

# Modelling fluidized dense phase conveying of Geldart A powders with MFiX-TFM: A case study

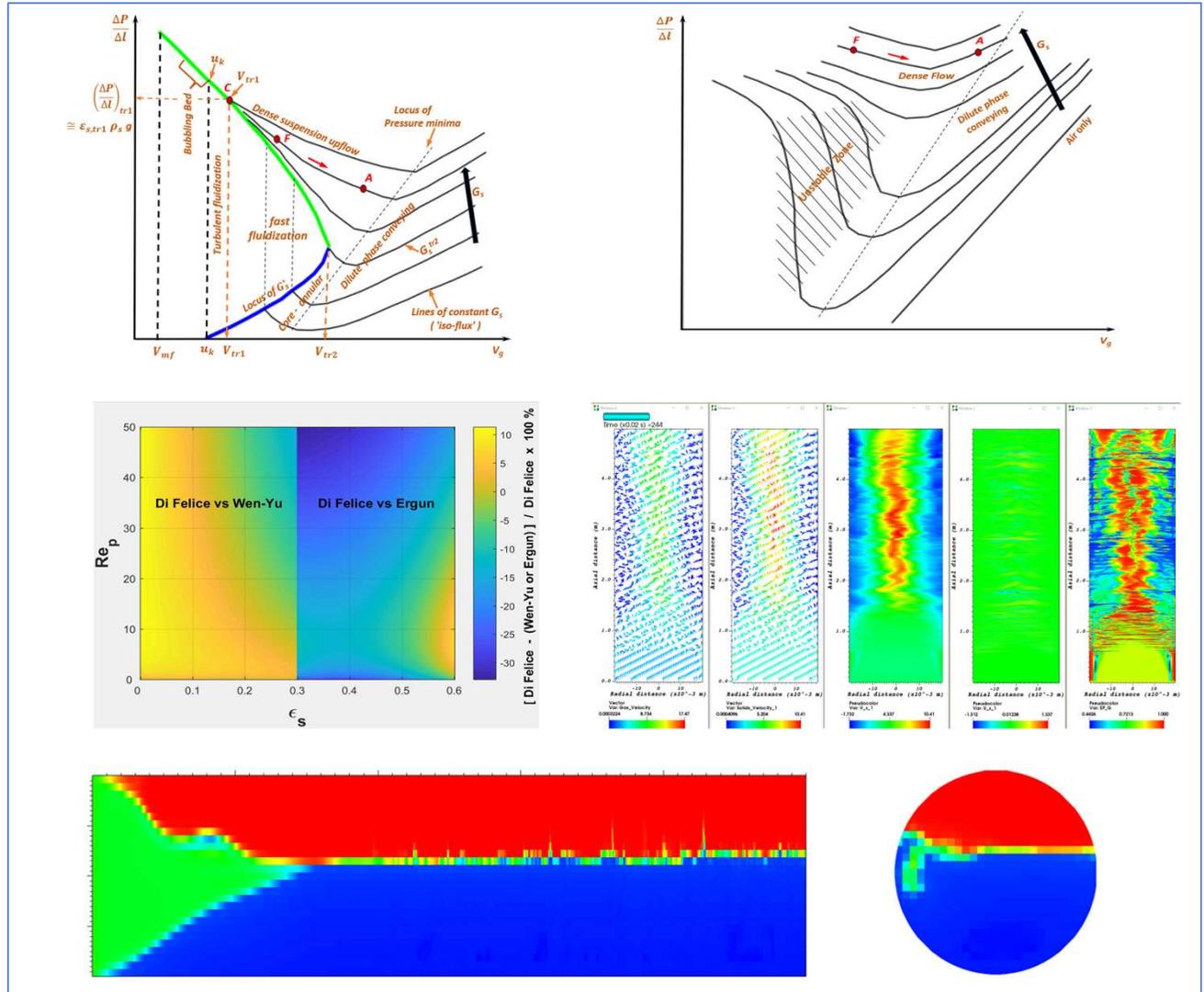
Prabu Balasubramanian, Andrew Cowell, Don McGlinchey

School of Computing, Engineering and Built Environment  
Glasgow Caledonian University, United Kingdom

# Outline

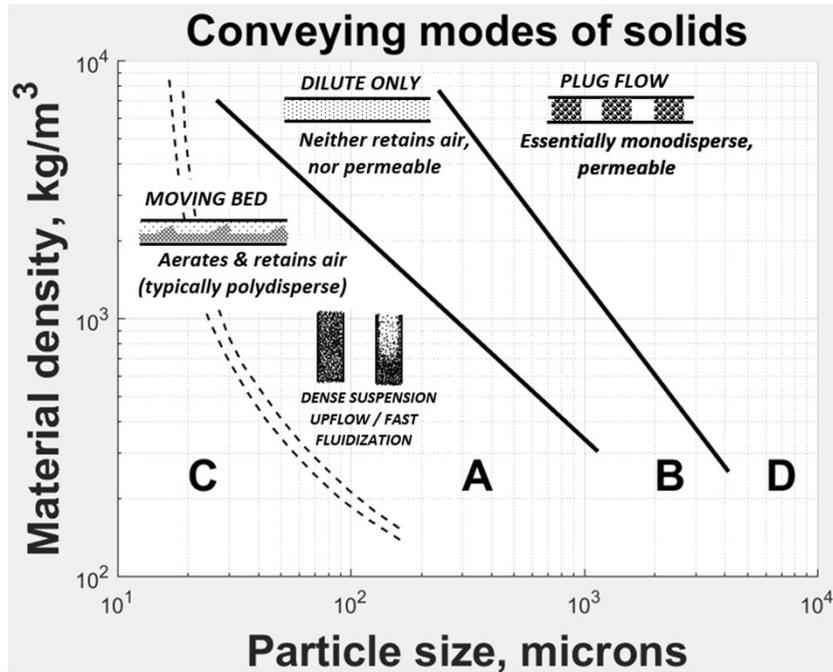
- Fluidized Dense Phase Conveying
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# Graphical Abstract

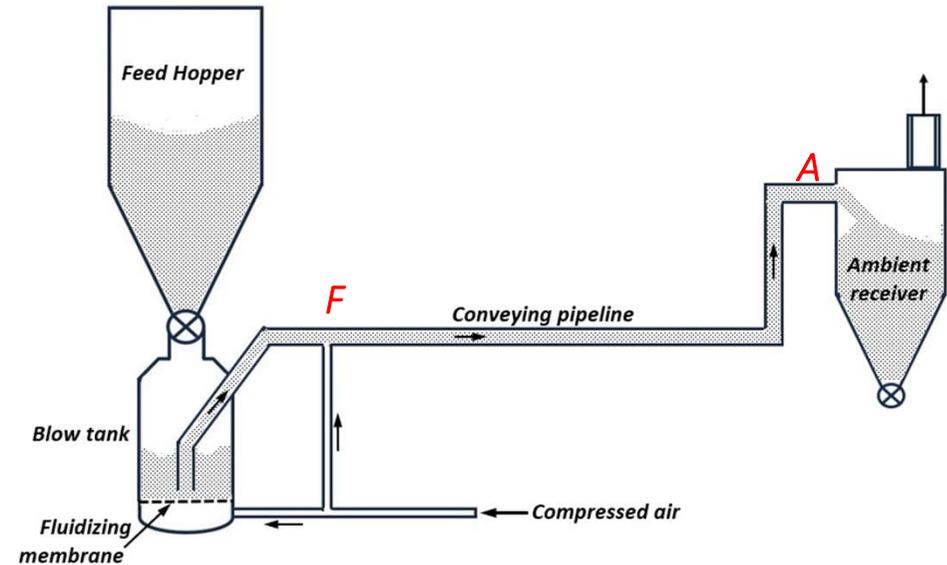


# Fluidized Dense Phase Conveying

# Fluidized dense phase conveying



- Suitable for fine powders (Typical Geldart A or C) that aerate and retain air well.
- Design remains largely empirical, requiring full-scale experiments with the product; Eulerian modelling is an attractive alternative.

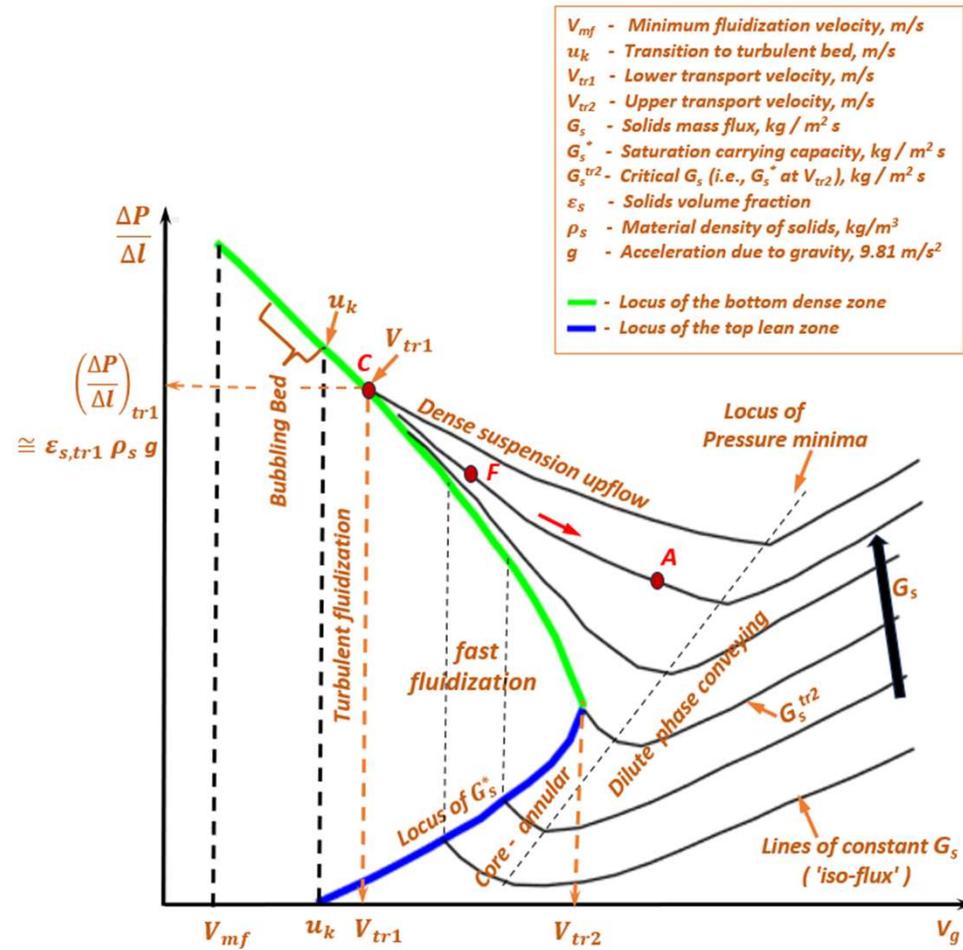


Typical Fluidized Dense Phase Conveying System and Operating Conditions Reference: Mills (2004)

Description		Feed zone ( <b>F</b> )	Ambient Receiver ( <b>A</b> )
Maximum Solids loading ( $m$ )	kg / kg of air	150 - 300	
Maximum Solids flux ( $G_s$ )	kg / $\text{m}^2 \text{ s}$	1000 - 3000	
Pressure	bar	2.5 - 4.0	Ambient
Solids volume fraction ( $\varepsilon_s$ )	-	0.12 - 0.30 *	0.04 - 0.14
Superficial gas velocity ( $V_g$ )	m / s	3 - 4	9 - 12
Conveying Pipeline	-	Typically, up to a few hundred meters long, > 80 % horizontal, with several bends	

\* - For powders that show clear pressure minima in the phase diagram.

# Fluidized Dense Phase Conveying on Vertical Flow Phase Map



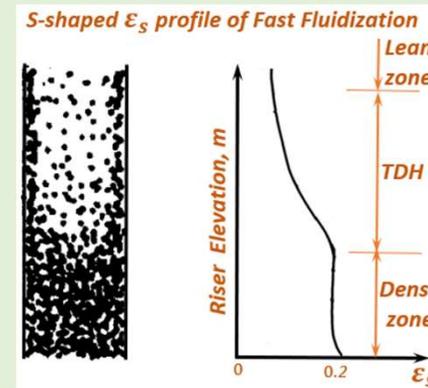
Vertical flow: Phase map of Wirth adapted for Geldart A powders

Reference: Adapted from Wirth (1988), with inputs from Yerushalmi & Avidan (1985), Kim et al. (2004), Cocco et al. (2010), Monazam & Shadle (2011), Breault (2023)

- Experimental data (Mills, 2004) suggests that, at high  $G_s$  the flow occurs at dense conditions (e.g.,  $F \rightarrow A$ ) wherein 'bed filling' is irrelevant; flow may not transition to dilute phase conveying ( $\epsilon_s < 0.02$ ) at the ambient receiver.

(Note: It is assumed here that the change in operating pressure does not affect the phase map.)

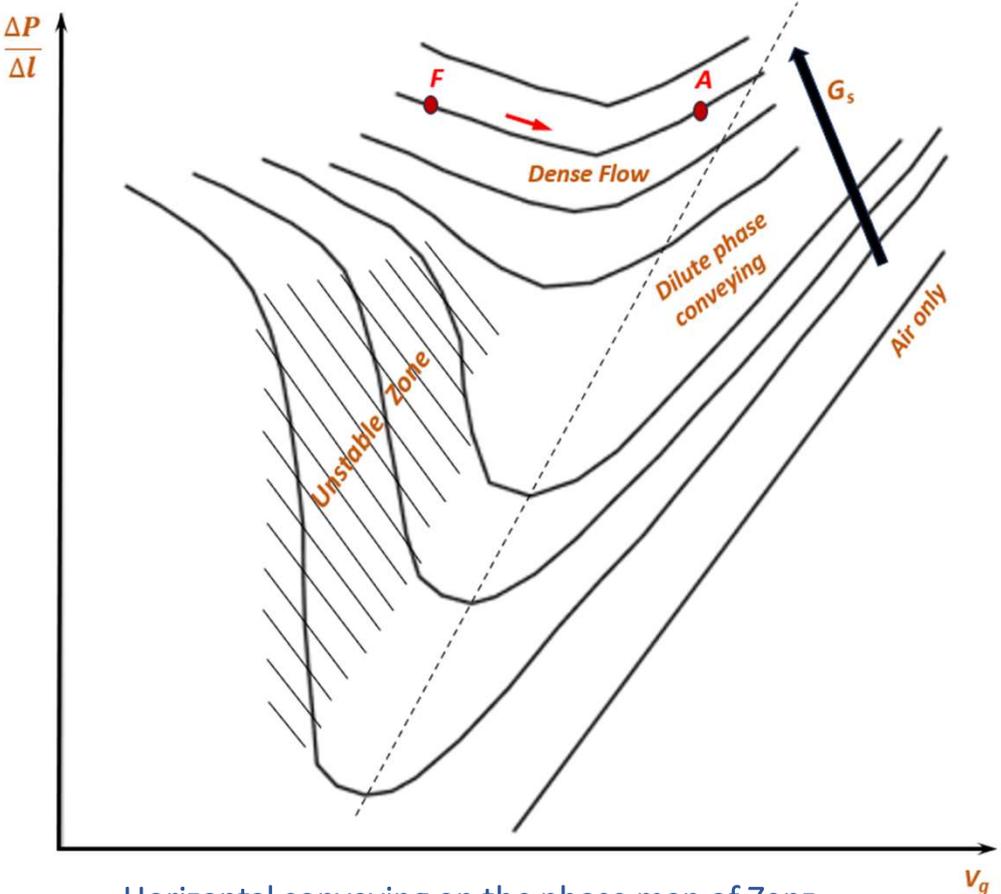
- Dense Suspension Upflow (DSU) is also broadly 'core-annular flow', with denser annulus and relatively dilute core, but with up flowing annulus. However, axial variation in  $\epsilon_s$  is limited to the expansion of air for the incurred pressure drop.
- As DSU operates at higher  $\epsilon_s$  than fast fluidization (0.07-0.25 against 0.03-0.10) for the same range of  $V_g$ , slip velocities are even higher (3-10 m/s against 2-6 m/s) Grace(2000).
- At lower  $G_s$ , the locus of  $G_s^*$  marks the 'onset' of accumulative choking'. Axial variation in  $\epsilon_s$  follows the 'S-shaped profile' with a Transport Disengagement Height (TDH) between the dense and lean zones. The operation (solids inventory) can be very sensitive to variations in  $G_s$  and/or  $V_g$  (Monazam & Shadle (2011)); however, it is a well-established operating regime in industry.



Reference: Kunii & Levenspiel (1991)

- For all cases choking is complete at  $C (V_{tr1}, \epsilon_{s, tr1})$ , wherein net entrainment has essentially stopped, and the solids have collapsed into a turbulent bed.

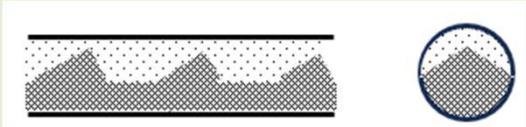
# Fluidized Dense Phase Conveying on Horizontal flow Phase Map



Horizontal conveying on the phase map of Zenz

Reference: Adapted from Zenz(1949) for fine powders, with inputs from Mills (2005), Canning & Thompson (1982) cited in Klinzing et al. (2010).

- Experimental data (Mills (2004), Canning & Thompson (1982) (cited in Klinzing et al. (2010)) suggests that, at high solids loading (1000 – 3000 kg/m<sup>2</sup>s) flow occurs at dense conditions (e.g.,  $F \rightarrow A$ ) where ‘saltation’ (unstable zone) is irrelevant.
- Experimental data (Mills, 2004) also indicates that dense flow at higher  $G_s$  occurs on either side of the pressure minima (intuitive as there is no static head of solids).
- Typical ‘moving bed’ dense horizontal flow pattern:



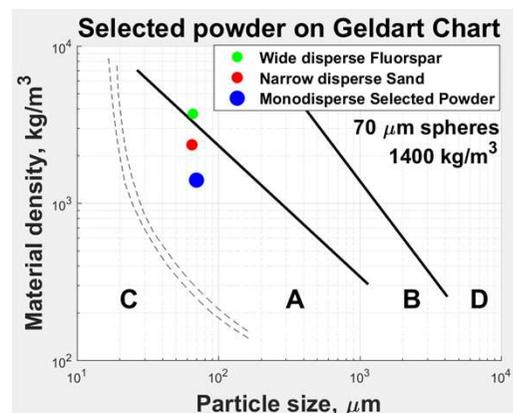
Reference: Klinzing et al. (2010)

*Dilute phase conveying ( $\epsilon_s < 0.02$ ) may coexist at the top of the pipe cross section with a moving dense bed of solids ( $\epsilon_s$  up to 0.6) at the bottom.*

- Given the very high  $G_s$  it may not be practical to pick up and accelerate solids fed to rest at the bottom of the pipe; instead, the solids are fed fluidized from the blow tank.

# Characteristics of the Geldart A powder

# Selection and Characteristics of the (hypothetical) powder



## For smaller $d_p$

- Ability of a powder to aerate and retain aeration is critical for fluidized dense phase conveying.
- Powders at the Geldart A-B boundary, may show interchanged flow behaviour depending on their ability to retain air, i.e., the width of size distribution.
- For a monodisperse Geldart A powder to flow by fluidized dense phase, it should be away from A-B boundary (low in  $\rho_s$  and  $d_p$ ).

Note: Geldart chart is based on ambient air. At higher pressures (such as at  $F$ ), Geldart A/B boundary may shift to the right (i.e., to higher mean particle size) (Yang (2007)).

## Against smaller $d_p$

- Cohesion due to van der Waals forces become significant at  $d_p < \sim 55 \mu\text{m}$  (Wang et al.(2011), Loezos et al. (2002)). Cohesion models are not available in standard MFiX-TFM.  
*(Askarishahi et al.(2022) have reported a custom implementation of the cohesion model of Gu et al.(2019) in MFiX)*
- Computationally prohibitive, as cells of  $\sim 10 d_p$  is required for reliable predictions and  $\sim 20 d_p$  for even reliable qualitative trends (Agrawal et al.(2001), Benyahia et al.(2007)).

## Characteristics of the selected powder at ambient conditions

Archimedes number	$Ar$		<b>17.5</b>	
Void fraction loose packed	$\epsilon_{s,max}$		<b>0.60</b>	Maximum packing limit
Interparticle restitution	$c_e$		<b>0.87</b>	Foerster et al. (1994), Drake (1991), (6 mm cellulose acetate spheres)
Particle – wall restitution	$e_w$		<b>0.89</b>	(Note-1)
Angle of wall friction	$\Phi_w$	°	<b>11.86</b>	
Angle of internal friction	$\Phi$	°	<b>30</b>	McKeen & Pugsley (2003)
Terminal settling velocity	$V_t$	m / s	<b>0.186</b>	
Min. fluidization velocity	$V_{mf}$	m / s	<b>0.004</b>	Kunii & Levenspiel (1991)
Min. bubbling velocity	$V_{mb}$	m / s	<b>0.012</b>	
Lower transport velocity	$V_{tr1}$	m / s	<b>1.95</b>	Yerushalmi & Avidan (1982) ('HFZ-20 catalyst', 49 $\mu\text{m}$ ,
Upper transport velocity	$V_{tr2}$	m / s	<b>&gt; 5.20</b>	1450 kg/m <sup>3</sup> , $D_r = 152 \text{ mm}$ ) (Note-2)
Critical $G_s$ (i.e., $G_s^*$ at $V_{tr2}$ )	$G_s^{tr2}$	kg / m <sup>2</sup> s	<b>&gt; 236</b>	Breault & Weber (2021)

Particles are non-cohesive, do not agglomerate or deform permanently, and there are no electrostatic effects.

An important criterion in the selection of powder is the availability of experimental data for model validation. The selected particle size and material density corresponds to FCC particles for which experimental data is widely reported (although all for vertical flow). However, one-to-one correspondence cannot be expected between the model which considers a monodisperse powder and experiments with polydisperse powders that contain a significant fraction of fines ( $d_p < 44 \mu\text{m}$ ).

Note-1: Restitution coefficients of 0.90 – 0.95 is widely used in the literature. Indicated values may be revised higher during model validation to match experimental radial profiles for solids fraction.

Note-2: The correlations available in the literature (such as Bi & Grace (1995) and Monazam & Shadle (2011)) underpredict  $V_{tr1}$  and  $V_{tr2}$  for fine powders.

Indicated  $V_{tr2}$  of 5.2 m/s from Yerushalmi & Avidan (1982) corresponds to the transition to 'Dense Conveying' (i.e., core-annular flow) at a  $G_s$  of 150 kg/m<sup>2</sup>s.

! ?  $Ar$  based correlations (e.g.,  $V_{tr1}$ ,  $V_{tr2}$ ,  $G_s^*$ ) are largely based on data at essentially atmospheric pressure. As  $Ar (= \rho_g (\rho_s - \rho_g) g d_p^3 / \mu_g^2)$  scales with pressure (i.e.,  $\rho_g$ ), it is not clear from the literature if the correlations are suitable for pressures higher than atmospheric, such as at the feed zone,  $F$ . ! ?

# Recent CFB experiments – HD-CFB or LD-CFB ?

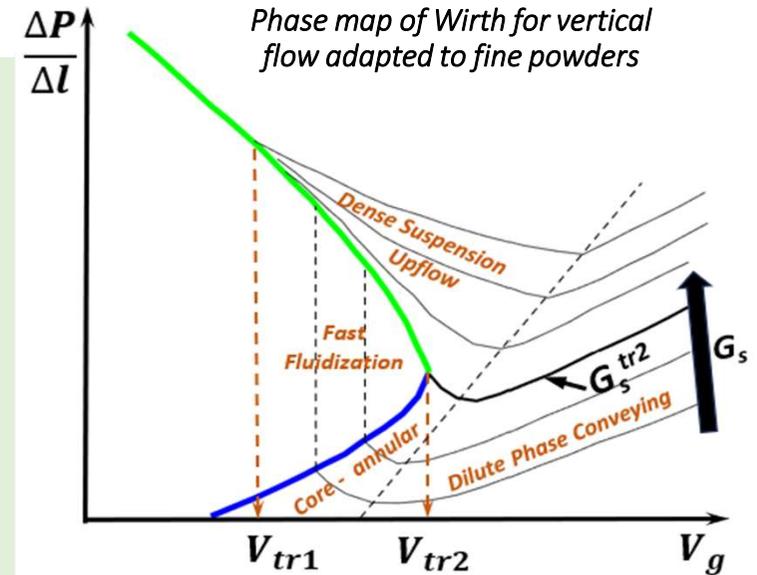
- Issangya et al. (2022) have recently reported S-shaped  $\varepsilon_s$  profile at as high as  $G_s$  as 636 kg/m<sup>2</sup>s and  $V_g$  of 9 – 16 m/s, with a riser diameter ( $D_r$ ) of 0.3 m. They have observed dense suspension at the bottom of the riser to coexist with dilute phase conveying at the top.
- Dense suspension upflow requires both  $V_g > V_{tr2}$  and  $G_s > G_s^{tr2}$ .
- Wang et al.(2022) have observed the S-shaped  $\varepsilon_s$  profile disappear only at a  $G_s \sim 1000$  kg/m<sup>2</sup>s and  $V_g \sim 9$  m/s, for a  $D_r$  of 0.08 m.
- As it can be seen in the correlation of Breault & Weber (2021),  $G_s^{tr2}$  scales directly with the riser diameter,  $D_r$ . (This correlation is based predominantly on FCC particles and covers data over  $5 < Ar < 20.1$ ,  $0.066 < D_r < 0.15$  m,  $1.09 < V_g < 4.00$  m/s,  $2.31 < G_s^* < 198$  kg/m<sup>2</sup>s.)

$$G_s^* = 318 \frac{D_r V_g^{(0.000716 d_p^2)}}{Ar}$$

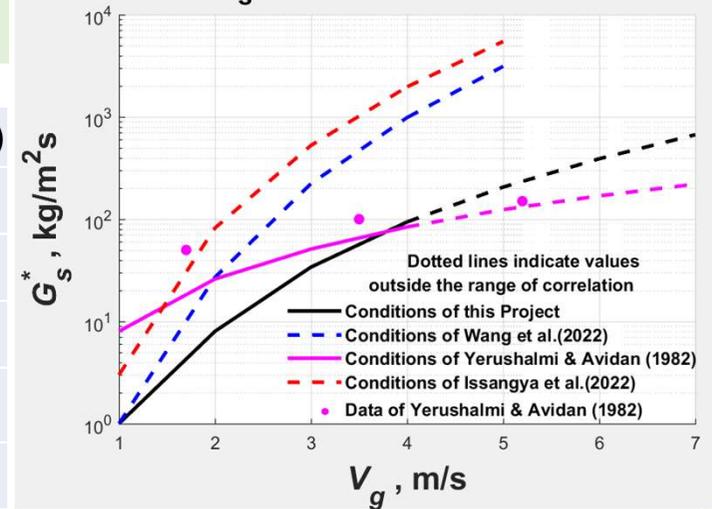
- Results of Wang et al.(2022) and the estimates for  $G_s^{tr2}$  based on Breault & Weber (2021) (extrapolated beyond the data range of the correlation) suggest that the maximum  $G_s$  of 636 kg/m<sup>2</sup>s used in the experiment was most probably below  $G_s^{tr2}$ .

## Conditions of the experiments

Description	This Project	Wang et al. (2022)	Yerushalmi & Avidan (1982)	Issangya et al. (2022)
Riser diameter ( $D_r$ ), m	0.04	0.08	0.152	0.303
Riser height, m	--	18.0	8.5	20.4
Mean particle size ( $d_p$ ), $\mu$ m	70	85	49	80
Material density ( $\rho_s$ ), kg/m <sup>3</sup>	1400	1500	1450	1490
Archimedes number ( $Ar$ ) (ambient)	17.5	33.6	6.2	27.8

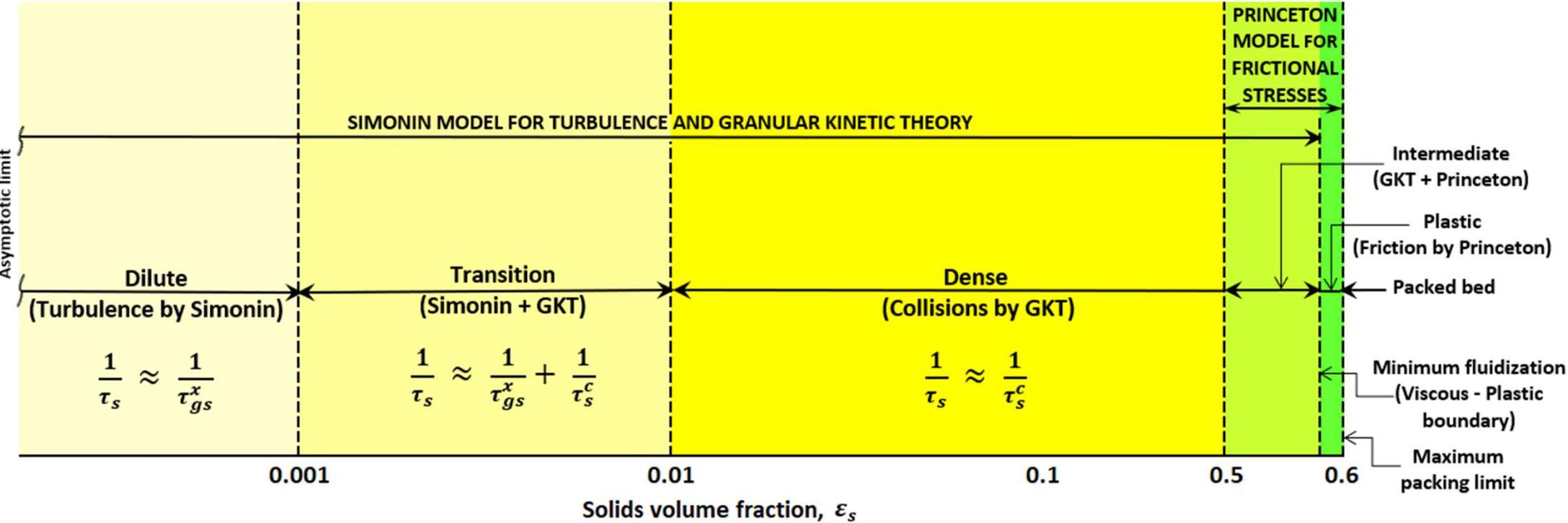


Predicted  $G_s^*$  based on Breault & Weber(2021)



# Modelling Options

# Model scheme



Simonin viscous stress model covers dilute turbulent through to the dense limit of viscous regime by a harmonic mean of collisional and particle relaxation time scales; Simonin's turbulence model and the GKT are recovered at the dilute and dense limits, respectively.

$\tau_s$  - Dissipation time scale, s

$\tau_{gs}^x$  - Particle relaxation time, s

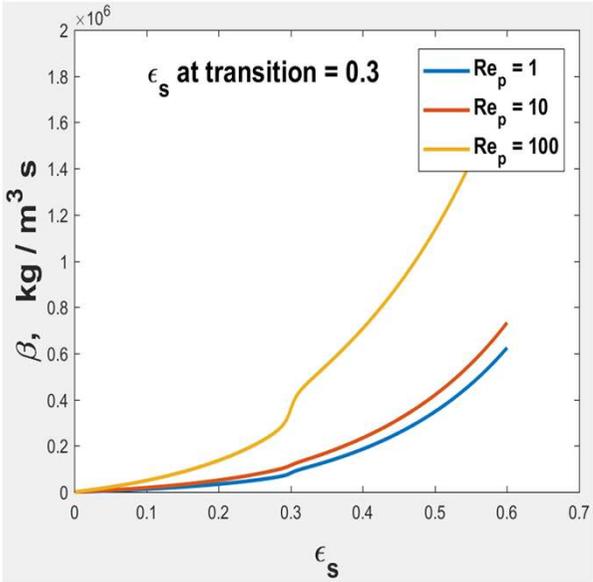
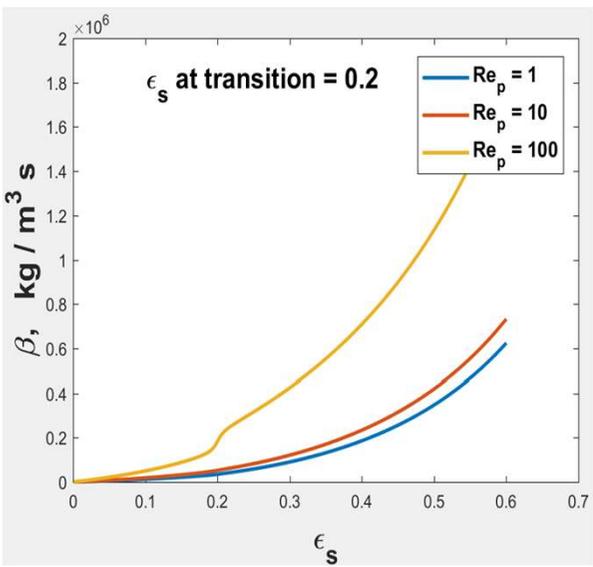
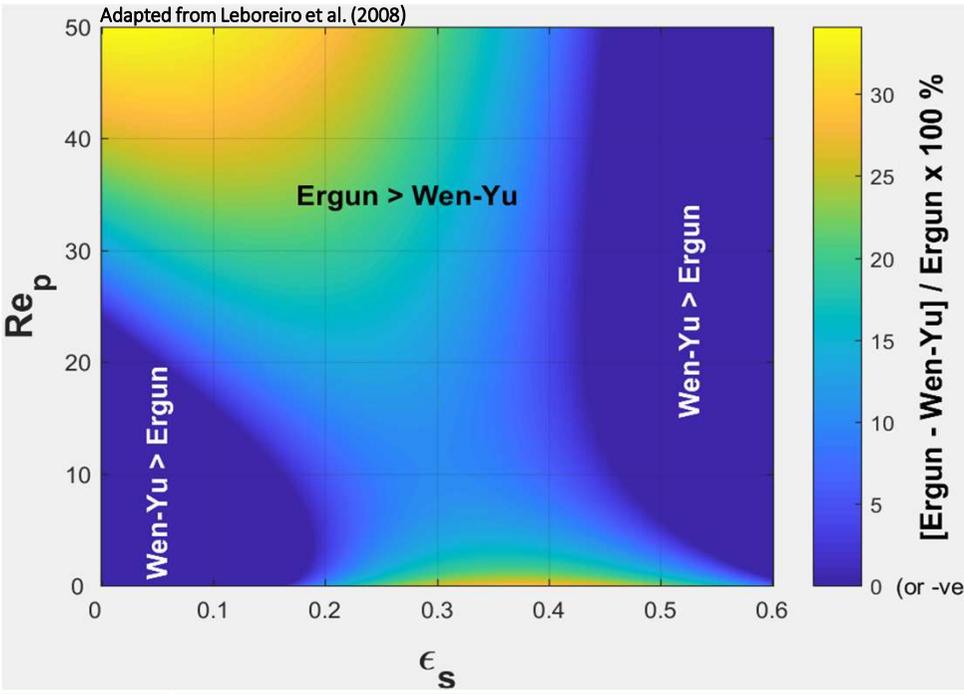
$\tau_s^c$  - Collisional time scale, s

Reference: Balzer et al.(1996) Benyahia et al.(2005) & (2007), Srivastava & Sundaresan (2003)

# Selection of drag model

## Transition in the Gidaspow blend drag model

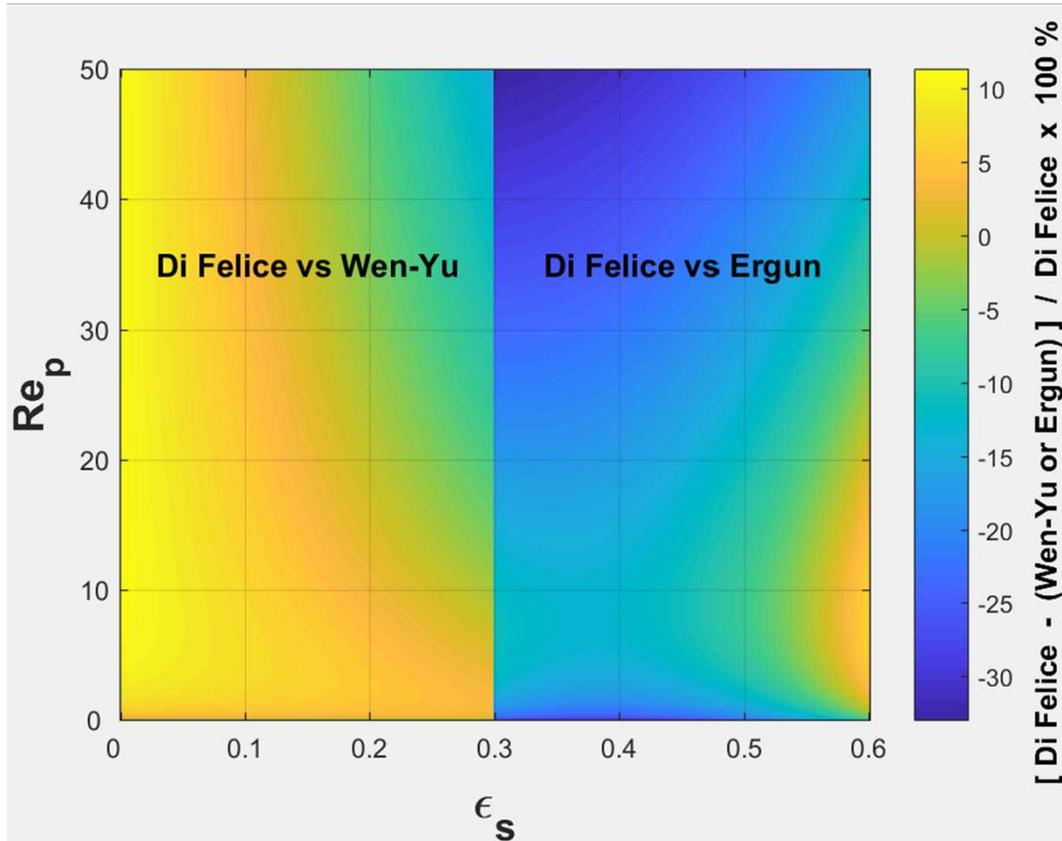
Type	Model	Applicable Range
Empirical	<b>Gidaspow blend</b> (Lathouwers & Bellan (2000)) (Smooth transition between Wen-Yu and Ergun at $\epsilon_s = 0.2$ )	$0 \leq \epsilon_s \leq 0.6$ $0.01 \leq Re_p \leq 5000$
	<b>Syamlal – O'Brien (1987)</b>	$0 \leq \epsilon_s \leq 0.6$ $0.1 \leq Re_p \leq 10000$
	<b>Di Felice (1994)</b> (Based on Dalla Valle isolated sphere correlation)	$0 \leq \epsilon_s \leq 0.6$ $0.01 \leq Re_p \leq 10000$
DNS	<b>Koch-Hill-Ladd (2001)</b>	$0 \leq \epsilon_s \leq 0.6$ $0 < Re_p < 120$
	<b>Beetstra et al. (2007)</b>	$0 \leq \epsilon_s \leq 0.6$ $0 \leq Re_p \leq 1000$
	<b>Tang et al. (2015)</b>	$0 \leq \epsilon_s \leq 0.6$ $0 \leq Re_p \leq 1000$
	<b>Tenneti et al. (2011)</b> (Hybrid with Schiller & Naumann isolated sphere correlation)	$0 \leq \epsilon_s \leq 0.5$ $0.01 \leq Re_p \leq 300$



- Drag force is a function of  $\epsilon_s$  and  $Re_p$  based on slip velocity.
- Project range:  $0 < \epsilon_s < 0.6$  and  $Re_p < \sim 100$  (high slip velocities in DSU).
- For the project purpose, a homogeneous drag law is essential; heterogeneous drag laws intended for macroscale models are excluded.
- DNS drag laws overpredict at dilute conditions ( $0 < \epsilon_s < 0.2$ ), constrained by computing power for modelling the unbounded condition of an isolated sphere. (Tang et al. (2015))
- Tenneti et al. hybrid model does not cover the full range of  $\epsilon_s$
- Syamlal-O'Brien drag law is suitable for higher velocities but may not be near close packed conditions (Bakshi et al. (2015), Arastoopour et al.(2017)).

- Transition between Wen-Yu and Ergun in Gidaspow blend is smooth with an arctan function but steep except at  $\epsilon_s = 0.2$  and  $Re_p < \sim 10$ .
  - Wen-Yu (based on Schiller and Naumann) better predicts at the limit of an isolated sphere. Furthermore, LBM simulations (Kandhai et al. (2003)) have shown that Wen-Yu predicts well up to  $\epsilon_s = 0.3$ , and that Ergun overpredicts at  $0.2 < \epsilon_s < 0.5$ .
  - Gobin et al. (2003) have proposed the following transition:
- $$C_D = \begin{cases} \min(C_{D,Wen-Yu}, C_{D,Ergun}), & \text{if } \epsilon_s > 0.3 \\ C_{D,Wen-Yu}, & \text{if } \epsilon_s \leq 0.3 \end{cases}$$
- I.e., essentially at the Wen-Yu = Ergun boundary on the right side, at  $\epsilon_s > 0.4$ . However, Wen-Yu may not be suitable at  $\epsilon_s > 0.3$ .

# Di Felice drag model



- Di Felice (1994) correlated the Ergun equation for closely packed conditions together with experimental data for dilute and intermediate  $\epsilon_s$ .
- A correction is applied to the Dalla Valle isolated sphere correlation in terms of void fraction, with an empirical exponent; the exponent is a (weak) function of  $Re_p$ .

$$\beta = \frac{3}{4} C_D \frac{\epsilon_s \epsilon_g \rho_g |\vec{u}_g - \vec{u}_s|}{d_p} \epsilon_g \left( -2.7 + 0.65 \exp \left\{ \frac{-(1.5 - \log_{10} Re_p)^2}{2} \right\} \right)$$

$$C_D = \left( 0.63 + \frac{4.8}{\sqrt{Re_p}} \right)^2$$

- Di Felice model predicts within 10 % of Wen-Yu at  $\epsilon_s < 0.3$  and also within 10 % of Ergun at  $0.5 < \epsilon_s < 0.6$  for the expected project range of  $Re_p$ ; underpredicts Ergun by up to 20% at  $0.3 < \epsilon_s < 0.5$  for the expected project range of  $Re_p$  (which may be desirable too, as Ergun is reported to overpredict in this range).
- The model is continuous over the full range of  $\epsilon_s$ .

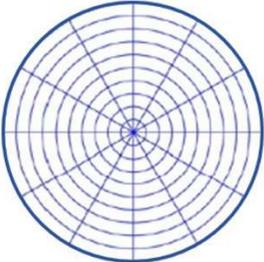
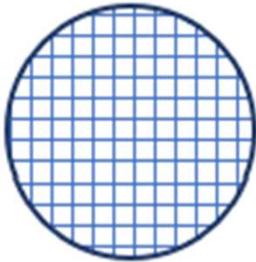
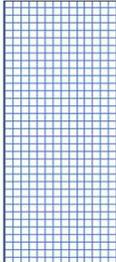
**Note:** As the Di Felice exponent was correlated using the Dalla Valle isolated sphere correlation, the model better conforms with Wen-Yu and Ergun at the applicable ranges of  $\epsilon_s$  with the Dalla Valle correlation than with the Schiller & Naumann correlation.

Amongst other interfacial forces (virtual mass, history, spin lift and slip-shear lift), the slip-shear lift force can be notable due to strong gradients in gas velocity, especially for horizontal flow (Massoudi(2003), Patro & Dash (2014)). However, it is not available in the standard MFiX-TFM.

# Coordinate system and Wall BC options

## Coordinate system options

## Wall BC options

Description	3D cylindrical	3D Cartesian cut-cell	2D Cartesian
Sectional views	 Radial section	 Radial section	 Axial section
Geometry	Exactly matches the pipe wall profile	Cartesian grid with peripheral cells cut to exactly match the pipe wall profile	Matches the wall profile in 2D
Wall BC for the solids phase	Johnson & Jackson partial slip BC, with Li & Benyahia variable specularity coefficient	Free slip (Johnson & Jackson BC is not available in standard MFiX-TFM)	Johnson & Jackson partial slip, with Li & Benyahia variable specularity coefficient
Advantages	Exactly matches with the wall profile and offers rigorous wall BC	Simplicity of Cartesian grid, without stairstep boundary at curved walls. Complex geometries can be modelled. Second order accurate in space (Kirkpatrick et al. (2003))	Qualitatively well predicts bed expansion, bubble rise, core-annular flow, clusters and streamers, etc. Lower computational cost for long pipe models (e.g., S-shaped profile). Offers rigorous wall BC.
Disadvantages	Axial BC, modelled as free slip wall with no normal flow through it, interferes with profile of gas bubbles and results in the overprediction of $\epsilon_s$ near the axis (Bakshi et al. (2014) & (2015)) High resolution grids result in very small cells near the axis	Does not offer a rigorous wall BC. Some cut cells (small size or high aspect ratio) may result in inaccuracies.	Not suitable for horizontal flow given variations in azimuthal direction too. Does not capture the inherent 3D nature of gas-solids flow. Numerical predictions can be affected by asymmetric flows, e.g., inlet and outlet configurations. (Li et al. 2014-I) May not simultaneously predict axial pressure profile and radial voidage accurately. (Li et al. 2014-II)

- Johnson & Jackson (1987) partial slip wall BC, with the variable specularity coefficient of Li & Benyahia (2012) is the best option for the project conditions. (Bakshi et al.(2015))  
However, it is not available for Cartesian Cut Cell coordinates in the standard MFiX-TFM.
- Free slip wall BC for the solids phase is a good approximation, as the specularity coefficient is generally very small for the higher velocities involved. (Benyahia et al.(2007))

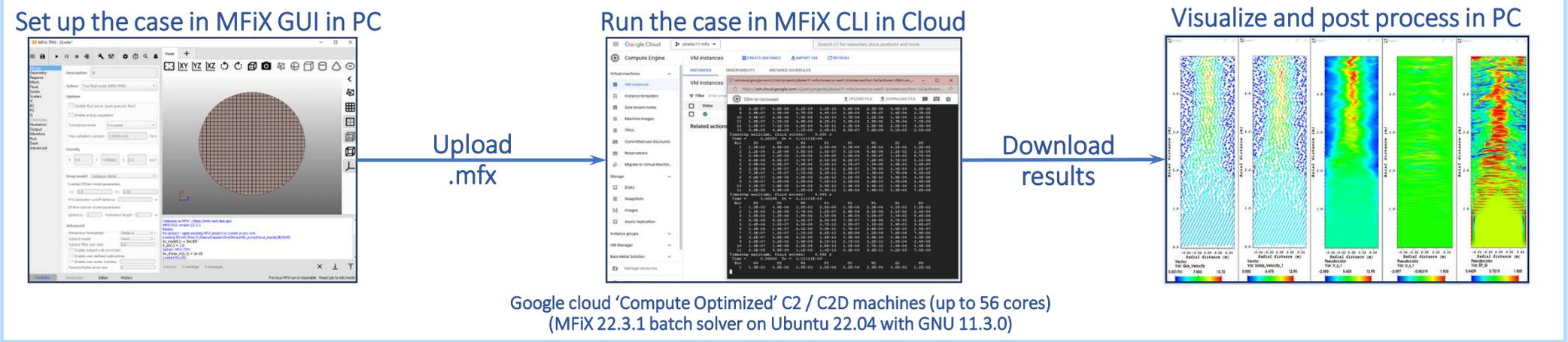
**!! Fede et al. (2016) have used no slip wall BC with zero granular energy flux at the wall to conform with PEPT experimental data. This study was based on a Geldart B solids (monodisperse 875  $\mu\text{m}$  & 740  $\text{kg}/\text{m}^3$ ) at 12 bar operating pressure. However, Geldart B solids tend towards Geldart A behaviour at high pressures (Yang, 2007). In fact, Sabatier et al. (2020) have used this wall BC to validate an upflow bubbling fluidized bed of Geldart A solids (polydisperse 73  $\mu\text{m}$  & 2640  $\text{kg}/\text{m}^3$ ). However, further validation studies for broader operating conditions may be required.!!**

- Cubic cells are selected as the solids distribution evolves strongly in the axial direction too (Lu et al. (2009), Benyahia (2012)), and as the flow field is turbulent.
- Some cartesian grids are inherently good (fewer small cut cells & good aspect ratios). 27x27 grid ( $\sim 21 d_p$ ) is used for first pass simulations; final confirmation runs by  $\sim 10 d_p$ .

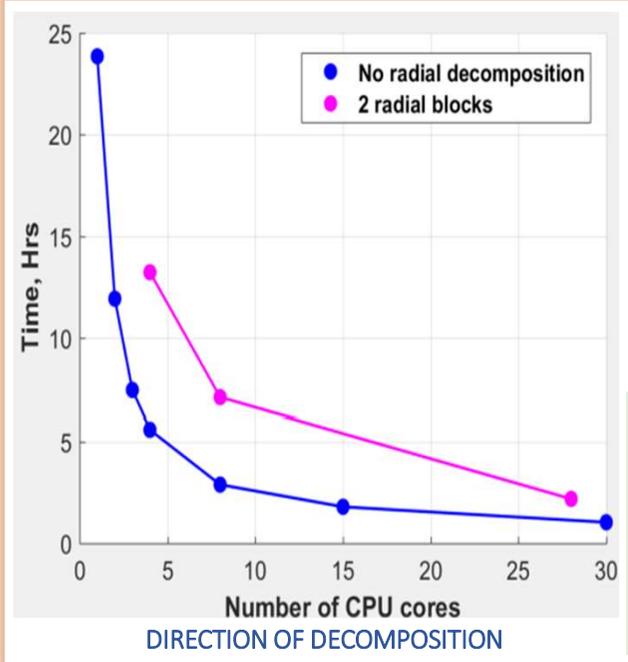
# Cloud computing and Parallel processing

Cloud computing

Parallel Processing by DMP



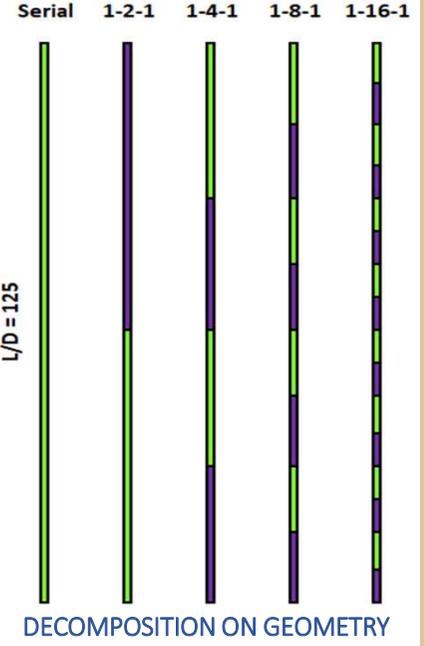
Google cloud 'Compute Optimized' C2 / C2D machines (up to 56 cores) (MFiX 22.3.1 batch solver on Ubuntu 22.04 with GNU 11.3.0)



RUN TIMES FOR A TEST CASE SIMULATION  
Google cloud C2 machines, FOUP, Preconditioner: 'NONE'

VCPU's	Physical cores	No radial decomposition		2 radial blocks		Folds increase in cores	Folds reduction in time
		Mode	Time, Hrs	Mode	Time, Hrs		
2	1	Serial	23.85			1	1
4	2	DMP-1-2-1	11.94			2	2
6	3	DMP-1-3-1	7.46			3	3
8	4	DMP-1-4-1	5.57	DMP-2-1-2	13.24	4	4
16	8	DMP-1-8-1	2.88	DMP-2-2-2	7.11	8	8
30	15	DMP-1-15-1	1.79			15	13
60	30	DMP-1-30-1	1.03	DMP-2-7-2	2.18	30	23

- For the geometry, it is optimum to decompose in the axial direction alone.
- Cases with 2 radial blocks require 4 times the cores for the same axial decomposition.
- Recommendation by Open MPI is to never specify more than the available physical cores. If 'oversubscribed', the performance is 'degraded'.
- Inter-processor communications incur a cost beyond DMP-1-8-1.
- Superbee took 60% longer than FOUP. Other higher order schemes were at the same ballpark.

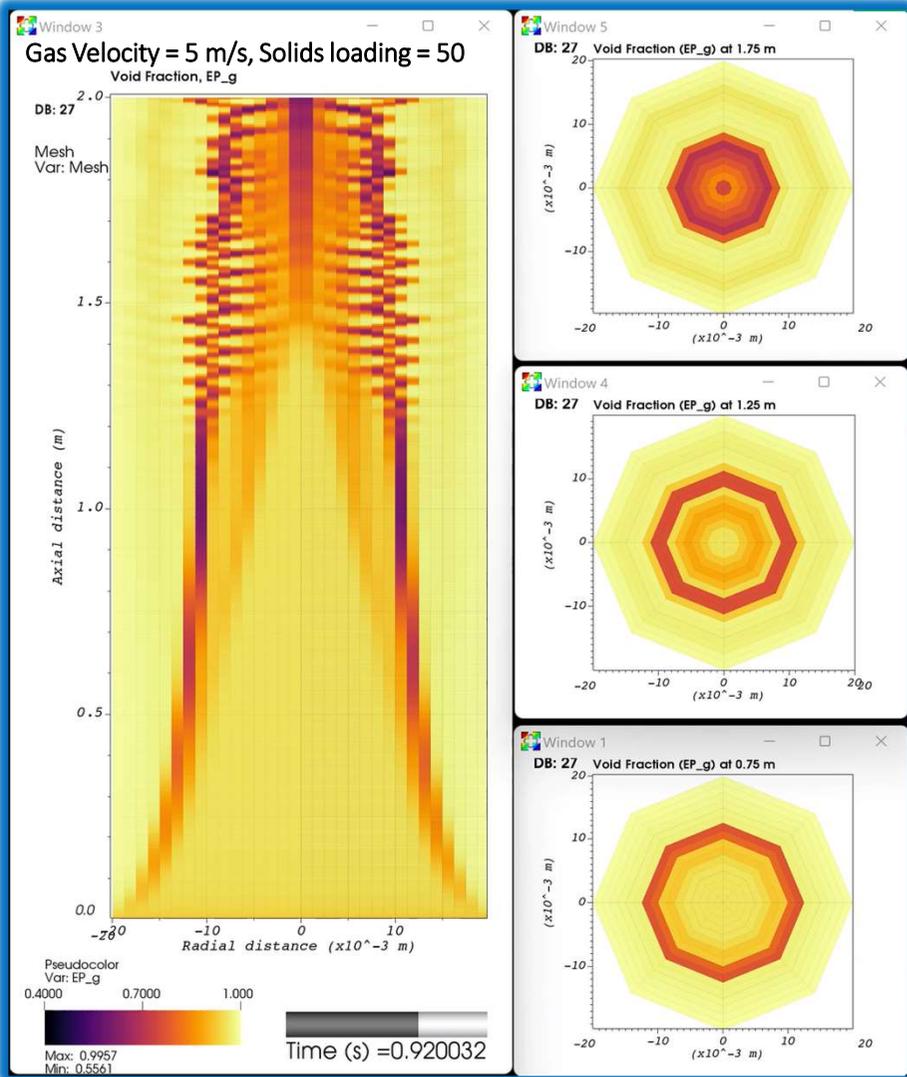


Reference: MFiX user manual, Google Cloud & Open MPI web pages.

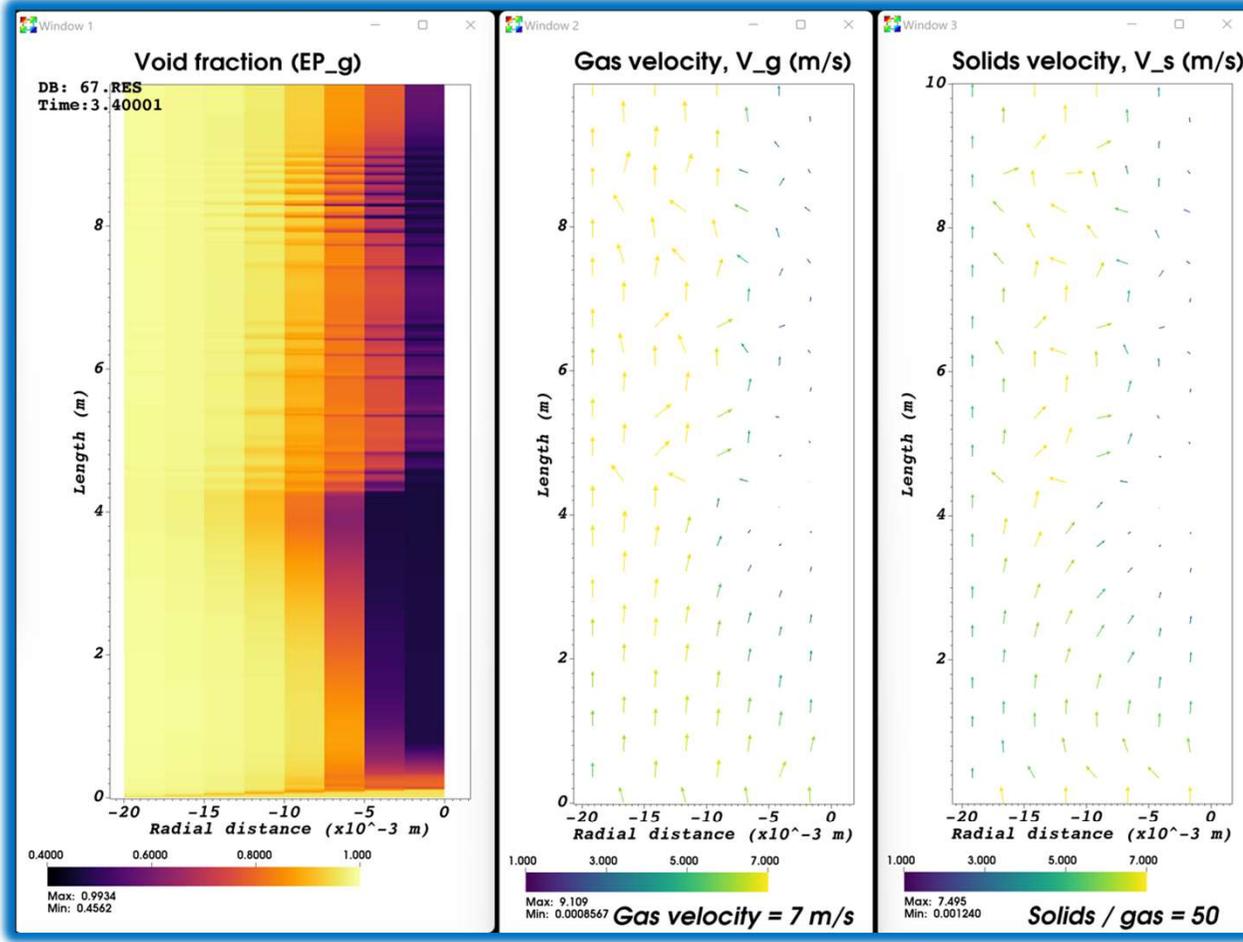


# Numerical modelling intricacies

# Numerical artifact: Solids accumulation at the axis with cylindrical coordinates



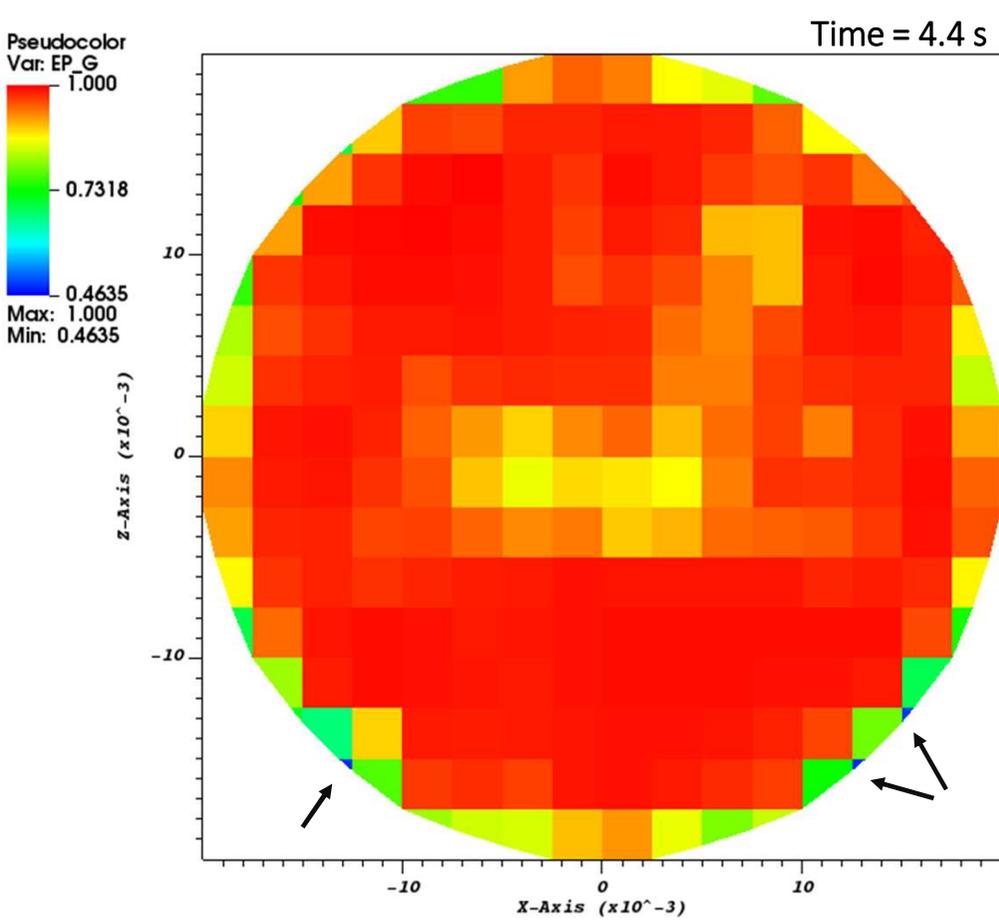
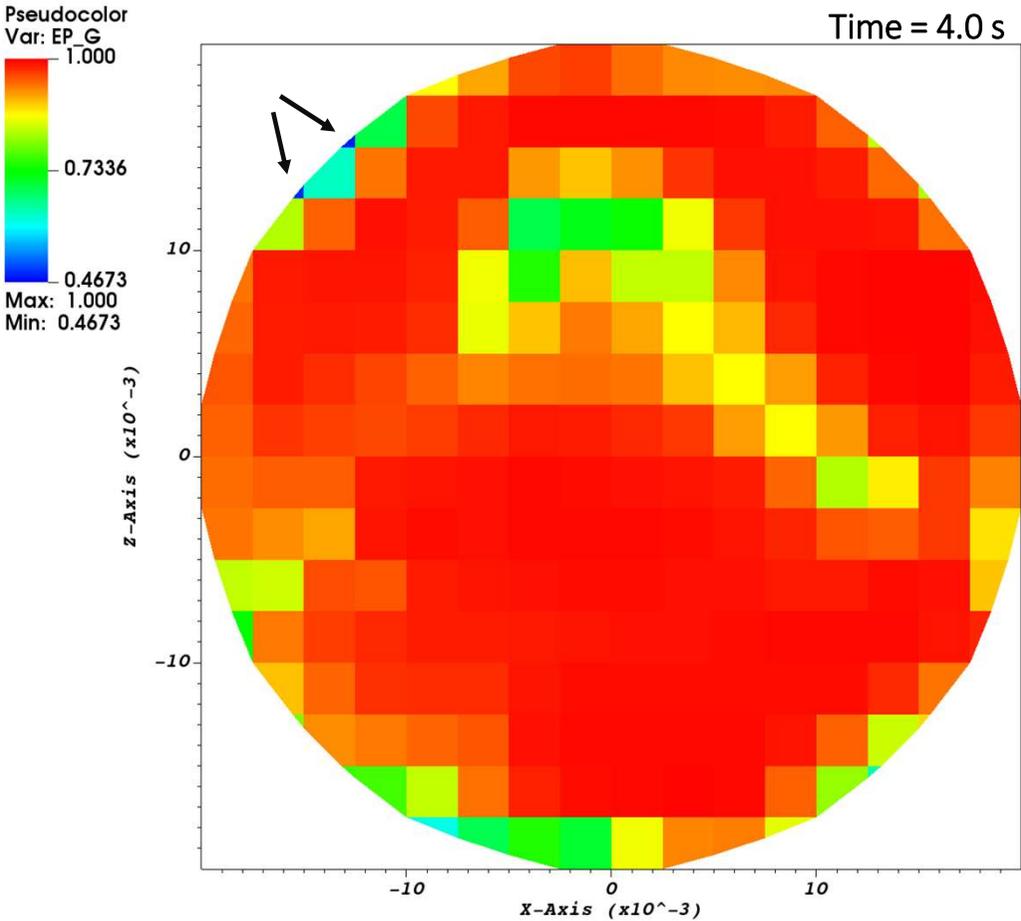
3D cylindrical, Grid: 16-512-8, diameter = 0.04 m, height = 2 m, Simonin + Srivastava,  $c_e = e_w = 0.90$ ,  $\Phi_w = 8.53$ , BC\_JJ\_M, Defaults but Superbee.



Grid: 8-2560-1, diameter = 0.04 m, height = 10 m, Simonin + Srivastava,  $c_e = e_w = 0.99$ ,  $\Phi_w = 11.31$ , BC\_JJ\_M, Defaults but Superbee.

Various parameter combinations / levels, with / without model components such as friction and turbulence, different wall BC's and IC's, etc. were tried – *In all cases solids accumulate at the axis.*  
The problem with axial BC in cylindrical coordinates is documented for dense beds by Bakshi et al. (2014) & (2015). Solids accumulate at the axis modelled as a free slip wall, e.g., axisymmetric 2D simulations Li et al. (2014-II)

# Numerical artifact: Solids accumulation at small cut-cells



Grid: 16 x 2000 x 16,  $\Delta x \sim 30 d_p$ ,  $\Delta t \le 5.0E-5$ , diameter = 0.04 m, height = 5 m, Lun + Srivastava, Superbee, Gas velocity = 3 m/s, Solids loading = 50, MI-PO, Free slip wall BC,  $c_e = 0.99$ , DMP, Preconditioner: 'NONE', (Run c7)

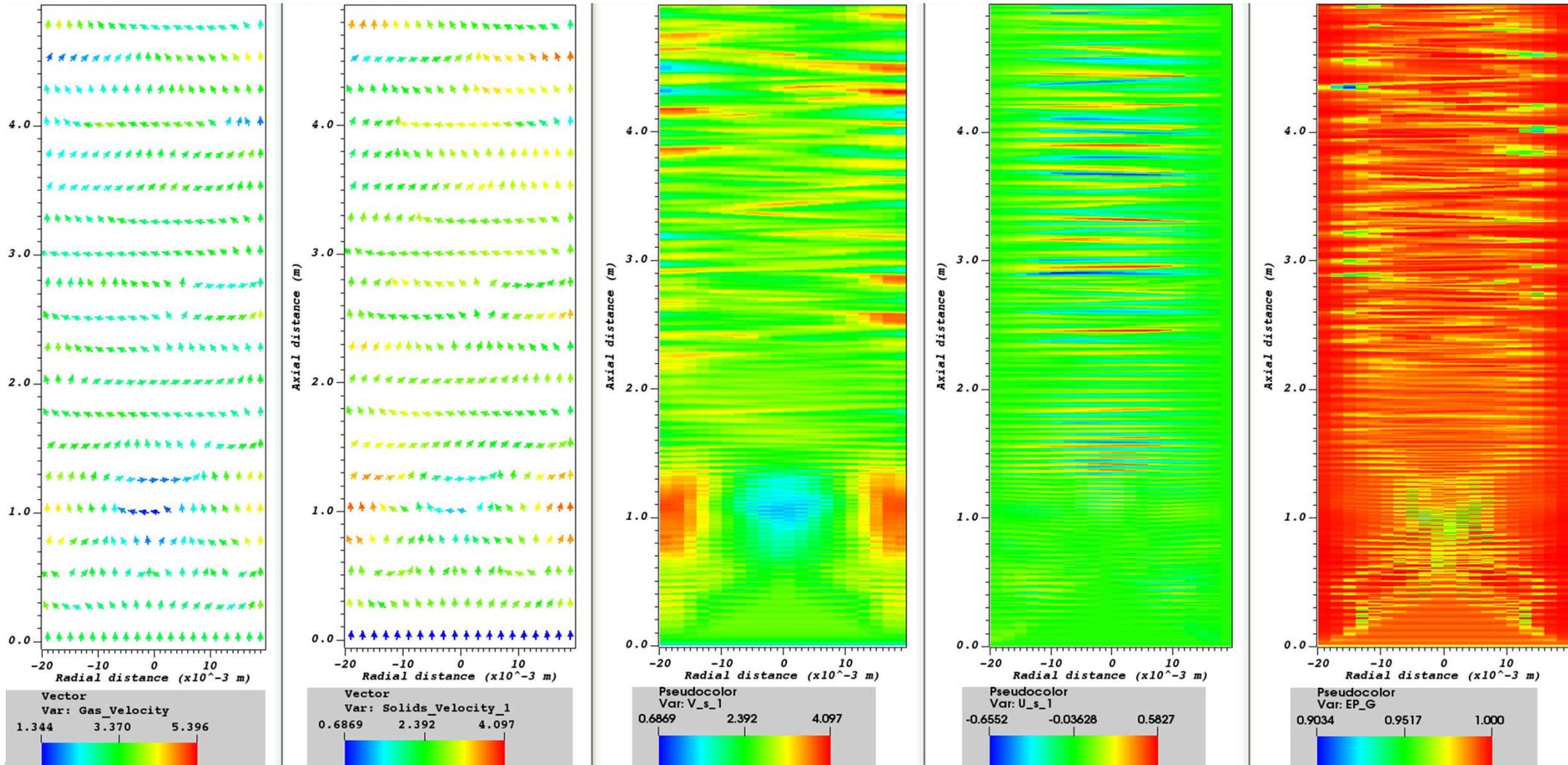
## Cross-sectional views at a height of 4.5 m

- Small cut-cells are frequently observed with higher solids concentrations than their neighbours with free slip wall BC.
- Observed with both FOUP and Superbee discretization (concentration gradient is sharp rather than diffuse).

# Numerical artifact: Radial oscillations in Cartesian 2D

- Benyahia et al. (2007) have observed similar wall to wall oscillations in 1D simulations.
- Syamlal et al. (2017) have attributed this to lack of grid convergence.

Results at 5 s

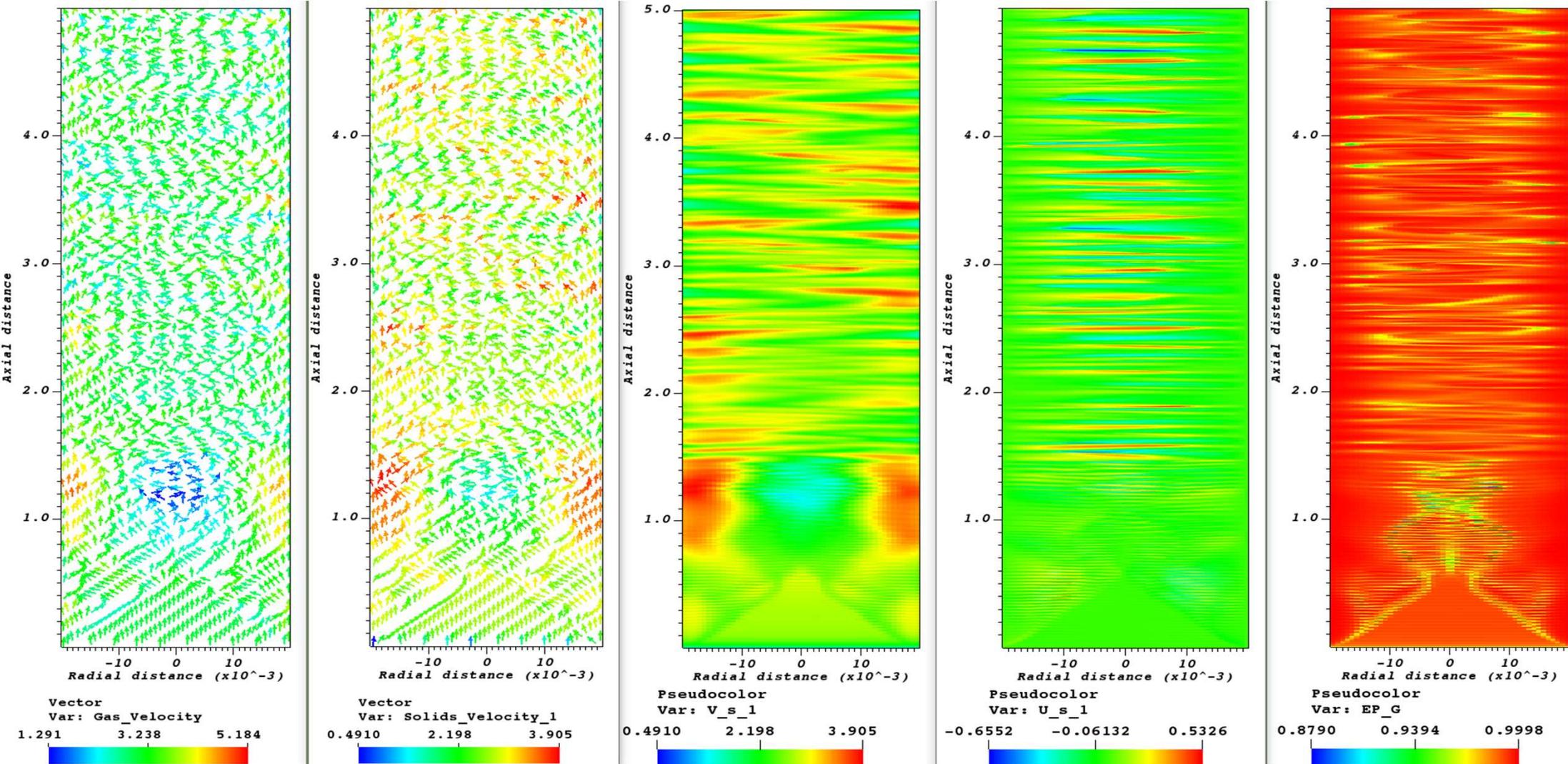


2D Cartesian, grid: 20 x 2500 x 1,  $\Delta x = 25 d_p$ ,  $\Delta t \leq 3.0E-5$ , diameter = 0.04 m, height = 5 m, Simonin + Srivastava, Superbee, Gas velocity = 3 m/s, Solids loading = 10, BC\_JJ\_M, c\_e = 0.99, e\_w = 0.99, DMP, Preconditioner: 'NONE', (Run urx24r)  
 URFAC(1,2,4,9) = 1.0, URFAC((3&5))=0.5, URFAC(8)=0.8

# Numerical artifact: Radial oscillations in Cartesian 2D

Results at 3.9 s

However, does not improve with finer grid ( $\sim 10d_p$ ) and smaller time step ( $1E-5$ ). Does not respond to Numerics either.



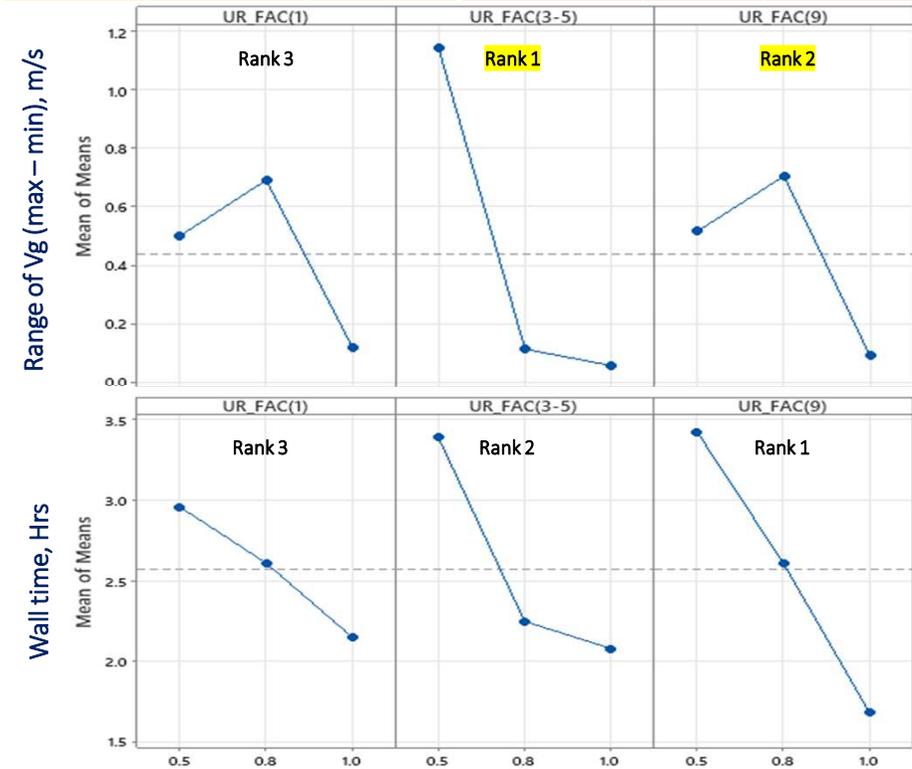
2D Cartesian, grid: 50 x 6250 x 1,  $\Delta x \sim 10 d_p$ ,  $\Delta t \leq 1.0E-5$ , diameter = 0.04 m, height = 5 m, Simonin + Srivastava, Superbee, Gas velocity = 3 m/s, Solids loading = 10, BC\_JJ\_M, c\_e = 0.99, e\_w = 0.99, DMP, Preconditioner: 'NONE', (Run urx24rr)  
 URFAC(1,2,4,9) = 1.0, URFAC((3&5)) = 0.5, URFAC(8) = 0.8

# Optimum underrelaxation factors to prevent backflow

- With 2D cartesian grid, Simonin viscous stress model and Pressure Outflow BC, back flow problem was encountered under gas only flow conditions, with the default underrelaxation factors. Outlet gas velocity and pressure were oscillatory, pressure drop was an order of magnitude higher and there were flow reversals.
- Underrelaxation factors are applied to rapidly changing field variables during iterations for stability of calculations. (Syamlal, 1998)
- Results of a statistical experiment with the underrelaxation factors for gas pressure (UR\_FAC(1)), V-momentums (UR\_FAC(4)) and k-e (UR\_FAC(9)) indicated that it is optimum to set all these factors at 1.0 for no/low solids flows. V-momentum (UR\_FAC(4)) is the most dominant factor (Rank 1), and it is intuitive: if the axial momentum is throttled relative to the other factors, backflow may occur!
- Considering the profound impact of underrelaxation factors on wall time and stability (measured as the number of stalls/divergences during a simulation), further statistical experiments were carried out to find the optimum values for other factors too.
- Not clear if optimizing underrelaxation factors would prevent backflow for all projects. Some researchers have adjusted the geometry to prevent back flow: Cloete et al. (2013) have used a porous zone at the top; Sabatier et al. (2020) have used a convergent head at the outlet to accelerate the suspension. These measures may increase the computational cost and introduce exit effects.

Note: Default Numerics were used for the simulations carried out for the statistical experiments except for Superbee discretization.

L9 - Taguchi – 3 factors x 3 Levels			Simulation Results		
Gas pressure	V-Momentums	k-e	Range of Vg	Wall time	Pressure drop
UR_FAC(1)	UR_FAC(4)	UR_FAC(9)	m/s	Hrs	Pa
0.5	0.5	0.5	1.33	8.36	-105
0.5	0.8	0.8	0.12	4.52	75
0.5	1.0	1.0	0.06	3.36	65
0.8	0.5	0.8	1.95	5.25	-135 / 415
0.8	0.8	1.0	0.06	3.17	65
0.8	1.0	0.5	0.06	5.16	65
1.0	0.5	1.0	0.15	3.31	65
1.0	0.8	0.5	0.16	5.46	65
1.0	1.0	0.8	0.06	3.78	65



Results from MiniTab

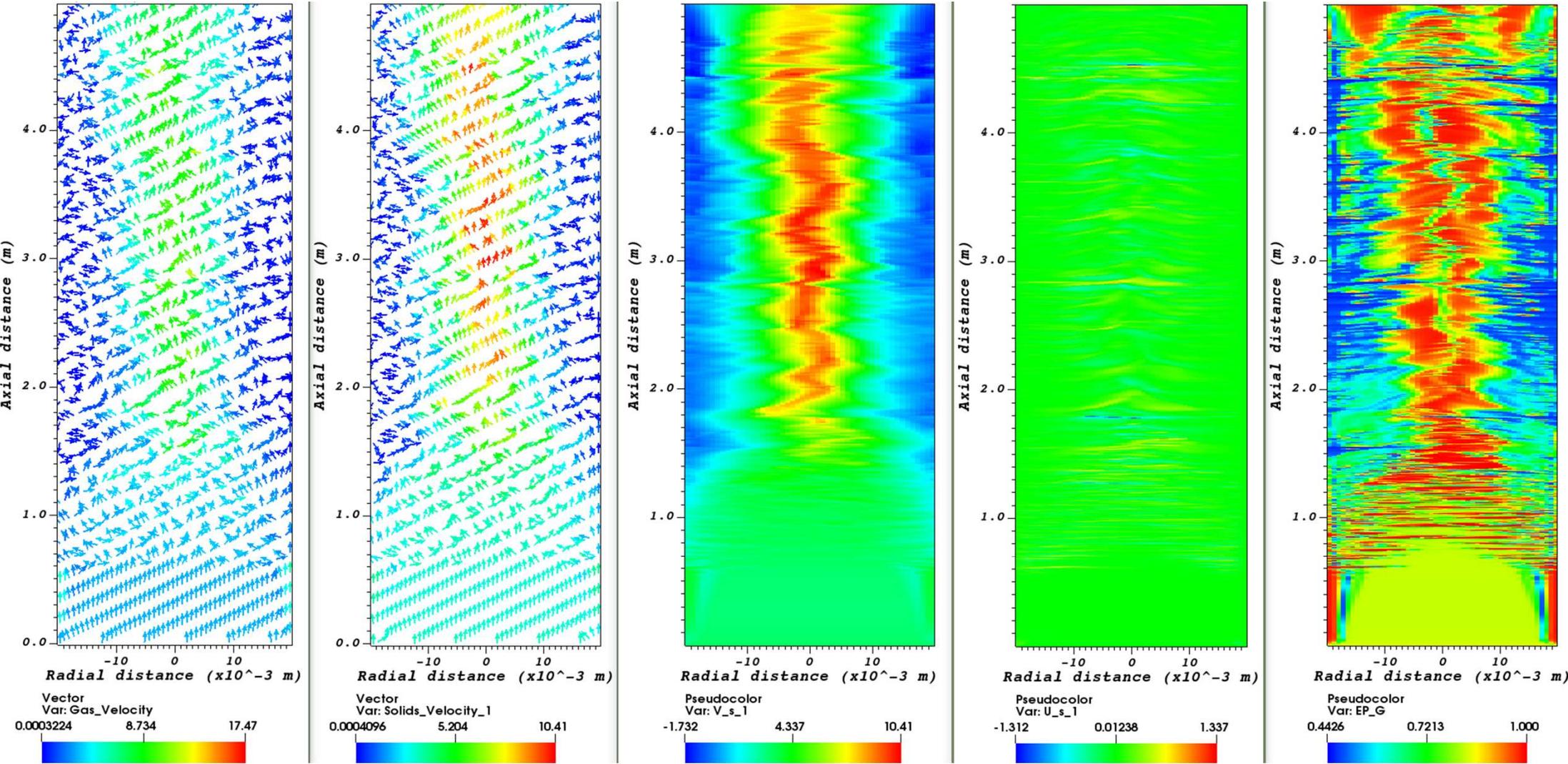
Optimum underrelaxation factors for 2D Cartesian grid simulations #				
Under relaxation factor	Default	Selected	Remarks	
UR_FAC(1)	Gas pressure	0.8	0.8	Improves stability
UR_FAC(2)	EP_s	0.5	1.0	
UR_FAC(3&5)	U&W-Momentums	0.5	0.5	Improves stability
UR_FAC(4)	V-Momentums	0.5	1.0	Set at 1.0 to avoid backflow at no / low solids loadings
UR_FAC(8)	Granular temperature	0.5	0.5	~ 1 in 3 runs diverges without underrelaxation
UR_FAC(9)	k-e	0.8	1.0	Set at 1.0 to avoid backflow at no / low solids loadings
UR_F_GS	Drag	1.0	0.0	Improves stability at ~ 3% increase in wall time

# - May not be suitable for other coordinate systems or simulation conditions

# Simulation results

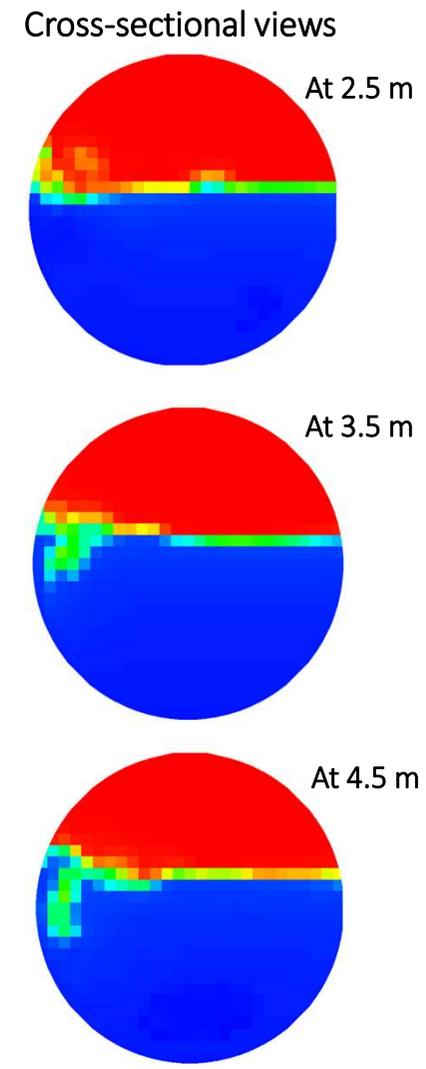
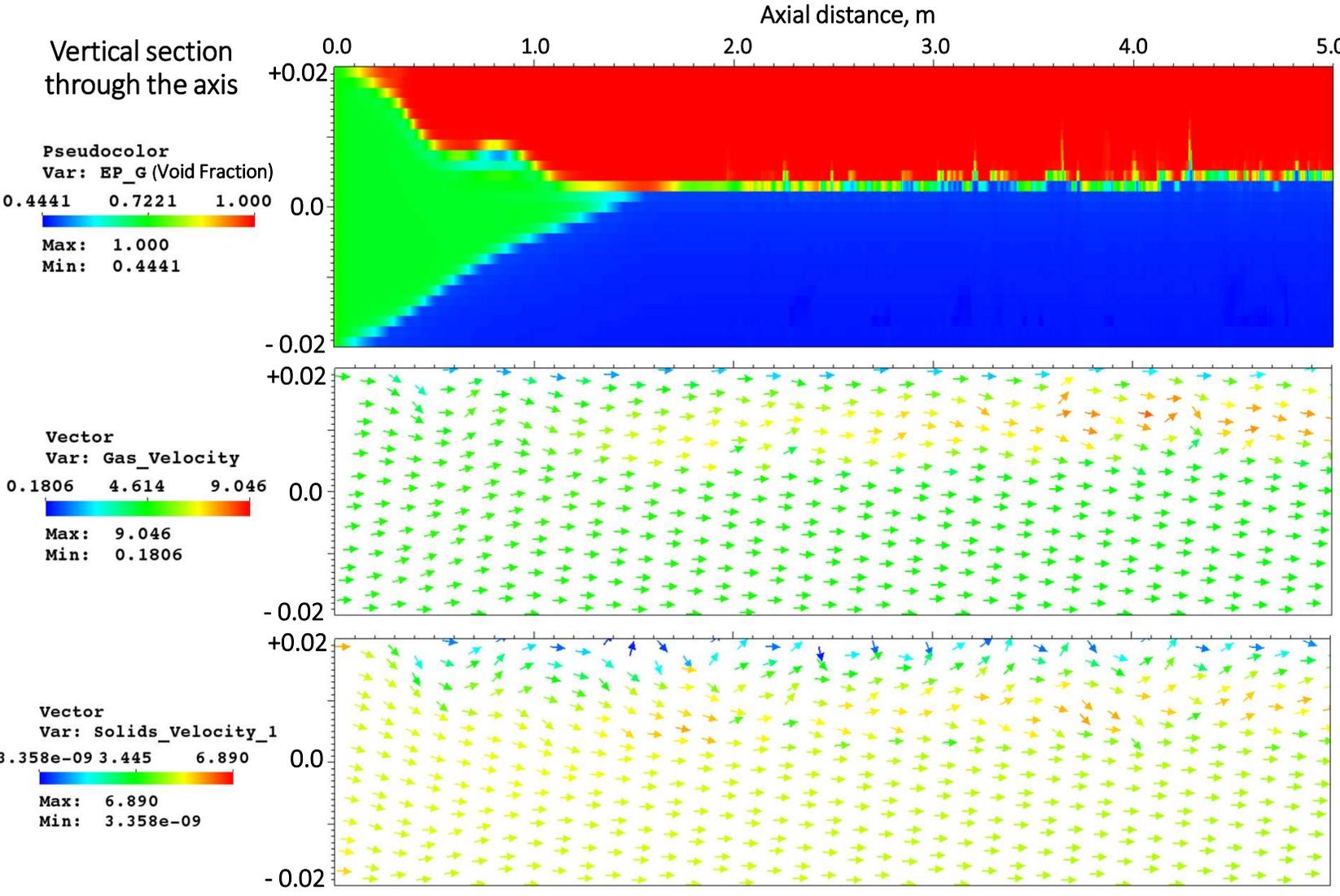
# Core-Annular flow in Cartesian 2D

Results at 5 s, Gas velocity = 3 m/s, Solids loading = 200



2D Cartesian, grid: 50 x 6250 x 1,  $\Delta x \sim 10 d_p$ ,  $\Delta t \leq 1.0E-5$  s, diameter = 0.04 m, height = 5 m, Simonin + Srivastava, Superbee, Gas velocity = 3 m/s, Solids loading = 200, BC\_JJ\_M,  $c_e = 0.99$ ,  $e_w = 0.99$ , DMP, Preconditioner: 'NONE', (Run urx28)

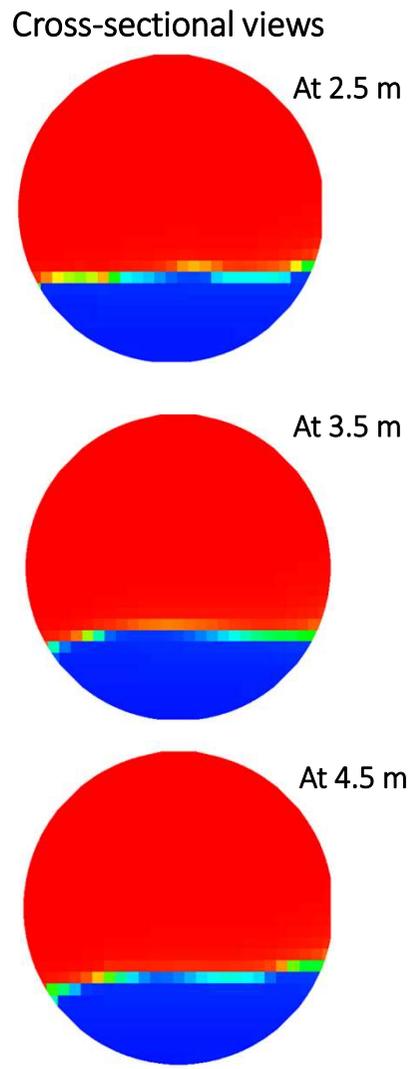
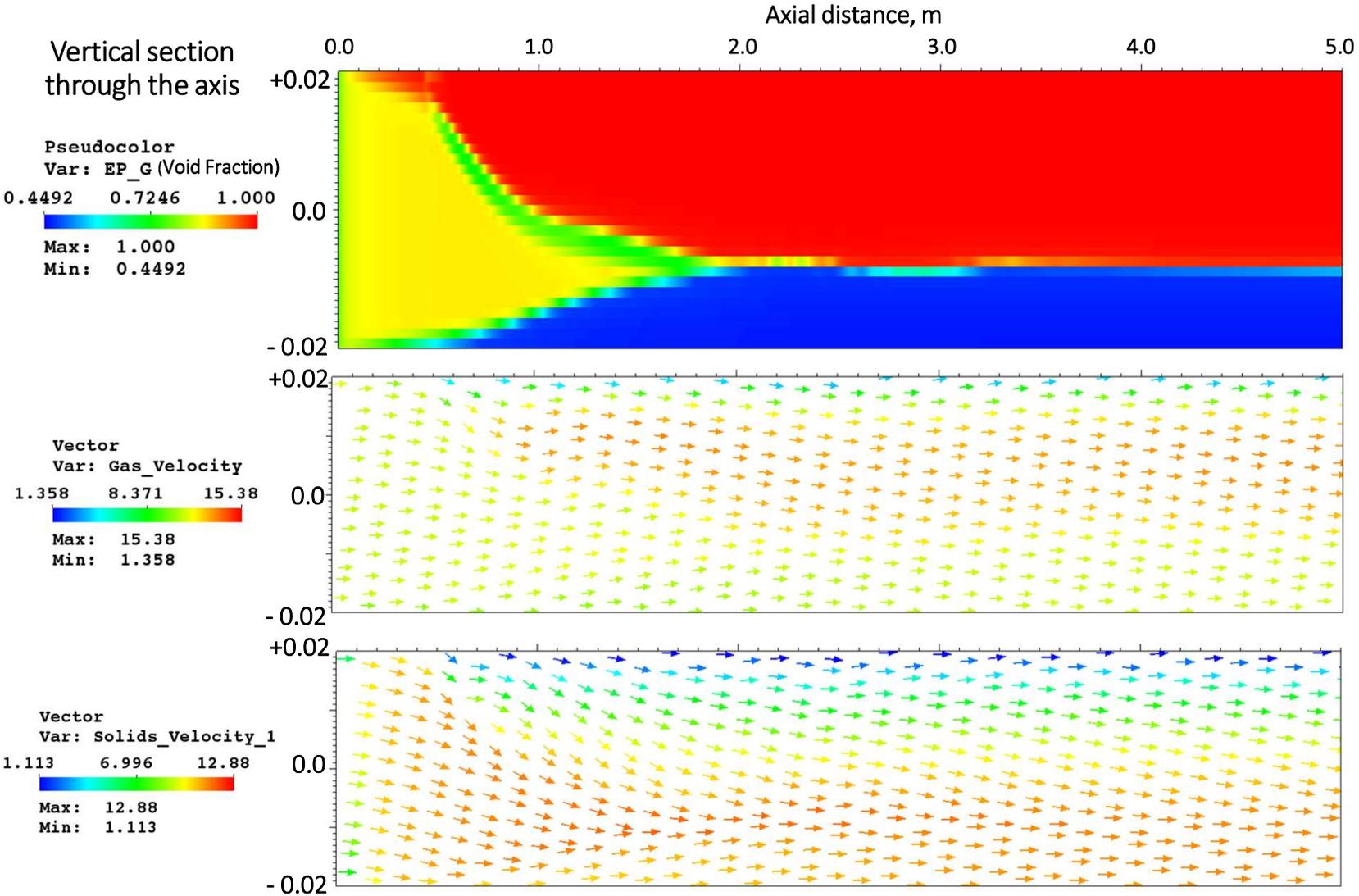
# Moving bed flow in cartesian cut-cell Feed Zone ( $F$ ), Pressure = 3 bar Results at 5 s, Gas velocity = 3 m/s, Solids loading = 166



Grid: 27x3375x27,  $\Delta x \sim 21 d_p$ ,  $\Delta t \leq 1.0E-4$  s, diameter = 0.04 m, length = 5 m, Simonin + Srivastava, Superbee, Gas velocity = 3 m/s, Solids loading = 166, MI-PO, Free slip wall,  $c_e = 0.87$ , DMP, Preconditioner: 'NONE', (Run Hori\_10)

# Moving bed flow in cartesian cut-cell Ambient receiver (A)

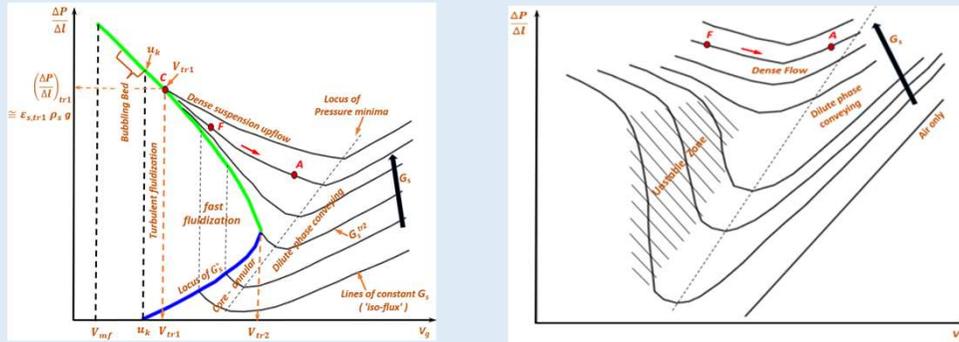
Results at 5 s, Gas velocity = 10 m/s, Solids loading = 166



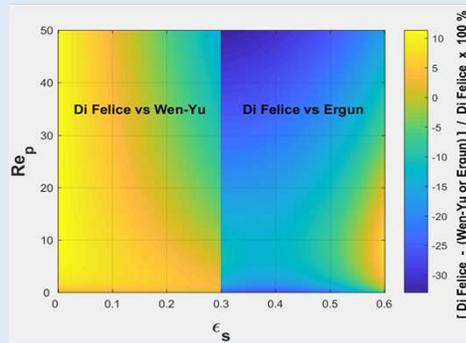
Grid: 27x3375x27,  $\Delta x \sim 21 d_p$ ,  $\Delta t \leq 1.0E-4$  s, diameter = 0.04 m, length = 5 m, Simonin + Srivastava, Superbee, Gas velocity = 10 m/s, Solids loading = 166, MI-PO, Free slip wall,  $c_e = 0.87$ , DMP, Preconditioner: 'NONE', (Run Hori\_9)

# Conclusions

- Fluidized dense phase conveying of fine powders situated on the vertical flow phase map of Wirth (1988) and the horizontal flow phase map of Zenz(1949), with inputs from other cited references.



- Suitability of the Di Felice (1994) drag model (based on the Dalla Valle isolated sphere drag correlation) to cover the full spectrum of solids volume fractions illustrated.



- Numerical artifacts encountered with 3D cylindrical, cartesian cut-cell and cartesian 2D coordinates highlighted.
- Optimum underrelaxation factors for V-momentums and k-e, to avoid backflow with pressure outlet BC proposed.
- Ongoing work: To generate rigorous data on spatiotemporal distributions of key parameters (such as solids volume fraction, gas and solids velocities and gas phase pressure) for horizontal and vertical fluidized dense phase conveying with MFiX-TFM.

### Wish list for MFiX-TFM features

- Johnson & Jackson (1987) partial slip wall BC for Cartesian cut-cell coordinates
- Slip-shear (lift) force model
- Cohesion model for mildly cohesive powders such as the Gu et al.(2019)
- Option to specify fully developed flow profile at the inlet BC to minimize the inlet transition length.

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# Thank you!

I acknowledge the support received at the MFiX forum.

Please forward your comments to [prabu.balasubramanian@gcu.ac.uk](mailto:prabu.balasubramanian@gcu.ac.uk)