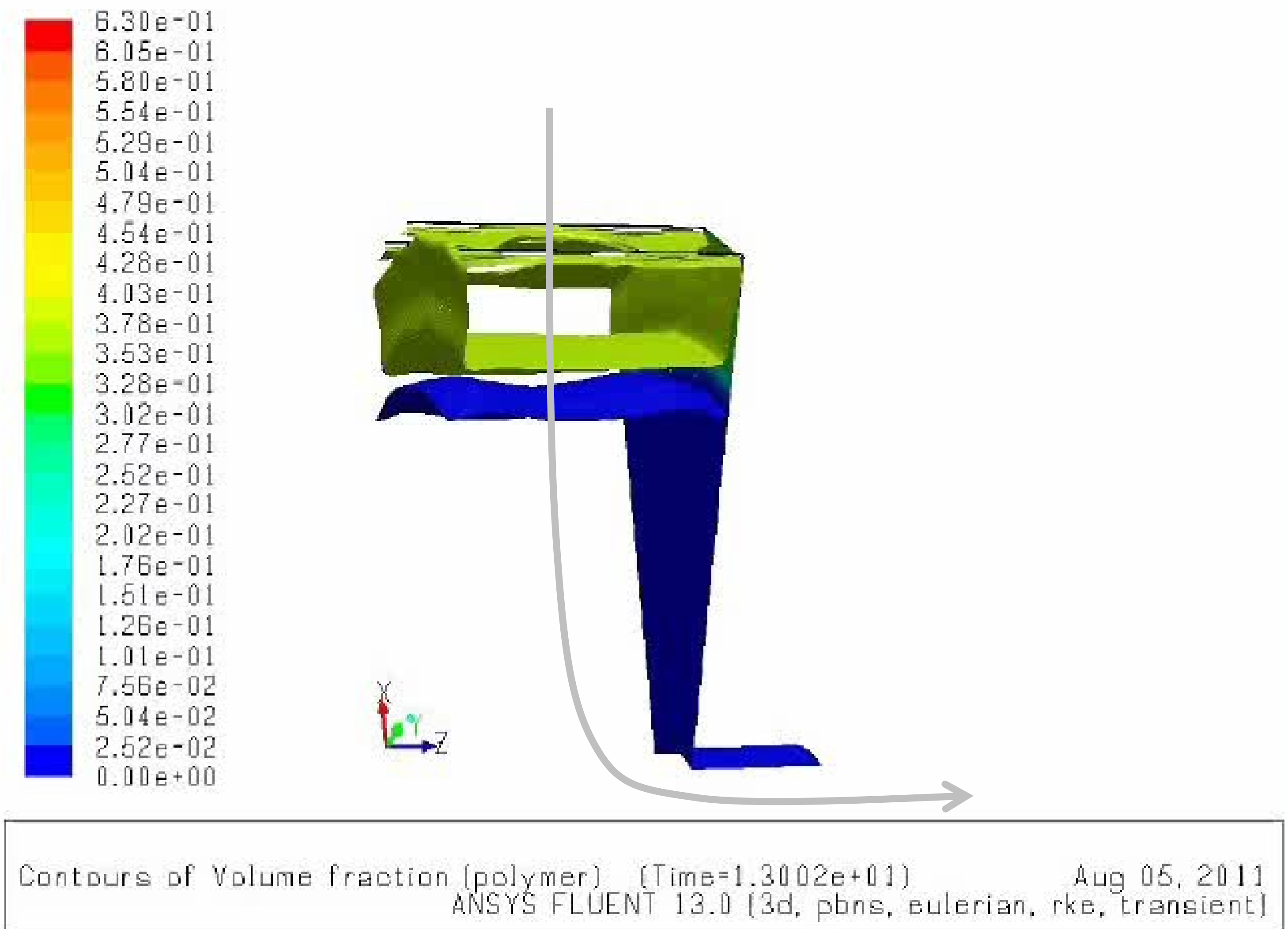
CFD Example Movies

2D (with gravity), 0.74 kg/s air, 3250 g bed



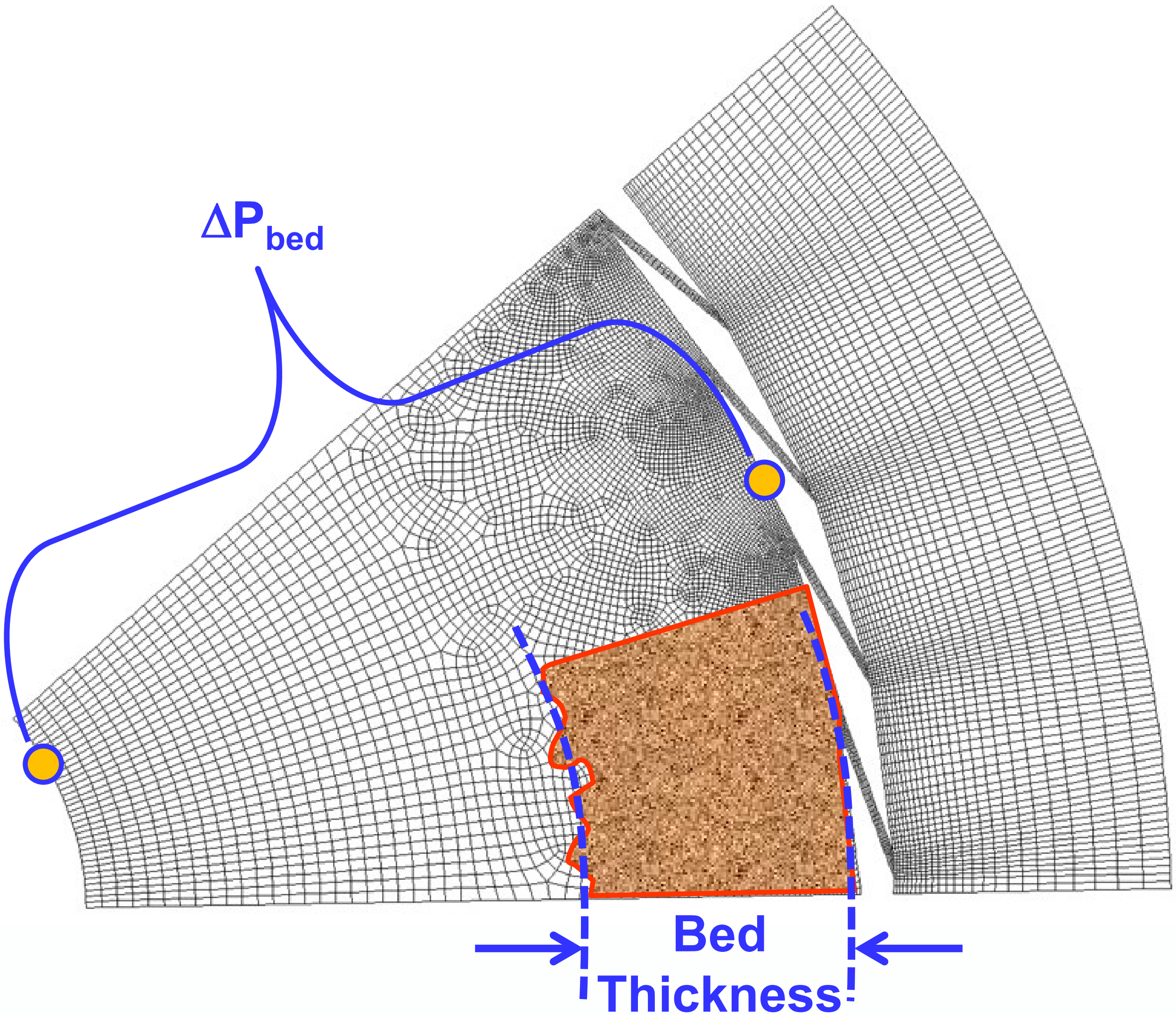
CFD Example Movies

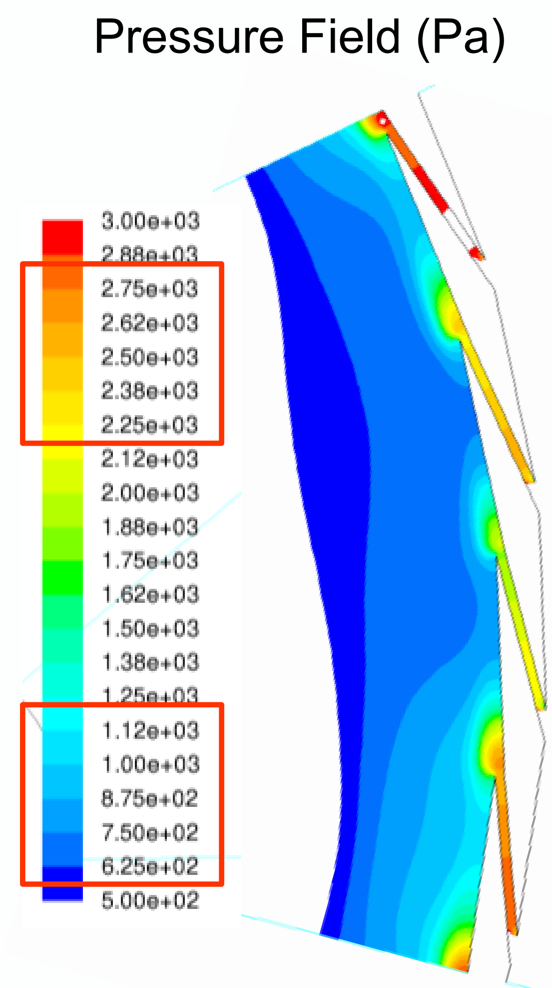
3D, 0.74 kg/s air, 3250 g bed
(iso-surfaces = 0.40 and 0.01 solids volume fraction)



Model Validation

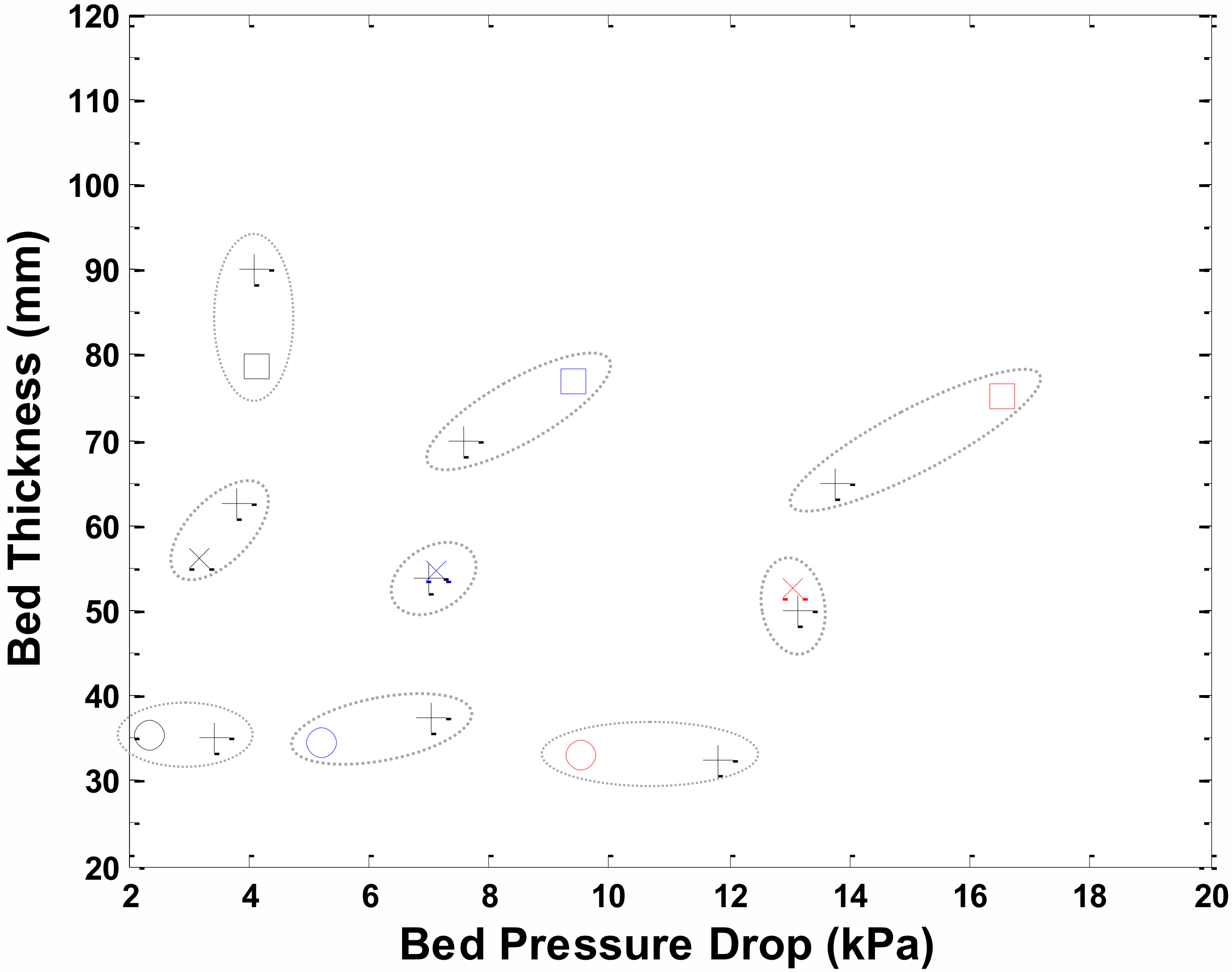
Bed Pressure Drop and Bed Thickness





Bed and Bed Thickness (2D)

Air flow: 0.5 kg/s 0.75 kg/s 1.0 kg/s



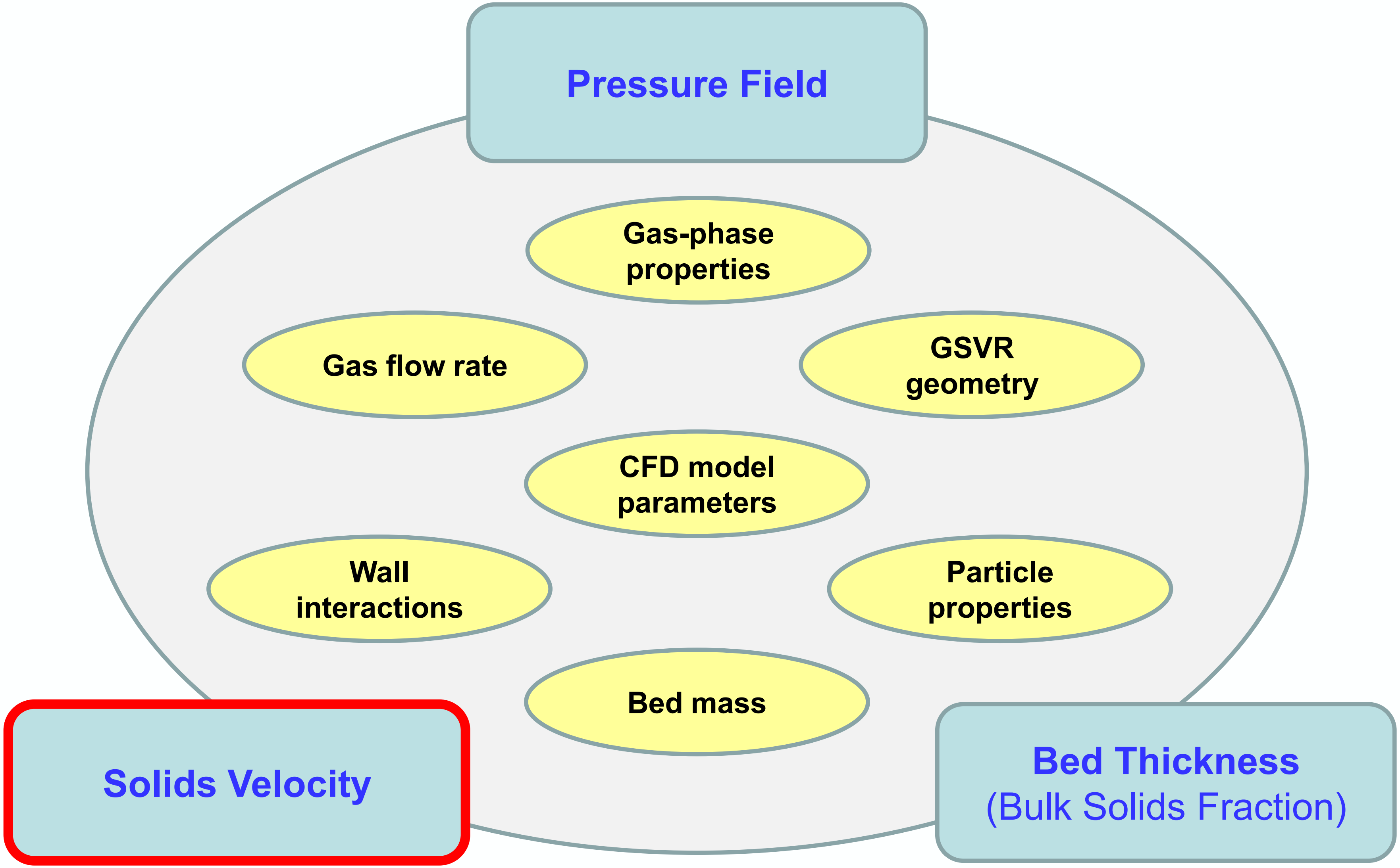
4.38 kg bed mass

3.25 kg bed mass

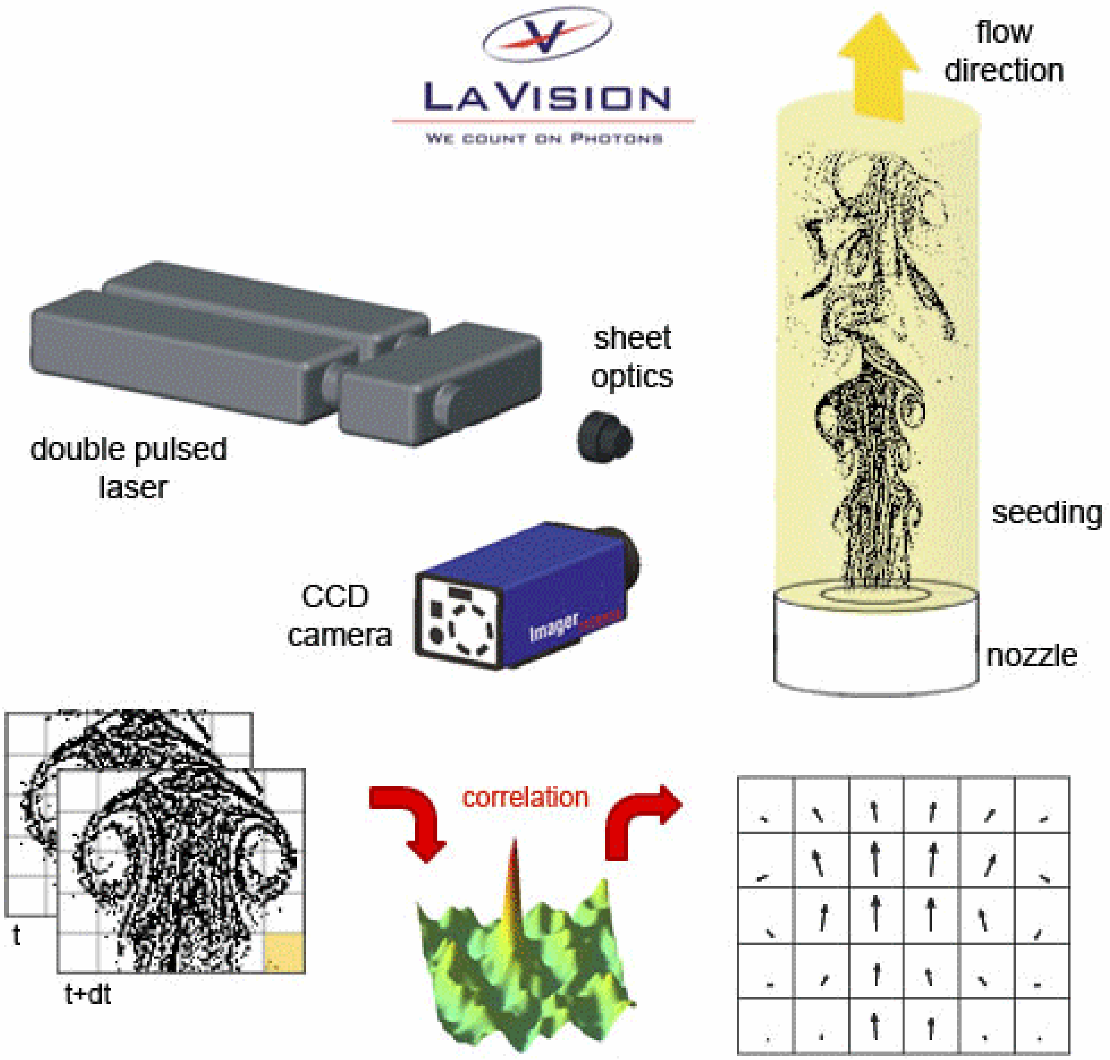
2.12 kg bed mass

Experimental data: (+) signs

Model Deficiencies & Refinement



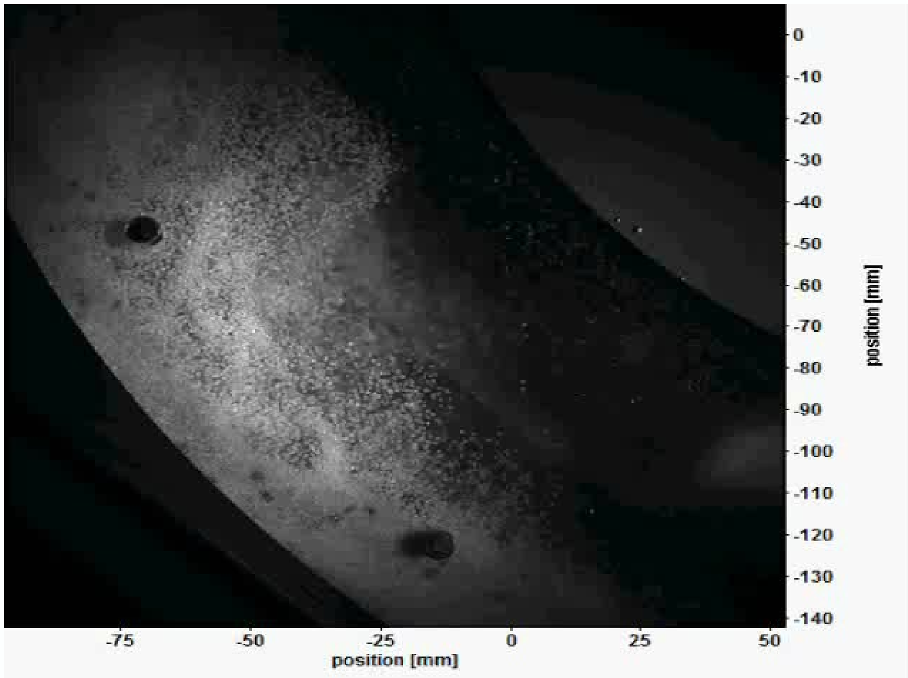
Particle Image Velocimetry (PIV)



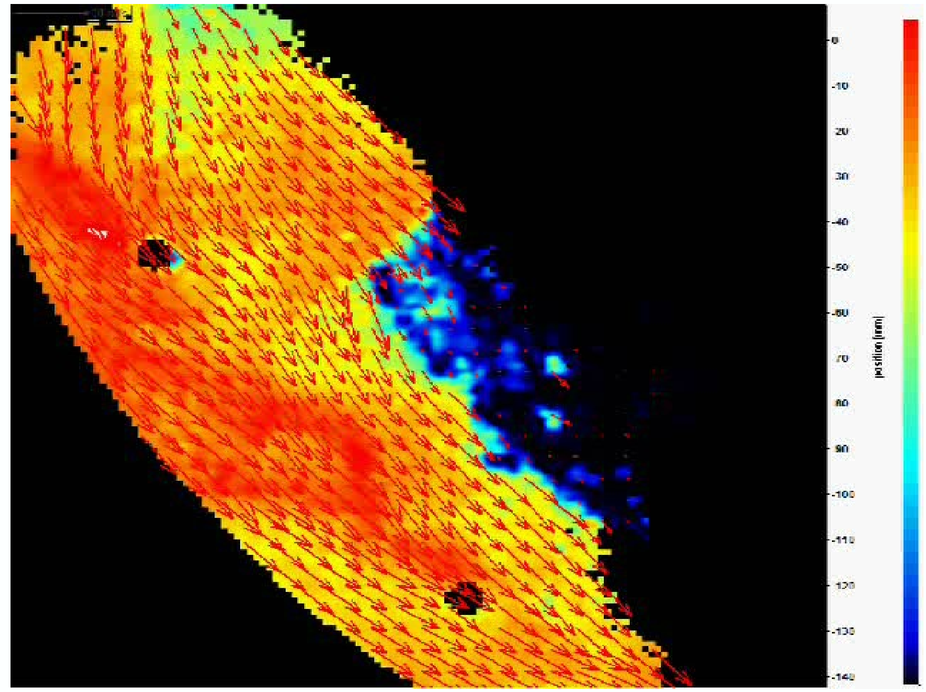
La Vision --- http://www.piv.de/piv/index.php

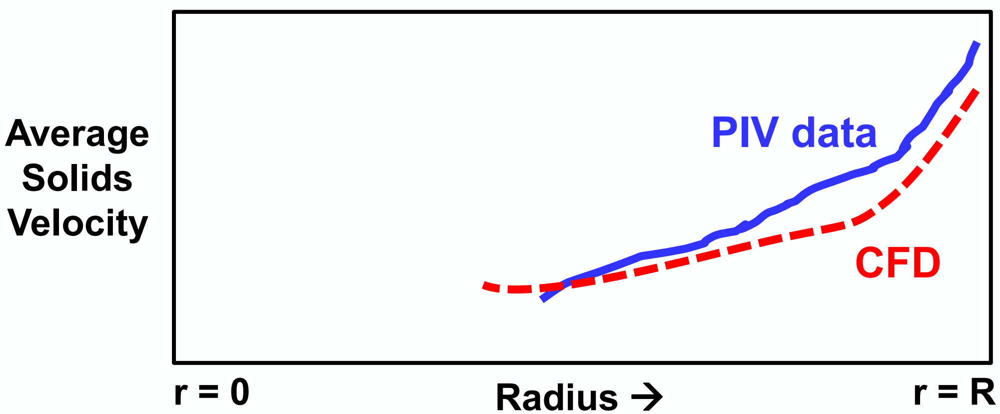
On-going Model Refinement - PIV

Raw image collection



Processed velocity field



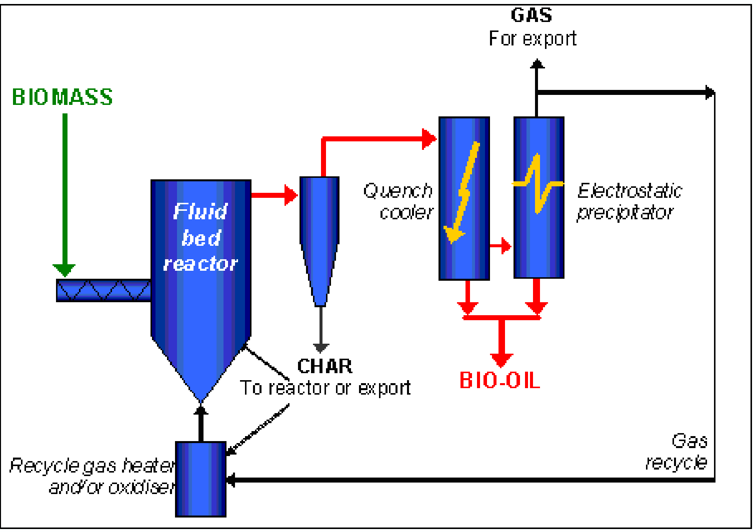


Goal:
Compare time-averaged data over many image pairs

Modeling Biomass Pyrolysis

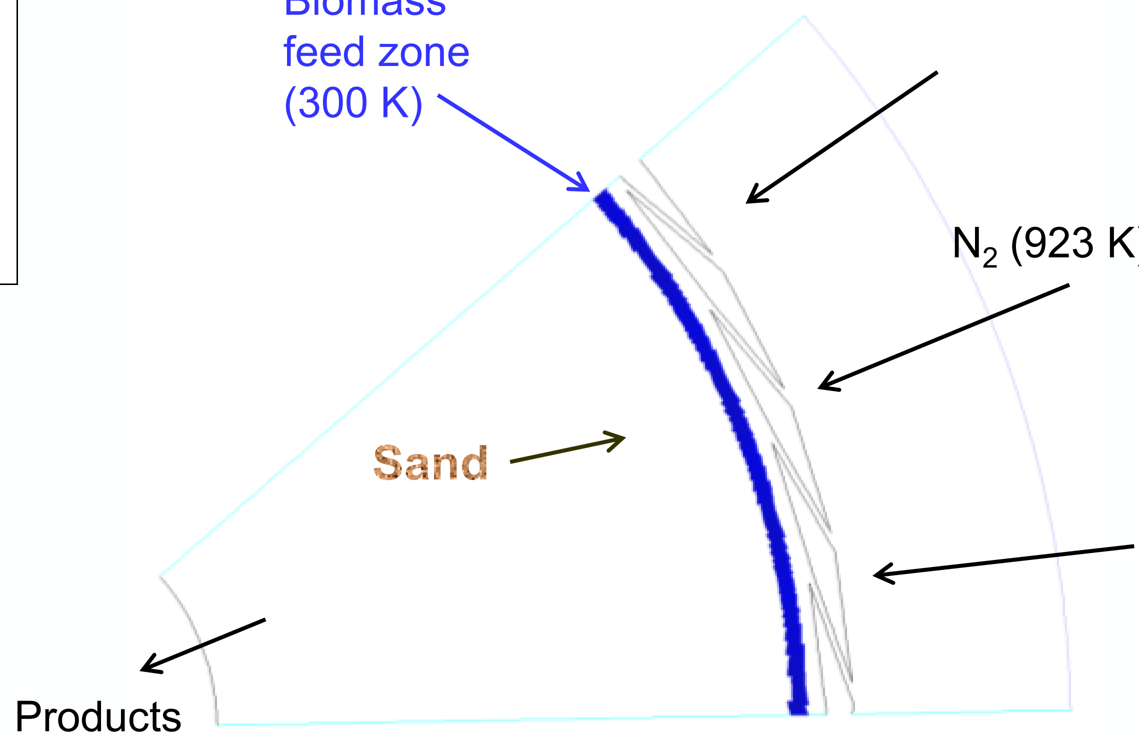
Biomass Pyrolysis in a GSVR

Traditional Static Fluidzed Bed [1]



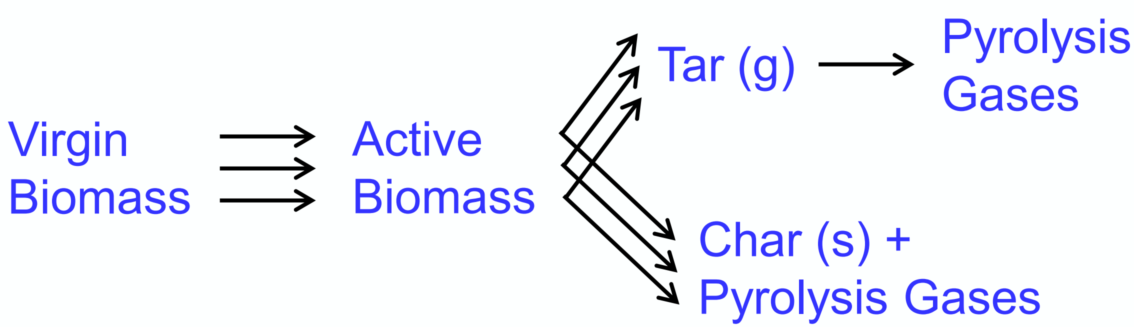
GSVR

D = 54 cm (solids region)
L = 10 cm

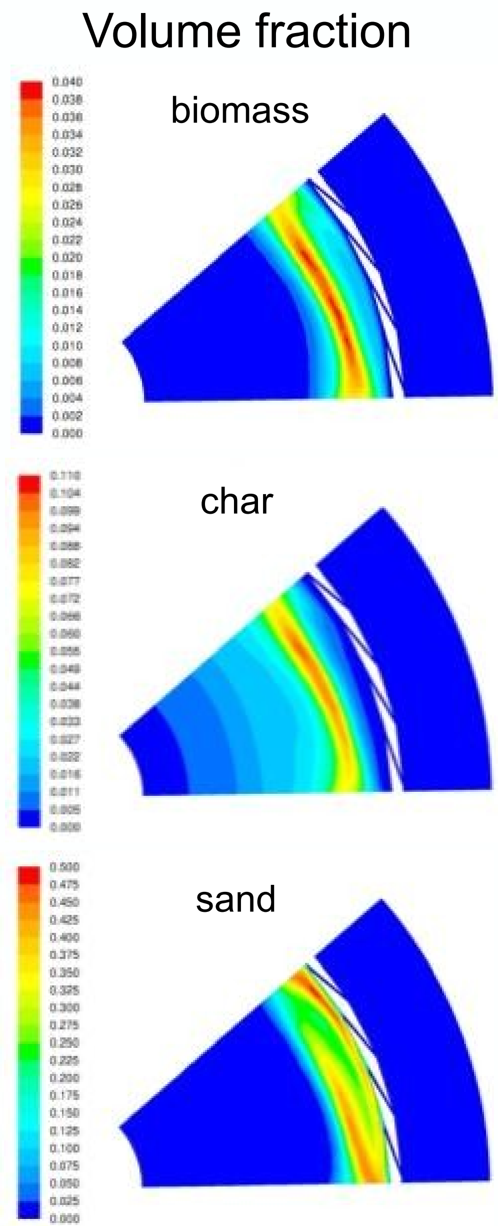


Pyrolysis Modeling in a GSVR

- 2D periodic GSVR simulations
- Heterogeneous reactions (solid → gas + char):
- 10-reaction network with psuedo-components [1]
- Continuous feeding of biomass
  - Cellulose, hemicellulose, and lignin
  - Different rates for each biomass component



- 4-phase Eulerian multiphase simulation (3 granular)
  - Gas, biomass, char, and sand
- Sand and biomass retained in reactor
- Char leaves with gas flow due to lower density



1. Xue, Heindel, and Fox, Chem. Eng. Sci. 66 (2011) 2440

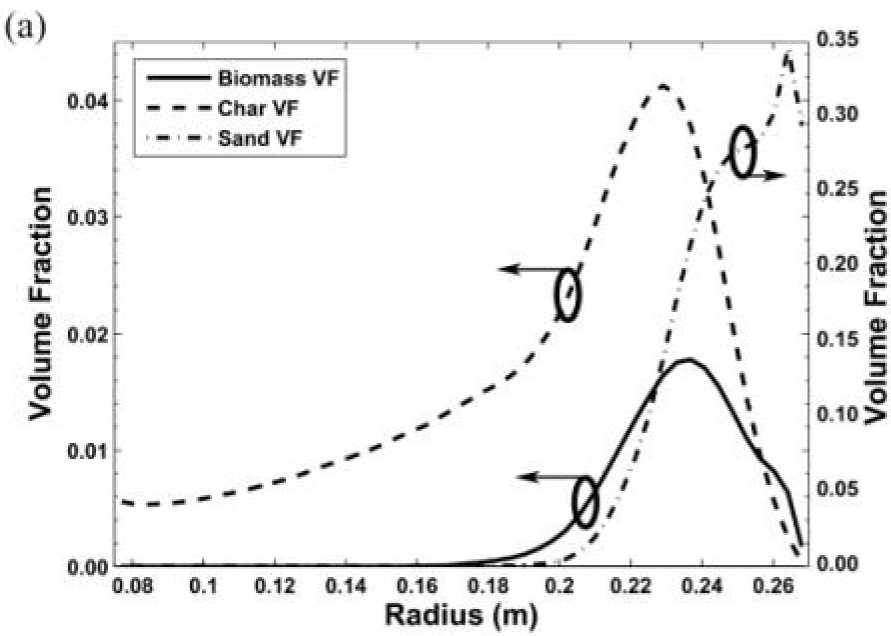
Base GSVR Operating Variables

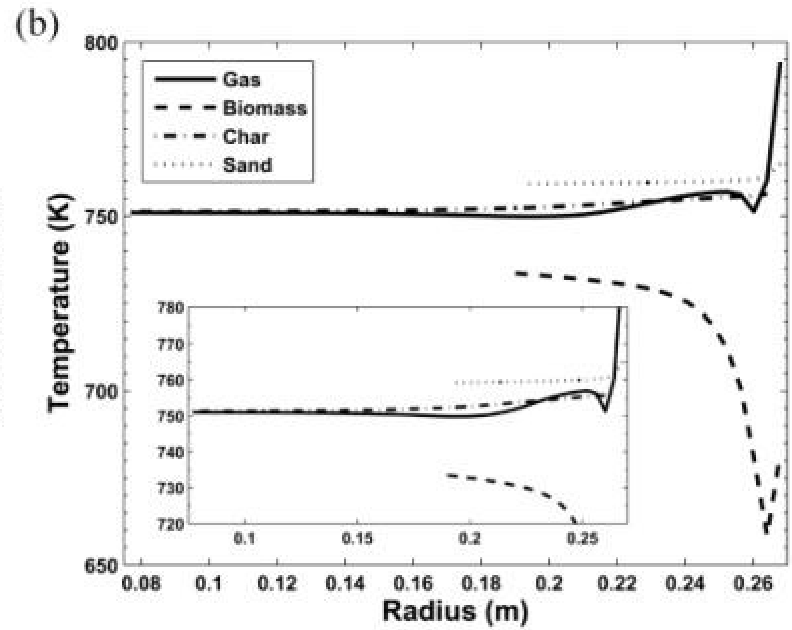
Volume (m^3)	**0.023**
Gas flow rate (kg/s)	0.22
Biomass feed rate (kg/s)	0.035
Biomass moisture content (wt%, dry basis)	10
Sand mass in reactor (kg)	5
Gas-to-biomass ratio ($kg_{gas}/kg_{biomass}$)	**6.4**
Gas feed temperature (K)	923
Biomass feed temperature (K)	300
Biomass feed rate/volume ($kg/m^3 \cdot s$)	1.5

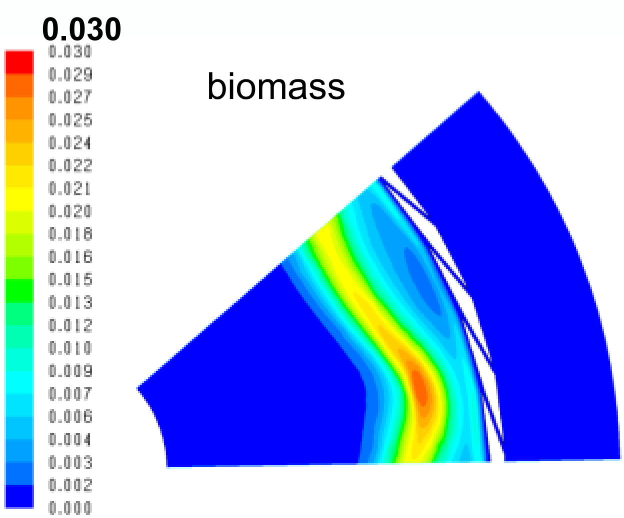
→ Biomass composition (wt% dry):

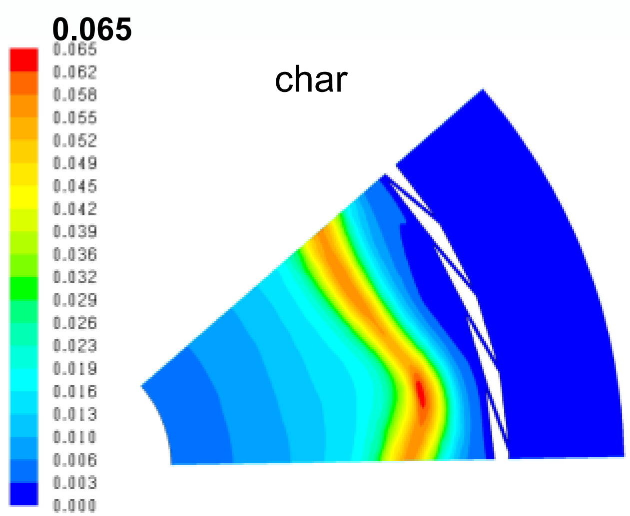
- 36% cellulose
- 47% hemicellulose
- 17% lignin

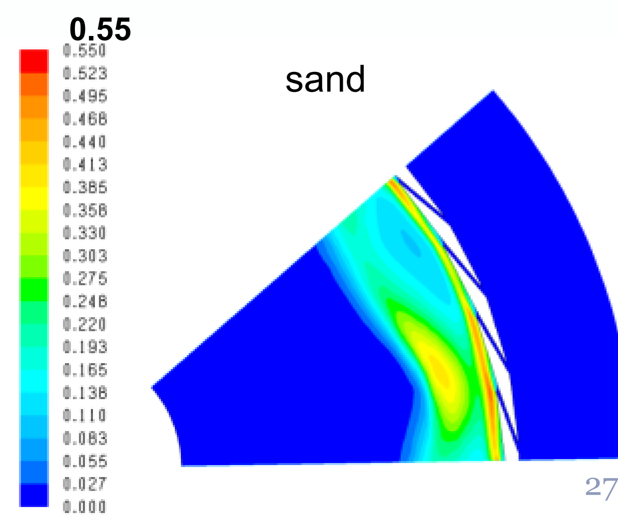
Volume Fraction and Temperature



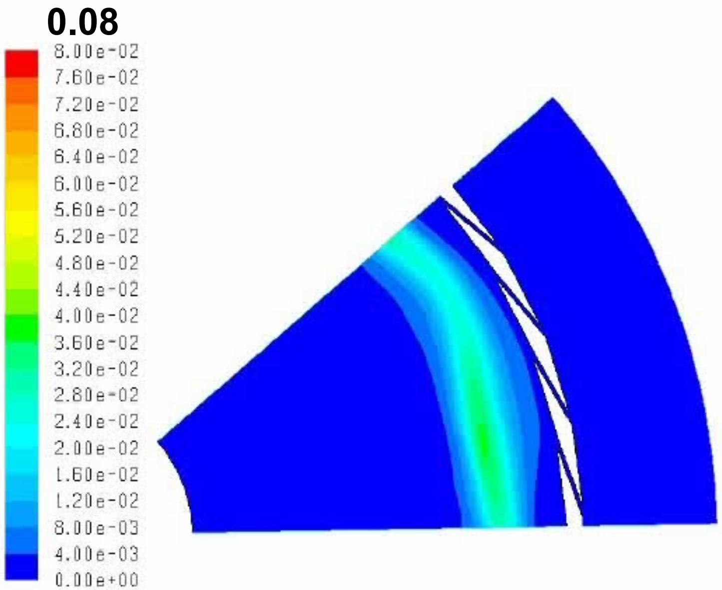




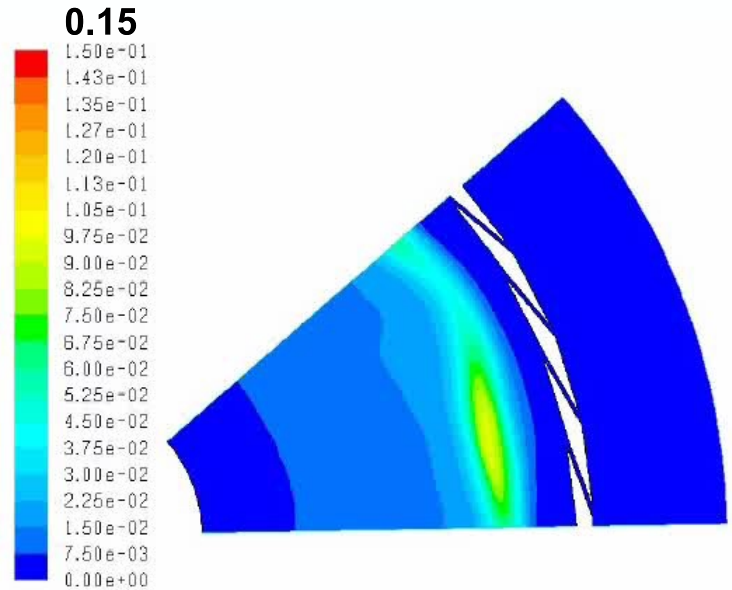




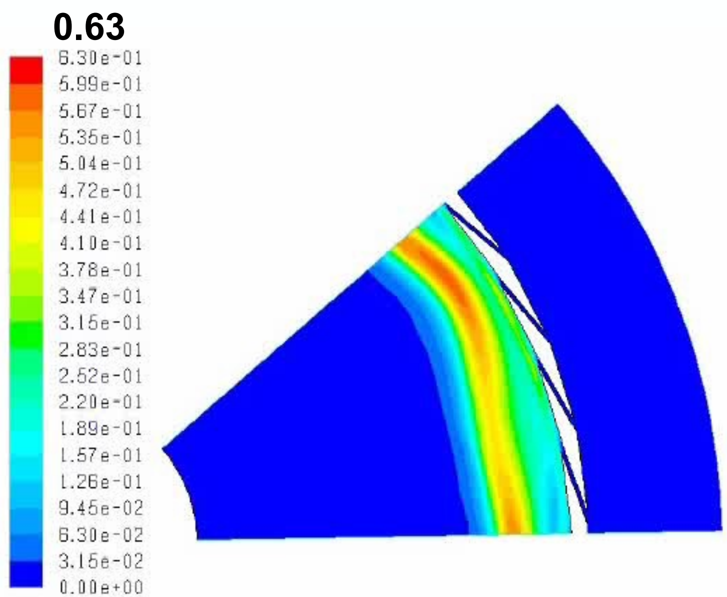
Volume Fraction Animation



Biomass



Char

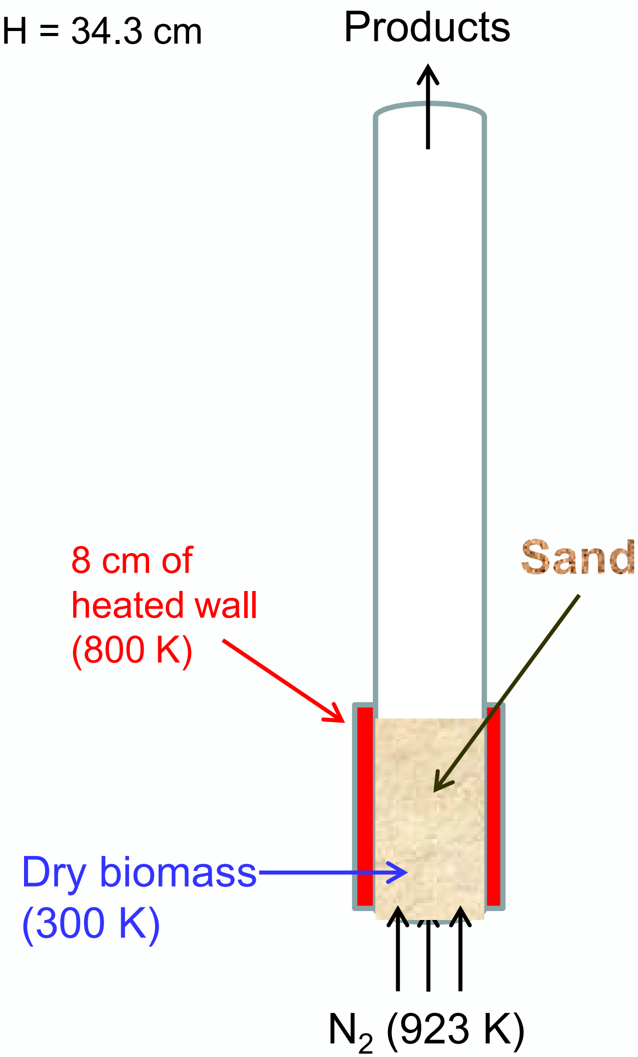


Total solids
(biomass, char, sand)

Comparison – GSVR vs Fluidized Bed

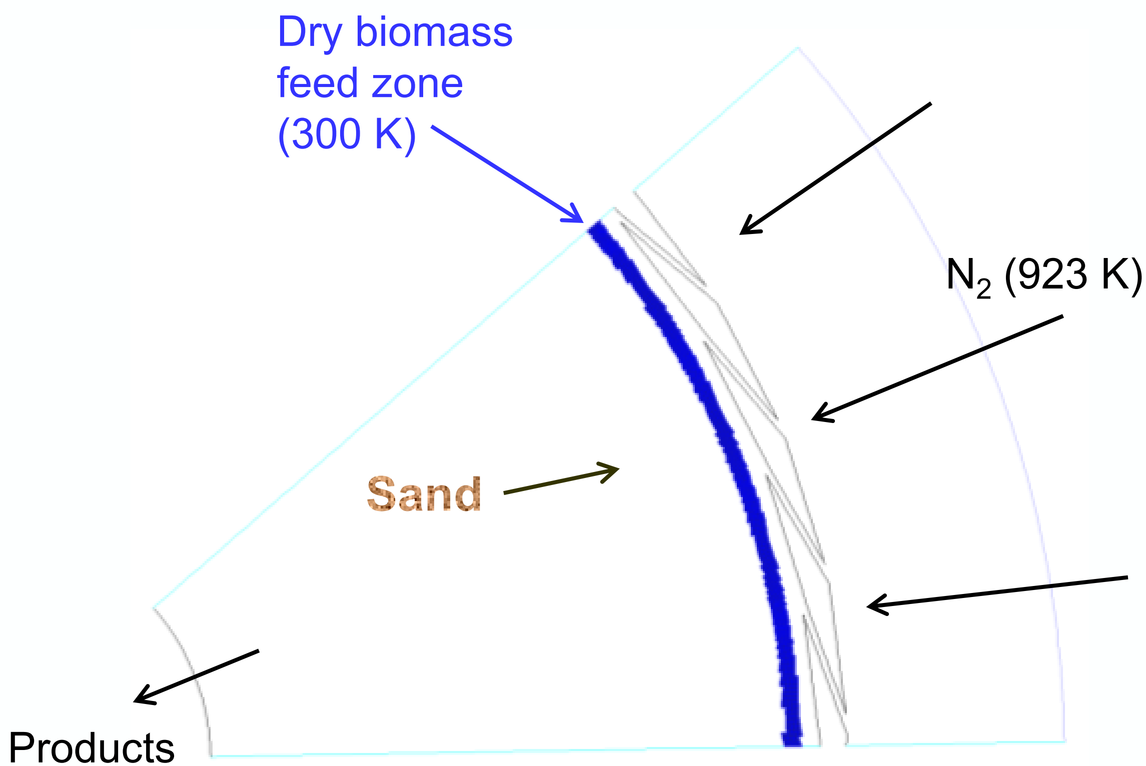
Static Fluidized Bed [1]

D = 3.81 cm
H = 34.3 cm



GSVR

D = 54 cm (solids region)
L = 10 cm



1. Xue, Heindel, and Fox, Chem. Eng. Sci. 66 (2011) 2440

Comparison – GSVR vs Fluidized Bed

	GSVR	Static FB [1]
Volume (m^3)	0.023	0.00039
Gas-to-biomass ratio ($kg_{gas}/kg_{biomass}$)	**6.4**	**6.4**
Sand mass in reactor/volume (kg/m^3)	217	322
Supplementary heating	no	yes
Outlet Temperature (K)	784	790
Gas-phase residence time (s)	~0.05	~0.75
Product Yields (wt% of fed biomass):		
Tar	76.0	63.4
Pyrolysis gas	8.9	21.5
Char	14.5	14.4
Biomass (unconverted)	0.0	0.6
Biomass conversion rate / reactor volume ($kg/m^3 \cdot s$)	1.5	0.07

1. Xue, Heindel, and Fox, Chem. Eng. Sci. 66 (2011) 2440

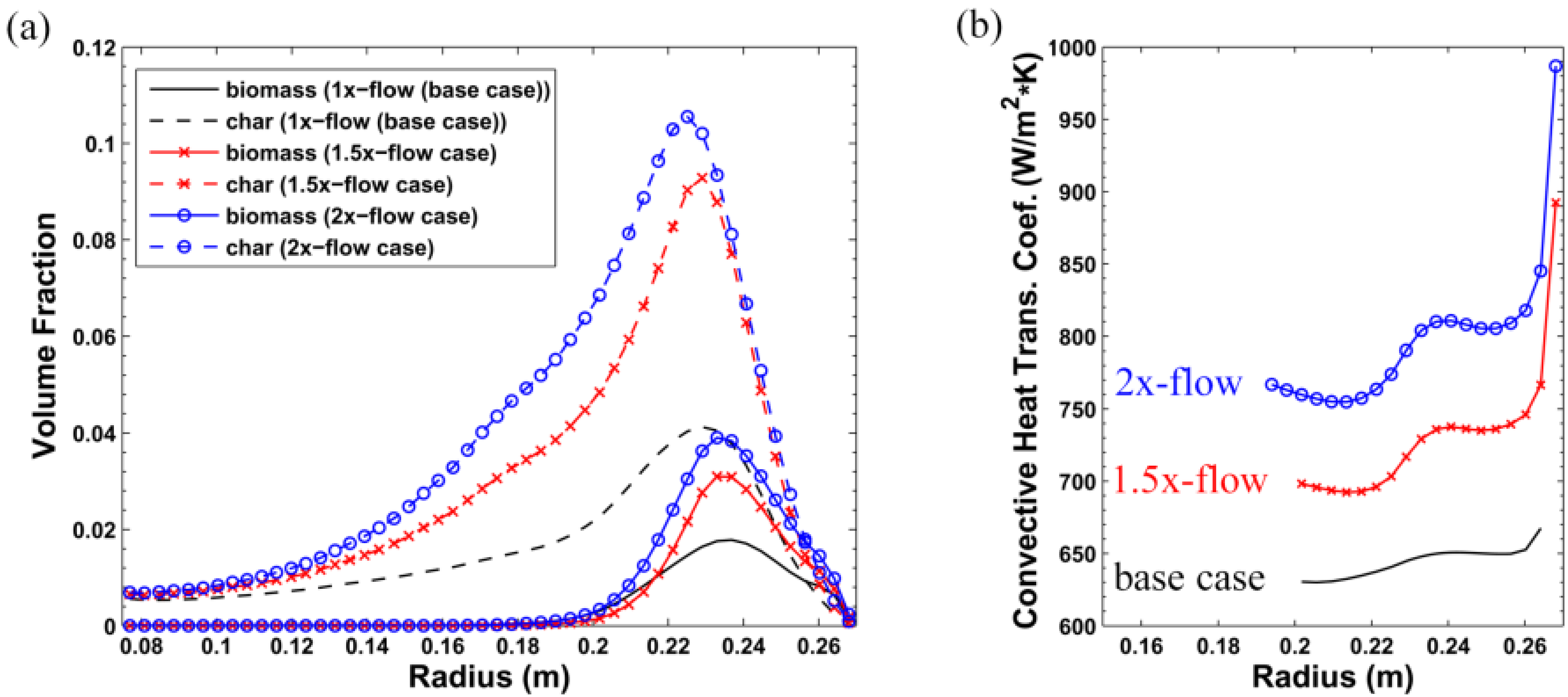
Process Intensification

GSVR Process Intensification

Increase gas and biomass feed rates proportionately

- Base feed rates:
  0.22 kg/s gas
  0.035 kg/s biomass

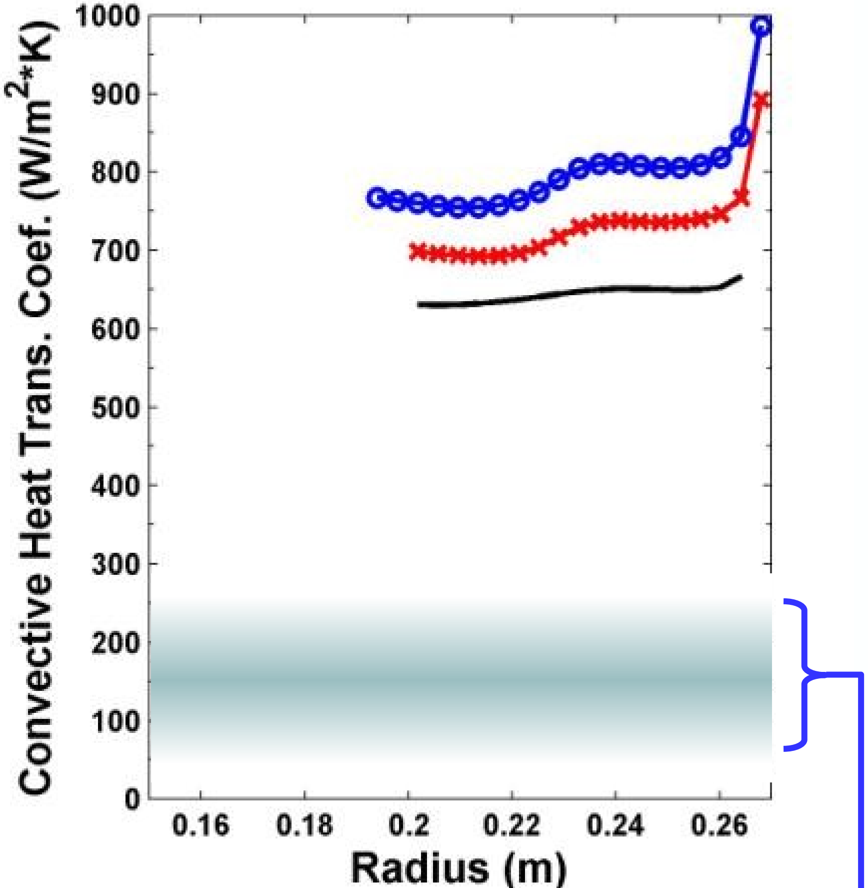
$$\mathrm{Nu}_p = \frac{h_p \cdot d_p}{\lambda_g} = (7 - 10\varepsilon_g + 5\varepsilon_g^2)(1 + 0.7 \cdot \mathrm{Re}_p^{0.2} \cdot \mathrm{Pr}^{\frac{1}{3}}) + (1.33 - 2.4\varepsilon_g + 1.2\varepsilon_g^2) \cdot \mathrm{Re}_p^{0.7} \cdot \mathrm{Pr}^{\frac{1}{3}}$$



→ Reactor performance and product yields ~ the same (but increased ΔP)

→ Plus, shorter gas residence time and higher heat transfer coefficients

GSVR Process Intensification



Typical range for static fluidized beds and risers/CFBs: [1,2]
~100 – 200 W/(m² K)

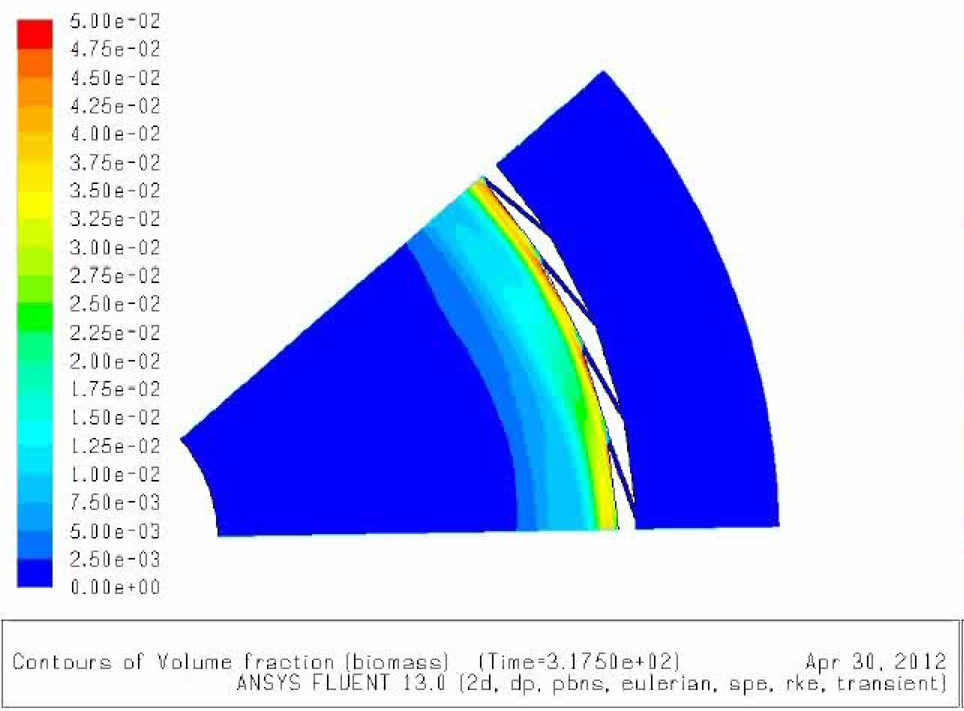
1. Z.Y. Zhou, A.B. Yu, P. Zulli, Particle scale study of heat transfer in … fluidized beds, AIChE J. 55 (2009) 868–884
2. Y. Ma, J.X. Zhu, Experimental study of heat transfer in a co-current downflow fluidized bed, Chem. Eng. Sci. 54 (1999) 41–50

Pyrolysis Reactor without Sand

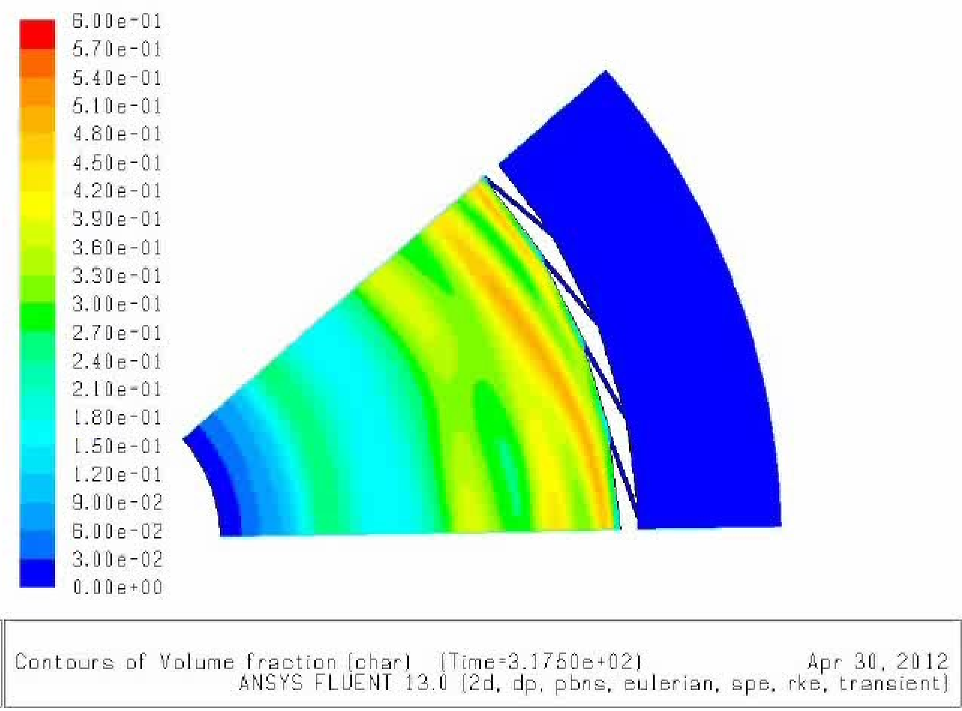
Operating the reactor with biomass as the only solid

- Much larger char mass accumulates
- Product distribution the same as in cases with sand
- Char removal occurs in pulsing, oscillatory pattern

Biomass



Char



Summary

GSVRs have the potential to intensify processes

- High intrinsic mass/heat transfer can yield improved overall rates
- High solid volume fractions can reduce equipment size

Biomass Pyrolysis Example

- Stratification of solid phases to retain sand & unreacted biomass
- Comparison to a static fluidize bed
  - Comparable degree of char formation
  - Increased tar and reduced pyrolysis gas formation
- Significantly opportunity for intensification in GSVR
  - 3x – 5x larger heat and mass transfer coefficients
  - Ability to increase feed rates without biomass loss, but more ΔP

Future Projects

- Direct measurement of solid velocities using PIV
- Experimental GSVR to examine heat transfer and reacting flows

Acknowledgements

Lab. for Chemical Technology

- Prof. Guy Marin
- Prof. Geraldine Heynderickx
- Prof. Kevin van Geem
- Jelena Kovacevic
- dr. Maria Pantzali
- dr. Maarten Sabbe
- Georges Verenghen

Ghent University Resources

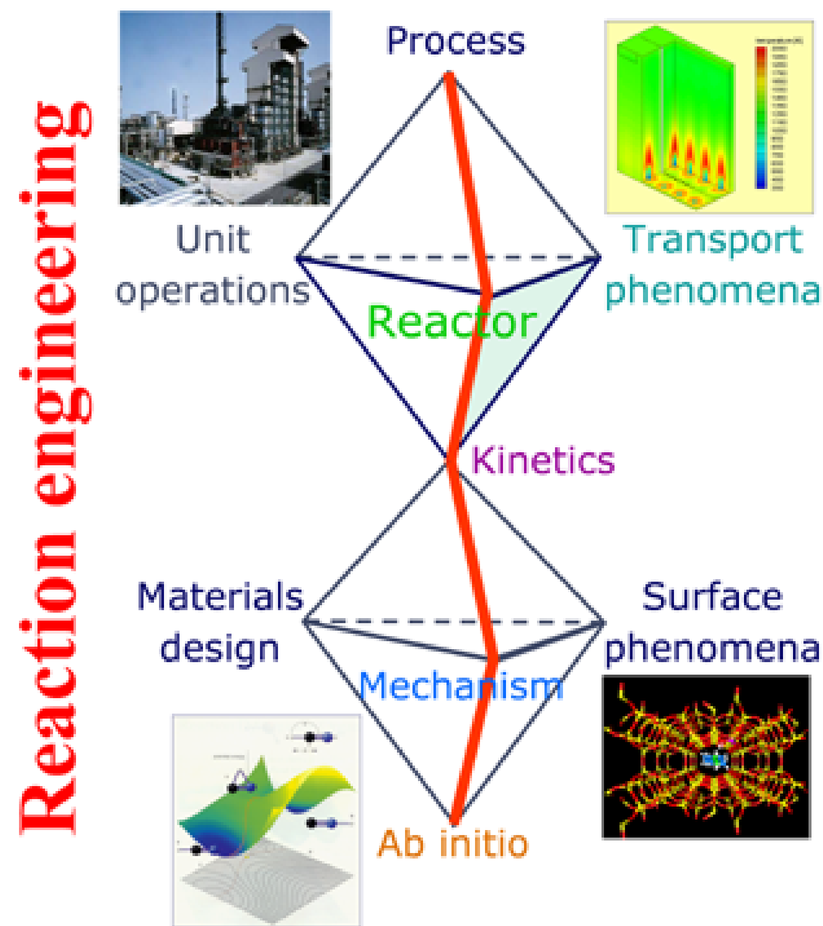
- High-Performance Computing Cluster

Funding

- Methusalem grant - Flemish government
- ERC Advanced Grant - MADPII

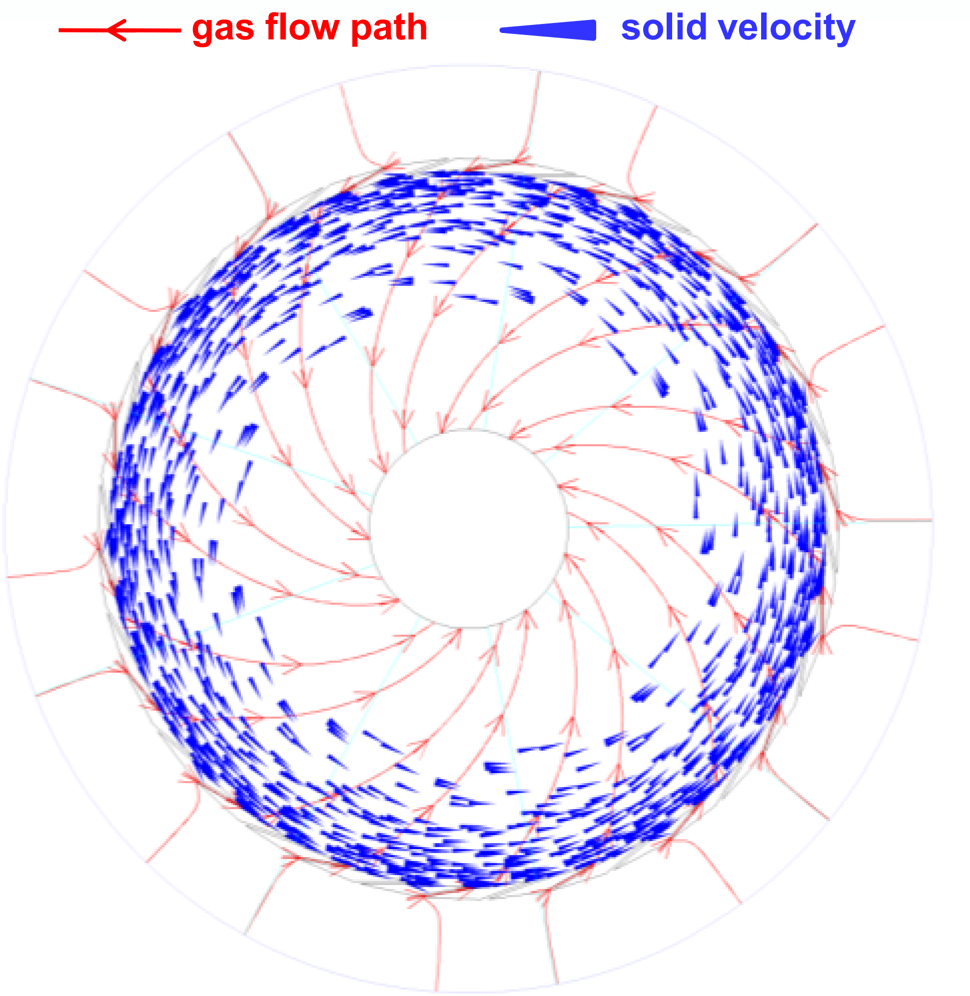
UNIVERSITEIT GENT

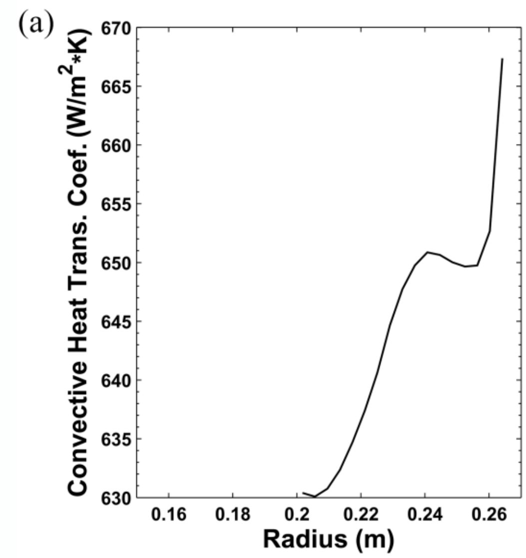
FACULTY OF ENGINEERING AND ARCHITECTURE

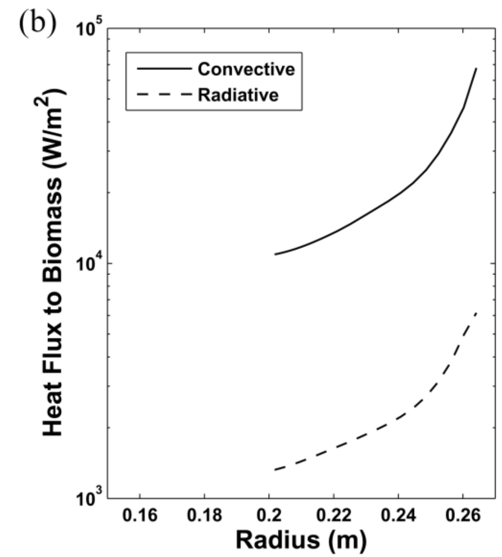


Backup Slides

Flow Paths and Heat Transfer







Biomass Kinetic Model

Table 1
Pyrolysis reaction mechanism and related data [9,47–49].

	Reaction[a,b]	ΔH_{rxn} (kJ/kg)	A_f (1/s)	E_A (kJ/mol)	k_{rxn} @ 773 K(1/s)
1a	$CL_v \rightarrow CL_a$	0	2.80×10^{19}	242.4	1170
1b	$HC_v \rightarrow HC_a$	0	2.10×10^{16}	186.7	5080
1c	$LG_v \rightarrow LG_a$	0	9.60×108	107.6	51.4
2a	$CL_a \rightarrow$ Tar	255	3.28×10^{14}	196.5	17.3
2b	$HC_a \rightarrow$ Tar	255	8.75×10^{15}	202.4	184
2c	$LG_a \rightarrow$ Tar	255	1.50×10^{9}	143.8	0.287
3a	$CL_a \rightarrow 0.35\ Char_c + 2.6\ Pgas$	−20	1.30×10^{10}	150.5	0.878
3b	$HC_a \rightarrow 0.6\ Char_h + 1.6\ Pgas$	−20	2.60×10^{11}	145.7	37.1
3c	$LG_a \rightarrow 0.75\ Char_l + Pgas$	−20	7.70×106	111.4	0.228
4	Tar $\rightarrow$ 4Pgas	−42	4.25×106	108.0	0.214

[a] Fractional char formation for CL, HC, and LG are 0.35, 0.60, and 0.75 kg char/kg, respectively.
[b] Subscripts "v" and "a" indicate the virgin and activated forms of biomass, respectively.

Table 2
Pyrolysis species and relevant thermochemical and physical properties.

	Component	Phase	MW [a] (g/mol)	ΔH_f^0 (kJ/mol)	ρ_s (dry kg/m^3)	C_p (J/(kg K))	λ (W/(m K))
1	CL_a	Biomass	100	0	500	1400	0.209
2	HC_v	Biomass	100	0	500	1400	0.209
3	LG_v	Biomass	100	0	500	1400	0.209
4	CL_a	Biomass	100	0	500	1400	0.209
5	HC_a	Biomass	100	0	500	1400	0.209
6	LG_a	Biomass	100	0	500	1400	0.209
7	$Char_c$	Char	100	−45.27	175	1100	0.071
8	$Char_h$	Char	100	−17.53	300	1100	0.071
9	$Char_l$	Char	100	−9.77	375	1100	0.071
10	Tar	Gas	100	25.5	–	Phenol	Phenol
11	Pgas	Gas	25	5.33	–	Ethylene	Ethylene
12	H_2O	Gas	18.02	–	–	–	–
13	N_2	Gas	28.02	–	–	–	–
14	Sand	Sand	–	–	2650	800	0.75

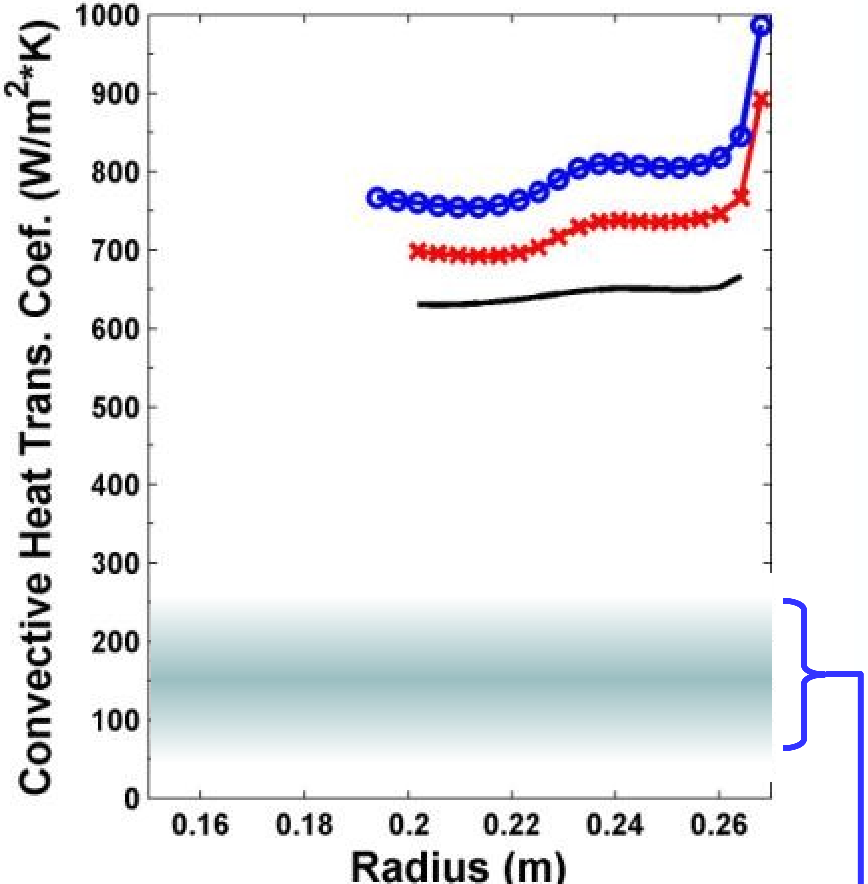
The emissivity of all particulate phases was assumed to be 0.75.
[a] The molecular masses of the biomass, char, and gas-phase pseudo-components are arbitrary and only affect the as-written stoichiometry of the reactions.

GSVR Biomass Simulations

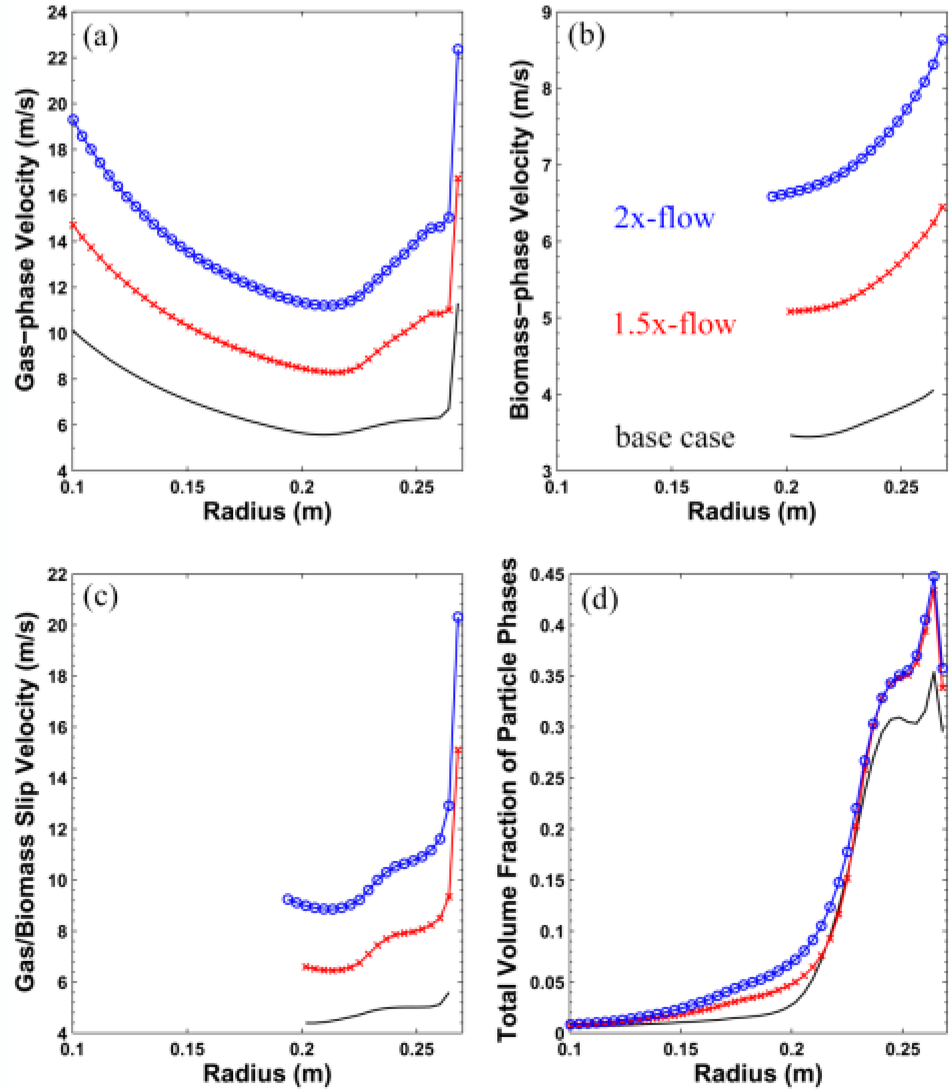
Case name	Air Feed Rate (kg/s)	Biomass Feed Rate (kg/s)	Biomass Water %
Base	0.22	0.035	10
No-H_2O (high-T)	0.22	0.035	0
1.5x-flow	0.33	0.052	10
2x-flow	0.44	0.070	10
No-sand	0.22	0.035	10
No-sand/No-H_2O (high-T)	0.22	0.035	0

→ Inlet Gas Temperature = 923 K
→ Biomass Feed Temperature = 300 K

GSVR Process Intensification

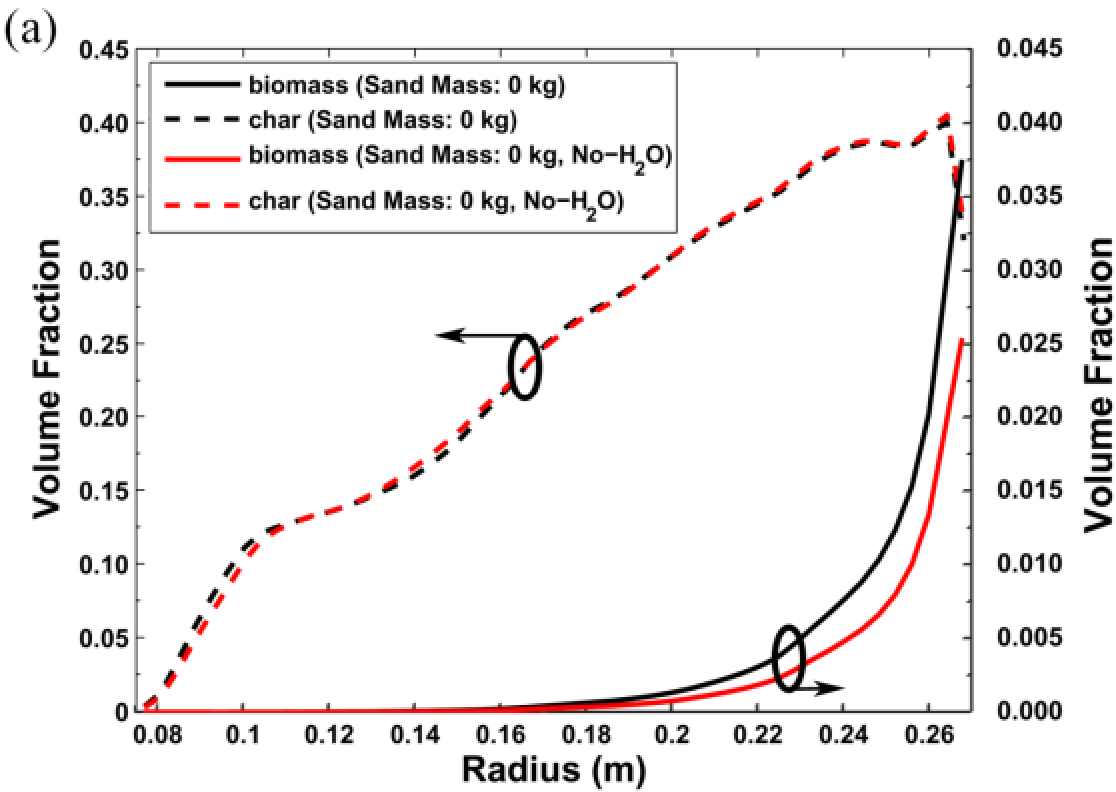


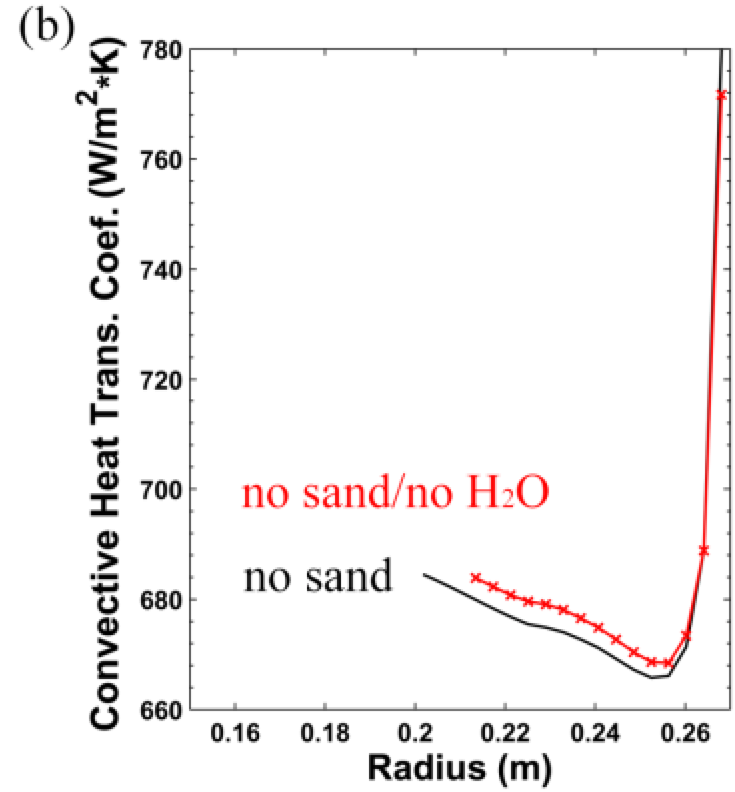
Typical range for static fluidized beds and risers/CFBs: [1,2]
~100 – 200 W/(m² K)



1. Z.Y. Zhou, A.B. Yu, P. Zulli, Particle scale study of heat transfer in … fluidized beds, AIChE J. 55 (2009) 868–884
2. Y. Ma, J.X. Zhu, Experimental study of heat transfer in a co-current downflow fluidized bed, Chem. Eng. Sci. 54 (1999) 41–50

No-Sand Cases Results





Case name	m^{ss}_{sand} (kg)	m^{ss}_{bio} (kg)	m^{ss}_{char} (kg)	T^{avg}_{bio} (K)	T^{avg}_{char} (K)	T^{avg}_{sand} (K)	T^{outlet}_{gas} (K)	$\dot{m}^{out}_{char}$ (kg/s)
Base	5.0	0.056	0.119	721	753	761	751	0.0056
No-sand	0.0	0.056	1.939	727	751	–	750	0.0060
No-H_2O	5.0	0.036	0.123	734	787	794	784	0.0050
No sand/No-H_2O	0.0	0.036	1.938	741	784	–	783	0.0056

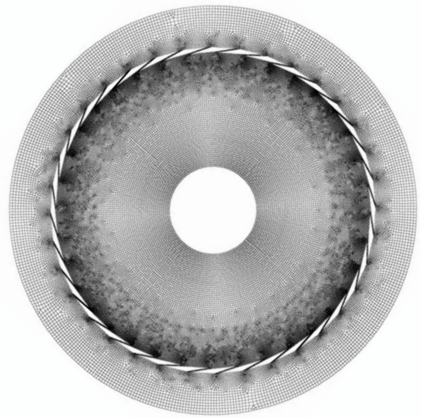
Biomass Pyrolysis Product Distribution

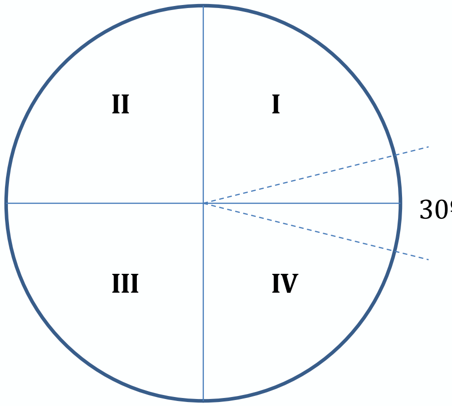
Case name	Char (%)		Tar (%)	Pyrolysis gas (%)
Base	16.1	(16.7%)[a]	73.8	9.5
973 K	14.6	(15.5%)[a]	75.6	8.9
No-H_2O	14.5	(15.1%)[a]	76.0	8.9
1.5x-flow	16.3	(17.0%)[a]	73.8	9.2
2x-flow	16.8	(17.6%)[a]	73.3	9.1
No-sand	17.1	(17.1%)[a]	73.6	9.3
No sand/No-H_2O	16.0	(15.7%)[a]	75.6	8.7

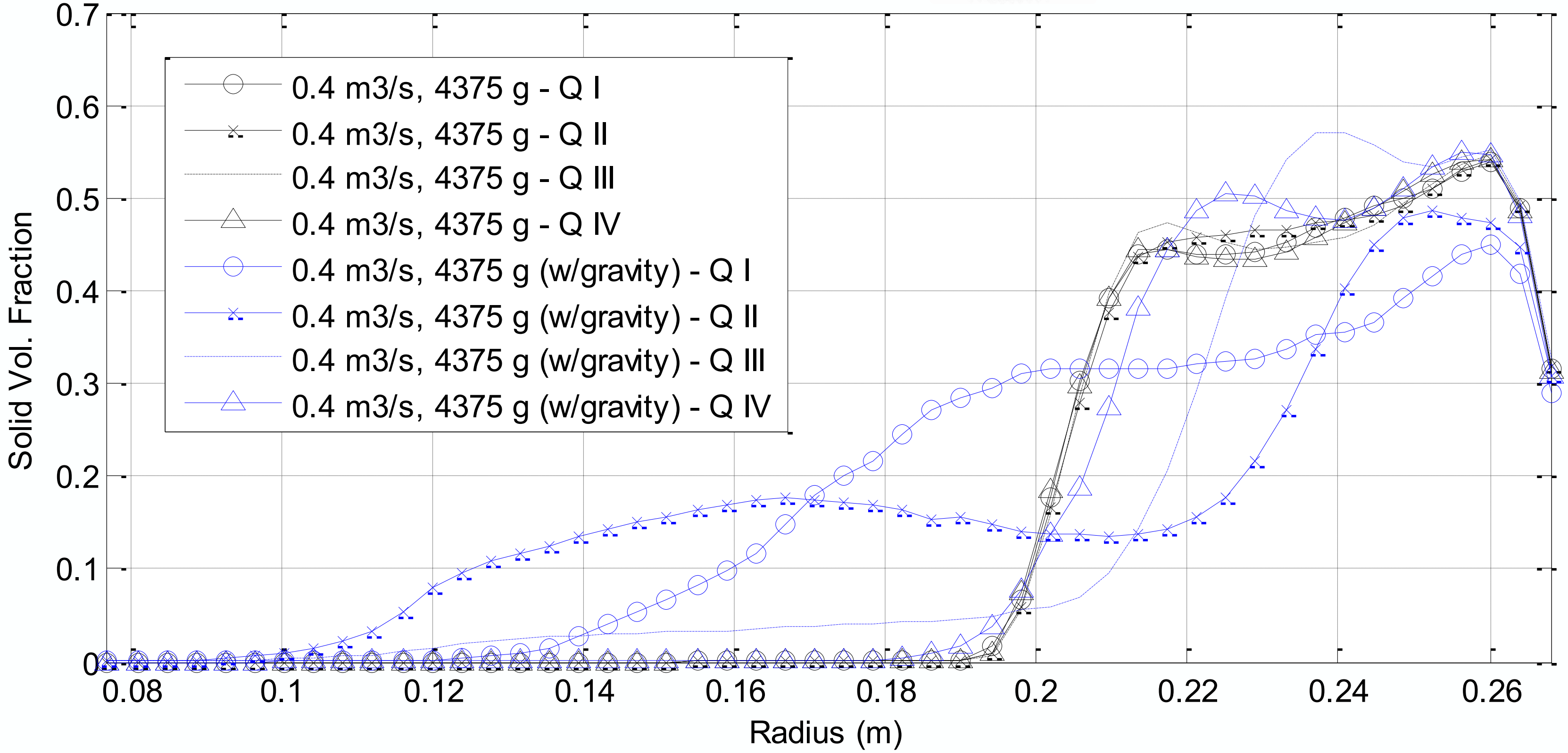
[a] Char production fraction necessary to achieve a perfect mass balance over the reactor; mass balance errors ranged from –0.9% to +0.3%.

"Full" 2D Simulations – Effect of Gravity

- 0.4 m^3/s air flow @ 1.225 kg/m^3 and 4.375 kg bed mass
- Run without gravity for 10 seconds
- Run 10 more sec. with/without gravity
- Quadrant view of solids VF:

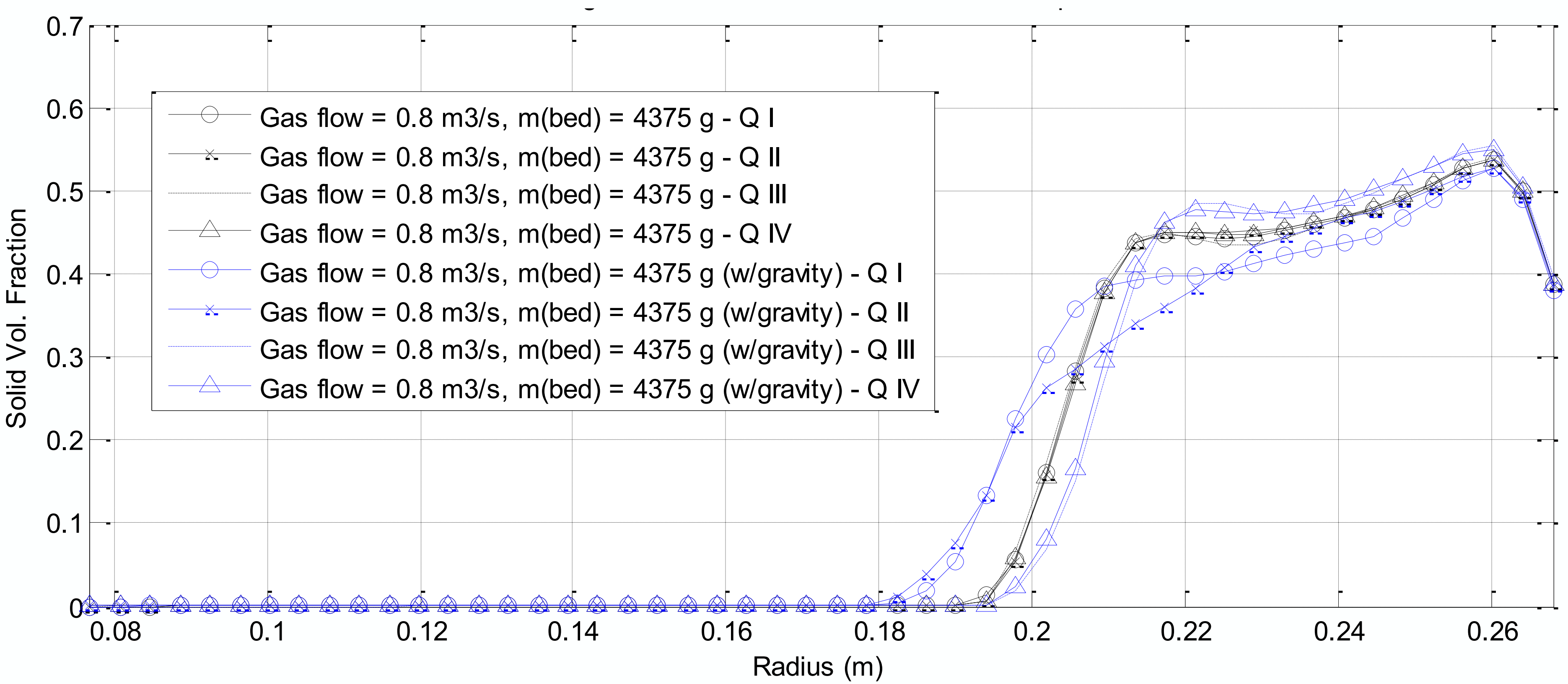


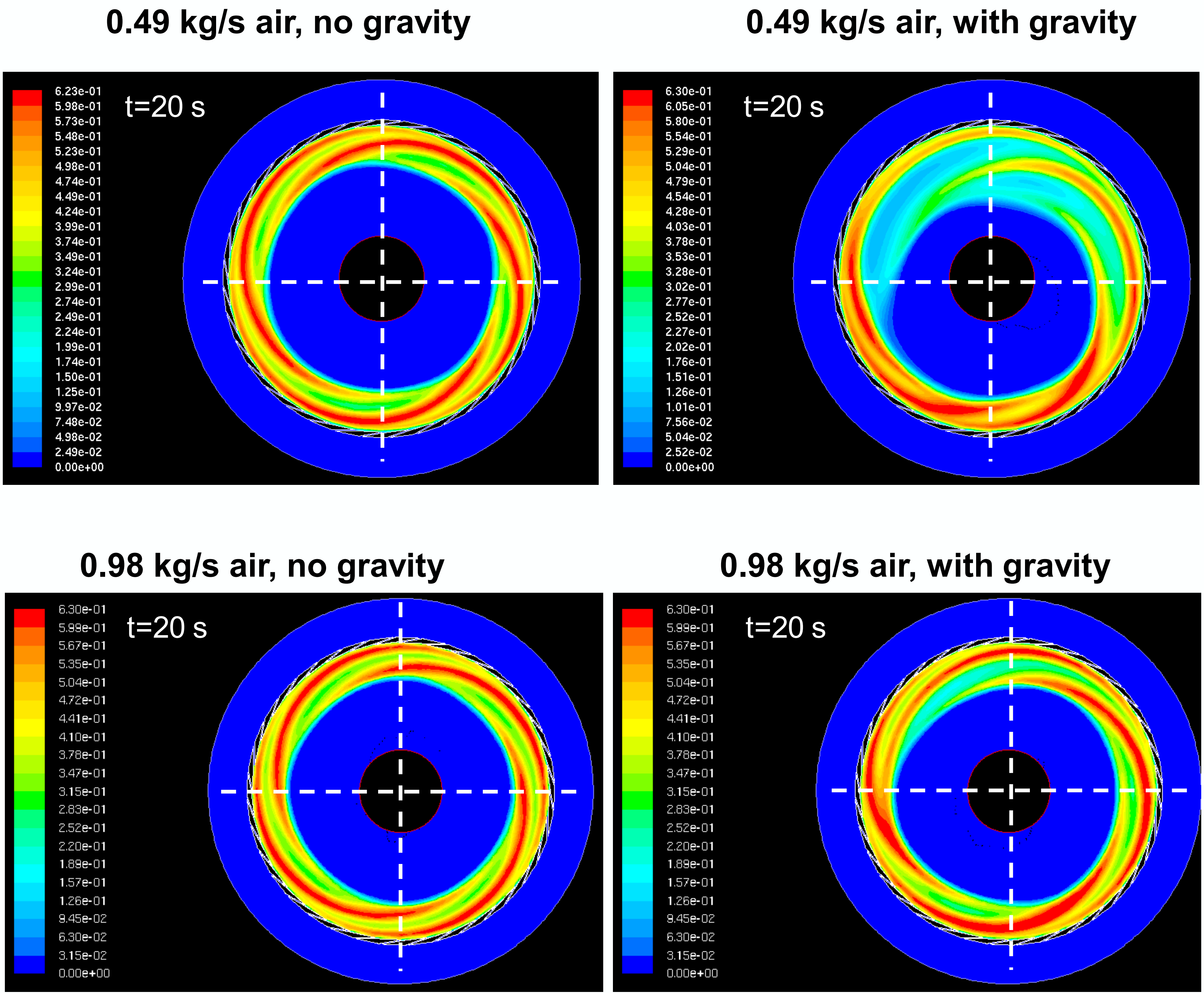


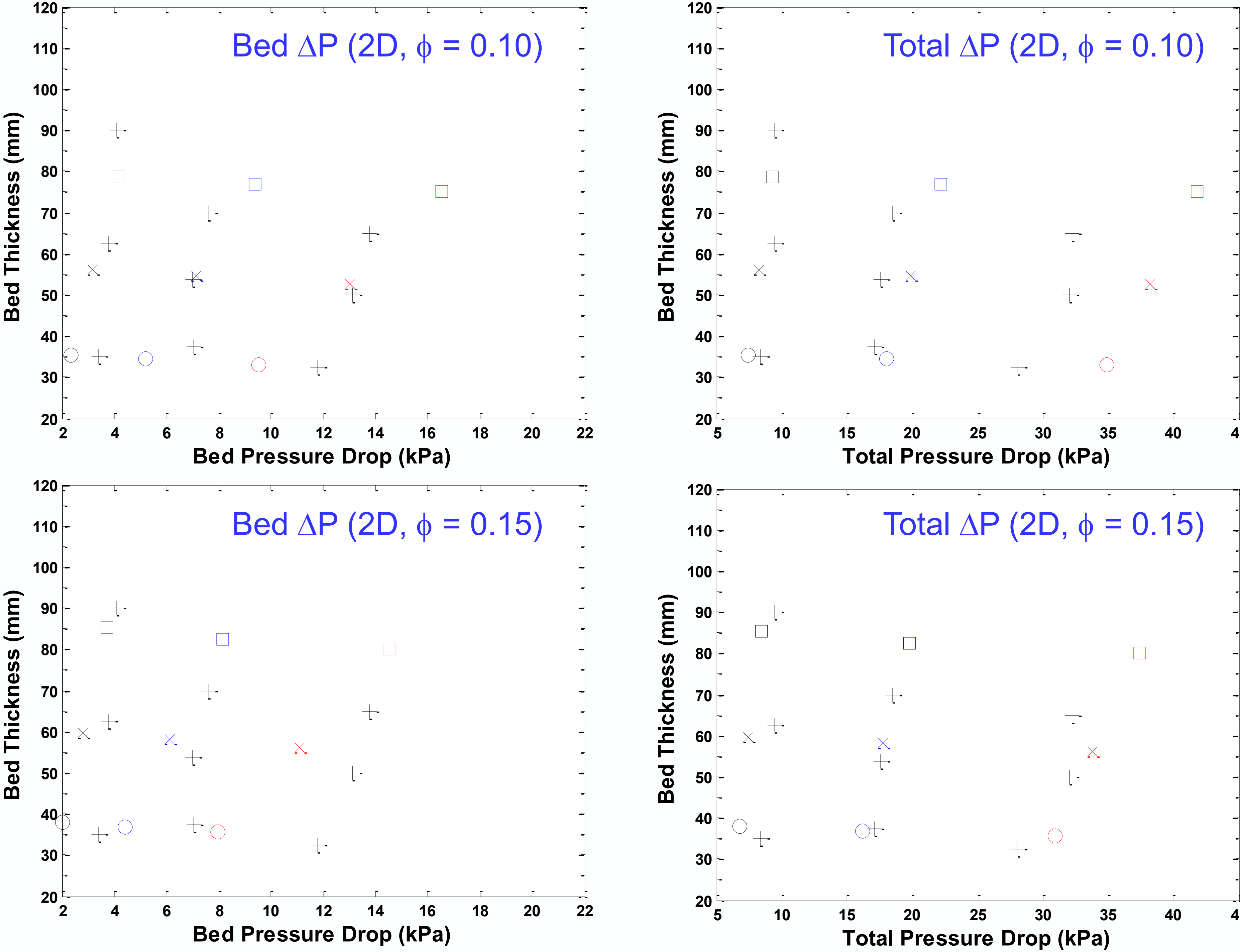


"Full" 2D Simulations – Effect of Gravity

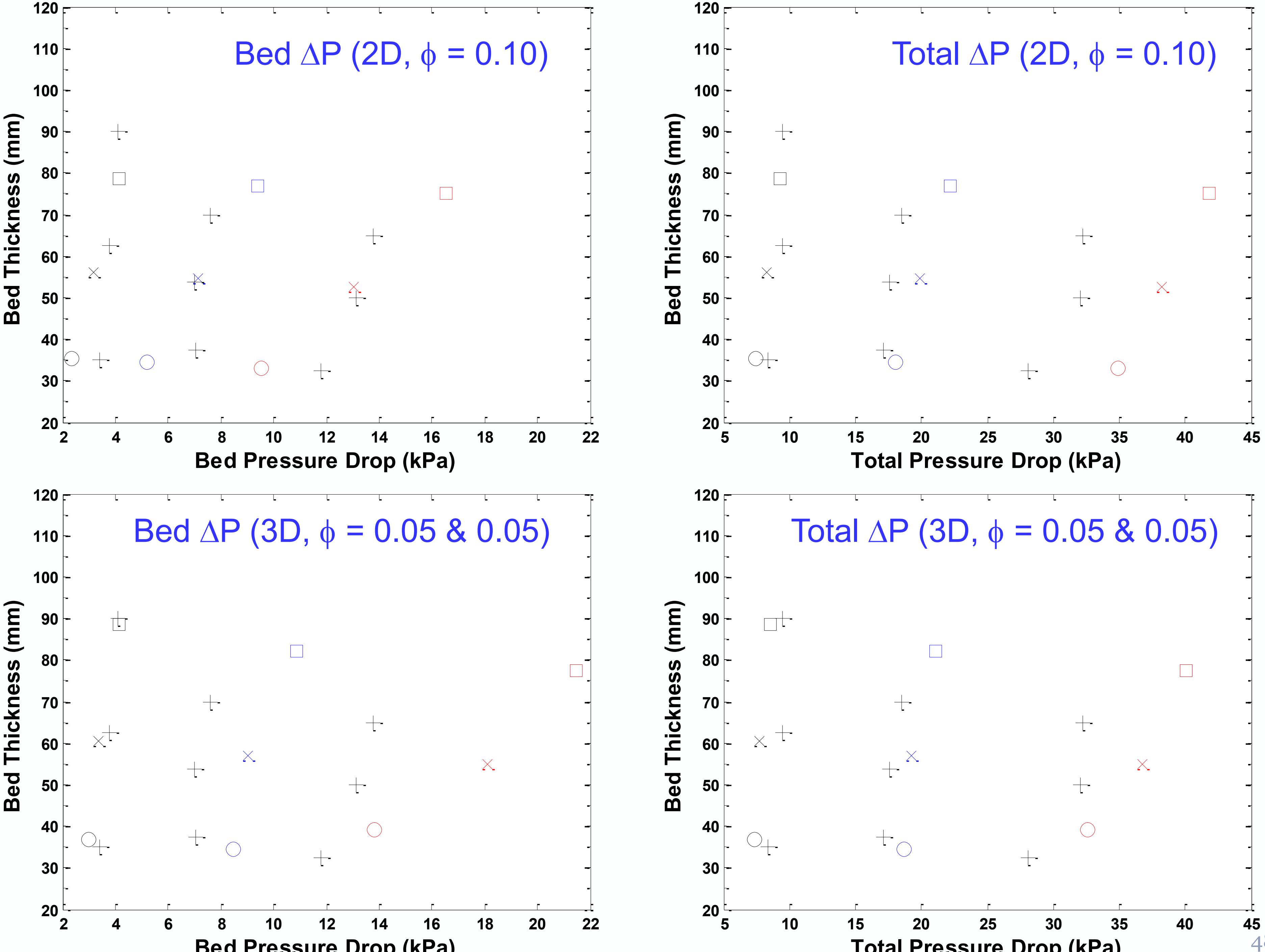
- 0.8 m^3/s air flow @ 1.225 kg/m^3 and 4.375 kg bed mass




0.49 kg/s air, no gravity
t=20 s
6.23e-01
5.98e-01
5.73e-01
5.48e-01
5.23e-01
4.98e-01
4.74e-01
4.49e-01
4.24e-01
3.99e-01
3.74e-01
3.49e-01
3.24e-01
2.99e-01
2.74e-01
2.49e-01
2.24e-01
1.99e-01
1.74e-01
1.50e-01
1.25e-01
9.97e-02
7.48e-02
4.98e-02
2.49e-02
0.00e+00
0.49 kg/s air, with gravity
t=20 s
6.30e-01
6.05e-01
5.80e-01
5.54e-01
5.29e-01
5.04e-01
4.79e-01
4.54e-01
4.28e-01
4.03e-01
3.78e-01
3.53e-01
3.28e-01
3.02e-01
2.77e-01
2.52e-01
2.27e-01
2.02e-01
1.76e-01
1.51e-01
1.26e-01
1.01e-01
7.56e-02
5.04e-02
2.52e-02
0.00e+00
0.98 kg/s air, no gravity
t=20 s
6.30e-01
5.99e-01
5.67e-01
5.35e-01
5.04e-01
4.72e-01
4.41e-01
4.10e-01
3.78e-01
3.47e-01
3.15e-01
2.83e-01
2.52e-01
2.20e-01
1.89e-01
1.57e-01
1.26e-01
9.45e-02
6.30e-02
3.15e-02
0.00e+00
0.98 kg/s air, with gravity
t=20 s
6.30e-01
5.99e-01
5.67e-01
5.35e-01
5.04e-01
4.72e-01
4.41e-01
4.10e-01
3.78e-01
3.47e-01
3.15e-01
2.83e-01
2.52e-01
2.20e-01
1.89e-01
1.57e-01
1.26e-01
9.45e-02
6.30e-02
3.15e-02
0.00e+00



Bed ΔP (2D, ϕ = 0.10)
Bed Thickness (mm)
Bed Pressure Drop (kPa)
Total ΔP (2D, ϕ = 0.10)
Bed Thickness (mm)
Total Pressure Drop (kPa)
Bed ΔP (2D, ϕ = 0.15)
Bed Thickness (mm)
Bed Pressure Drop (kPa)
Total ΔP (2D, ϕ = 0.15)
Bed Thickness (mm)
Total Pressure Drop (kPa)


Bed ΔP (2D, ϕ = 0.10)
Total ΔP (2D, ϕ = 0.10)
Bed ΔP (3D, ϕ = 0.05 & 0.05)
Total ΔP (3D, ϕ = 0.05 & 0.05)
Bed Thickness (mm)
Bed Pressure Drop (kPa)
Total Pressure Drop (kPa)

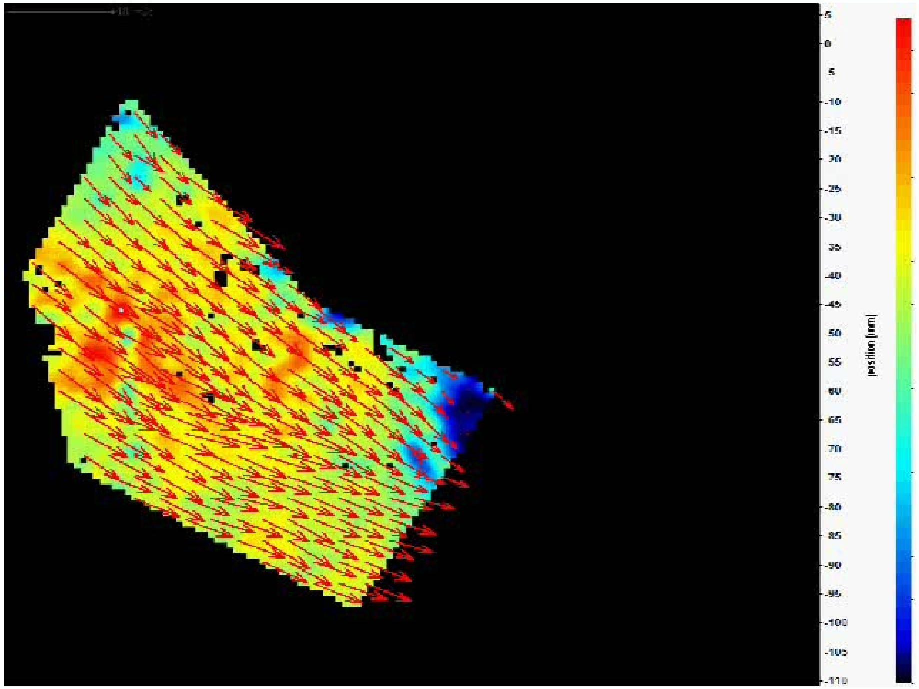
On-going Model Refinement - PIV

Particle Image Velocimetry (PIV)

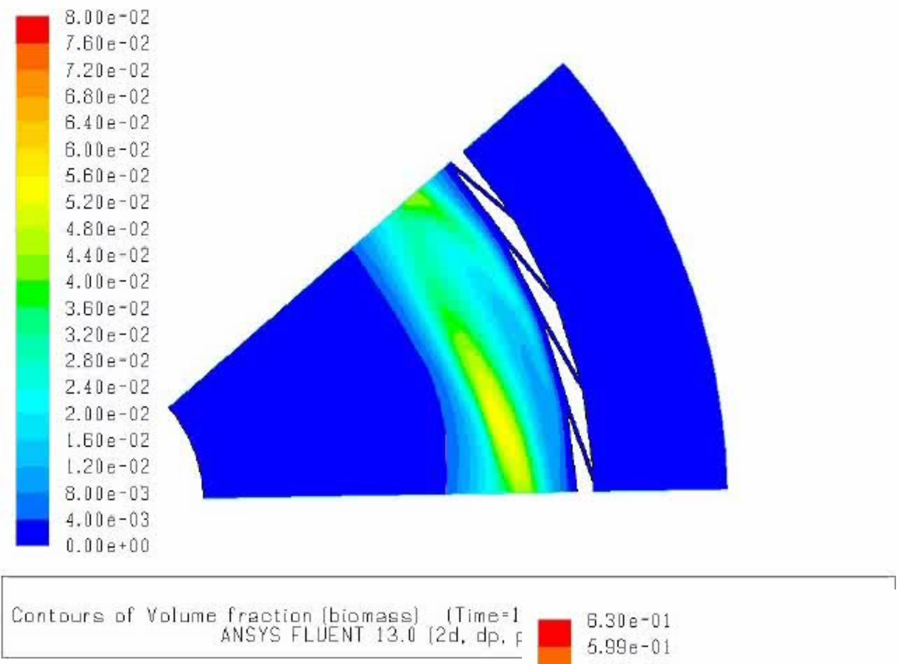
- Allows for 2D particle velocity field near end-wall
- Final “major” observable for bulk validation

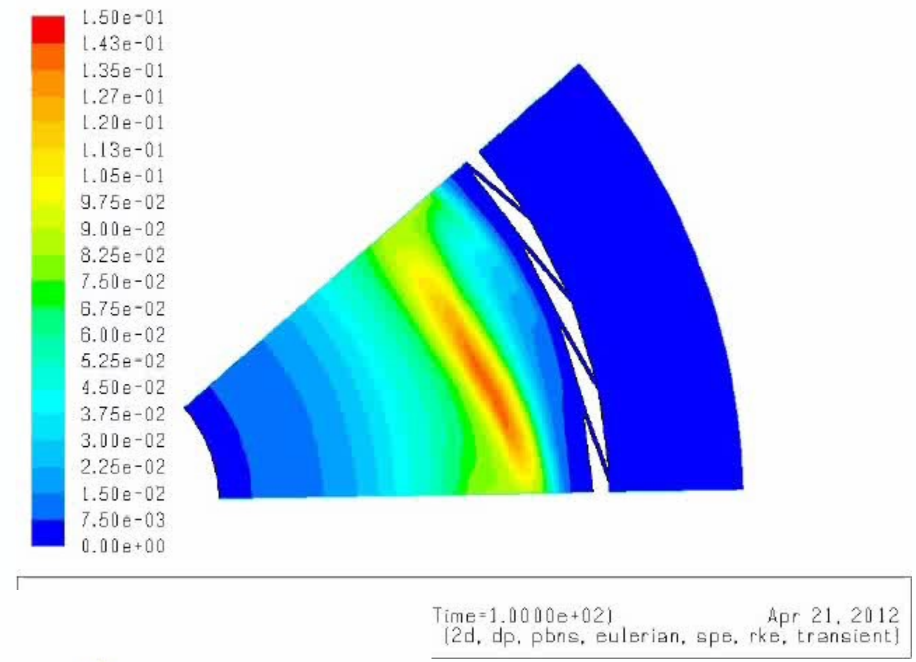
Raw image collection

Processed velocity field



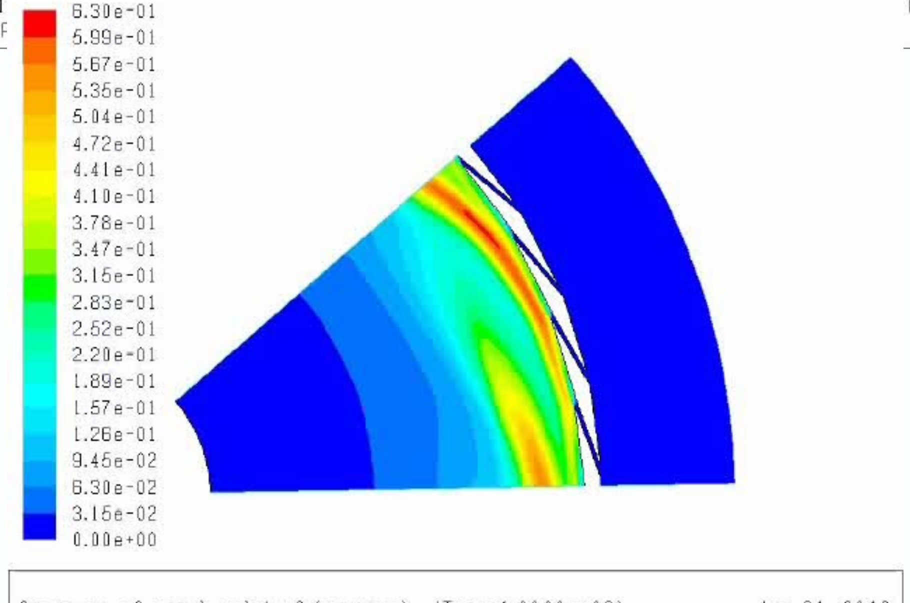
2x-Flow VF Animation (back-up slide)



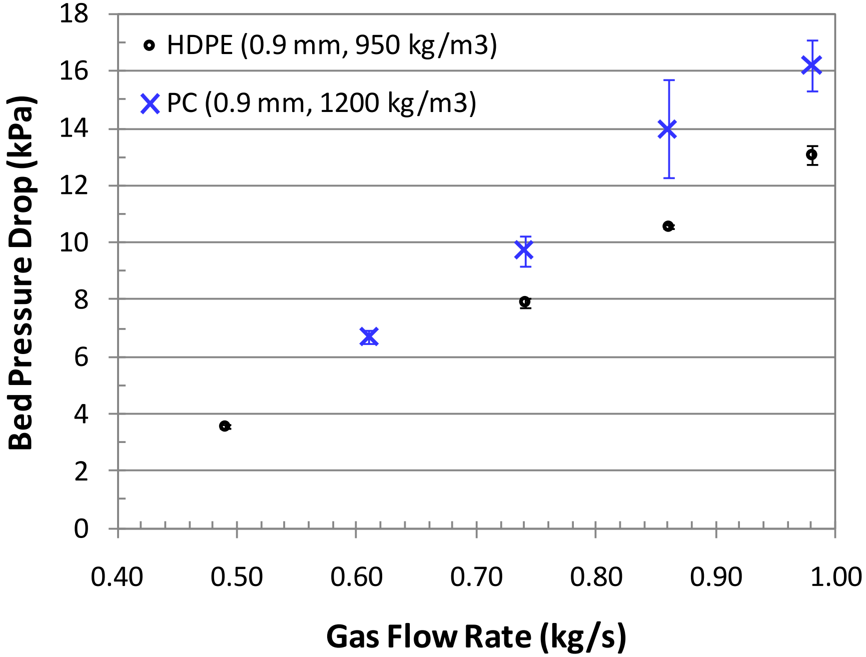


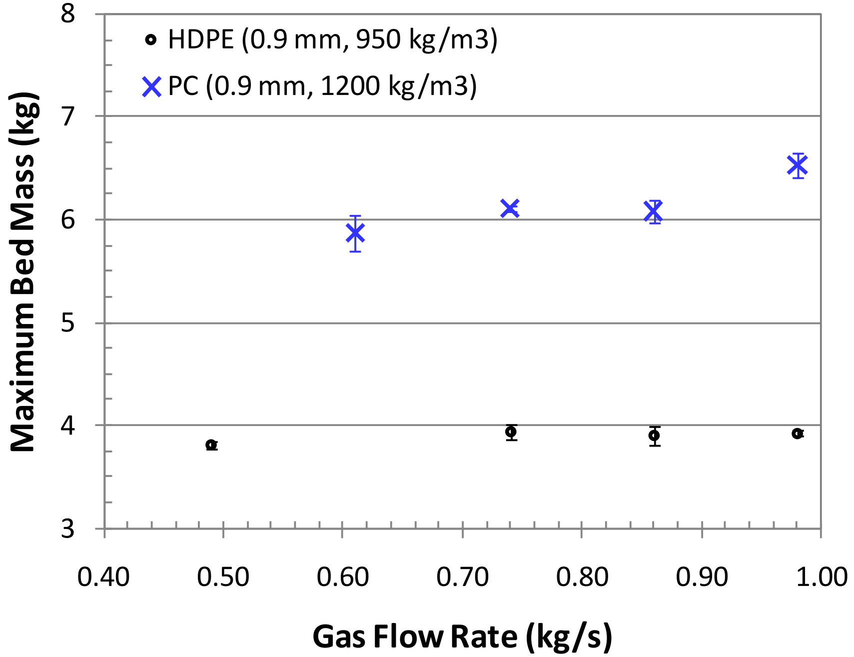
Biomass

Char



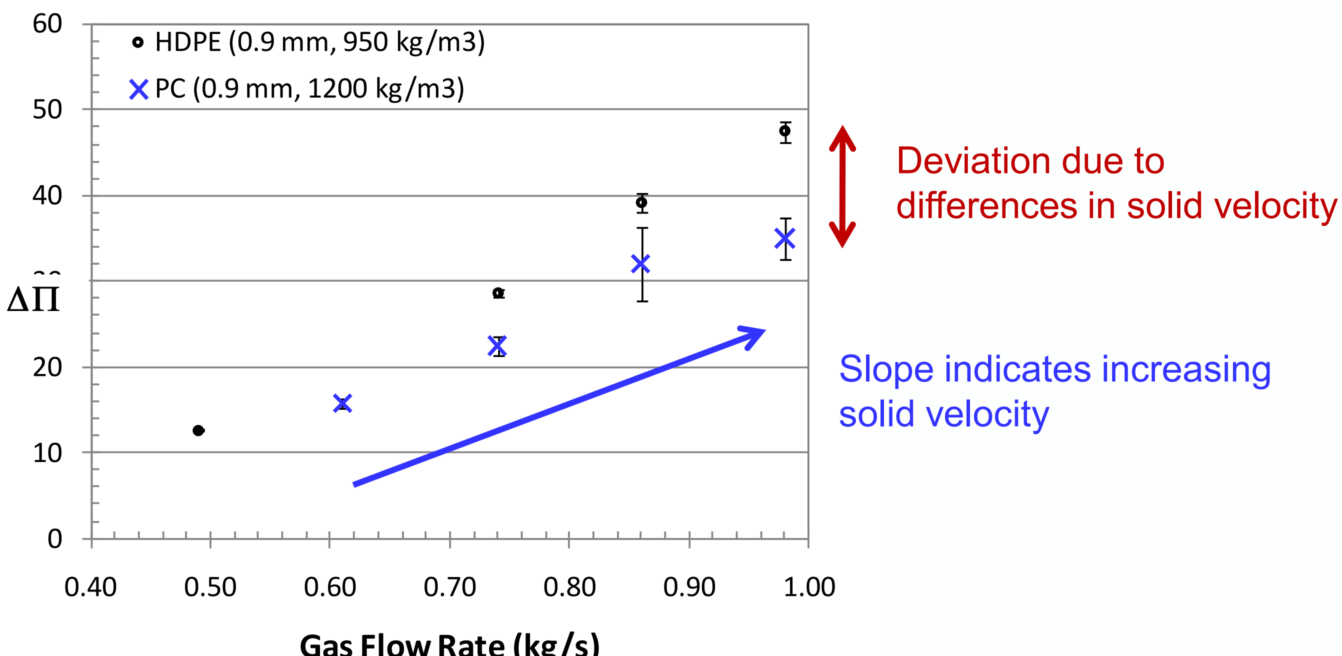
Total solids
(biomass, char, sand)





Scaled Bed Pressure Drop

$$\Delta\Pi = \frac{\Delta P_{bed}}{\rho_s \, g \, H_{bed} \, \varepsilon_s}$$



CFD Example Movies

3D, 0.74 kg/s air, 3250 g bed