

# 1D and 3D numerical simulations of a 100kWth coal CFB combustor

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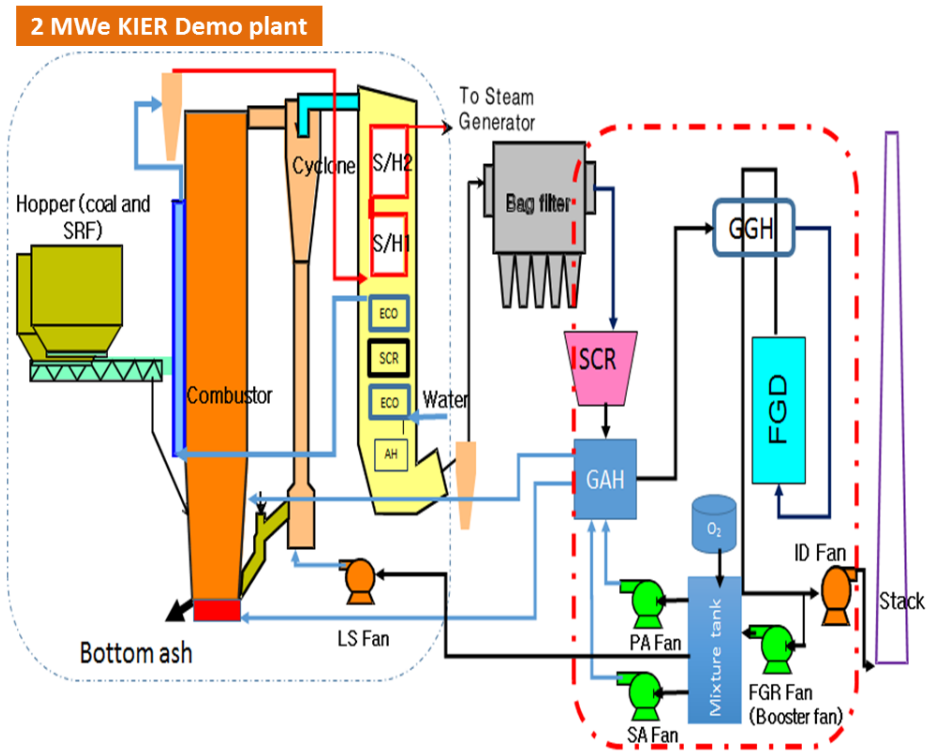
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2019 BARRACUDA USER CONFERENCE

# Circulating fluidized bed



2 MWe CFBC Demo plant  
(FEP Convergence Research center, KIER)

## -CFB advantages:

- \* **Fuel flexibility**-Capability to burn almost any fuel  
Wide range of coals, biomass, and RDFs.

- \* **High combustion efficiency**

  - Good solid mixing

  - Low unburned loss by cyclone, fly ash recirculation

- \* **Environmental friendliness**

  - In situ and very convenient desulfurization

  - Very low NO<sub>x</sub> generation

- \* **Low Operation & Maintenance costs**

  - Lower O&M costs due to elimination of SO<sub>x</sub> and NO<sub>x</sub> removal equipment's, pulverizer, and erosion issues.



A comprehensive understanding of the hydrodynamic characteristics in CFB is essential.

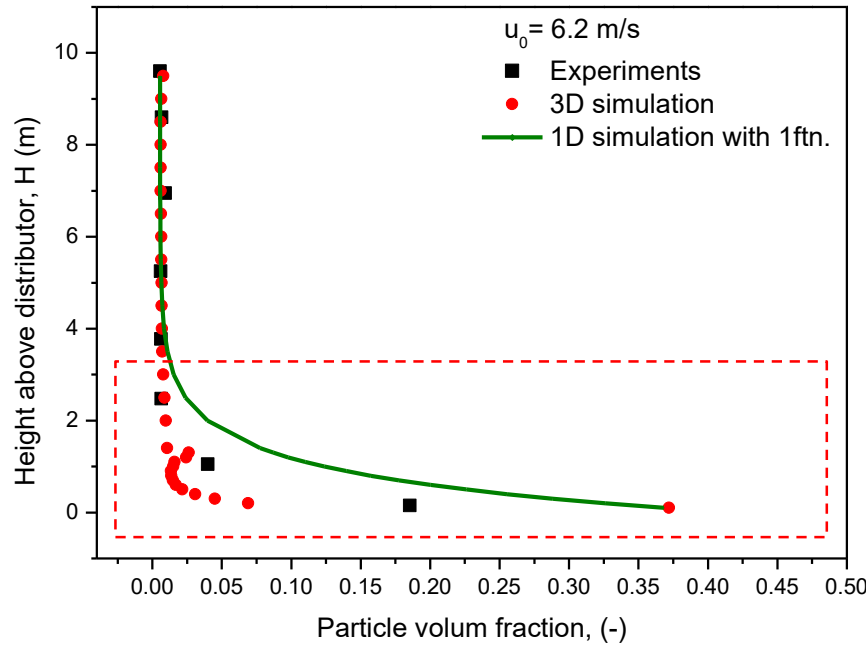
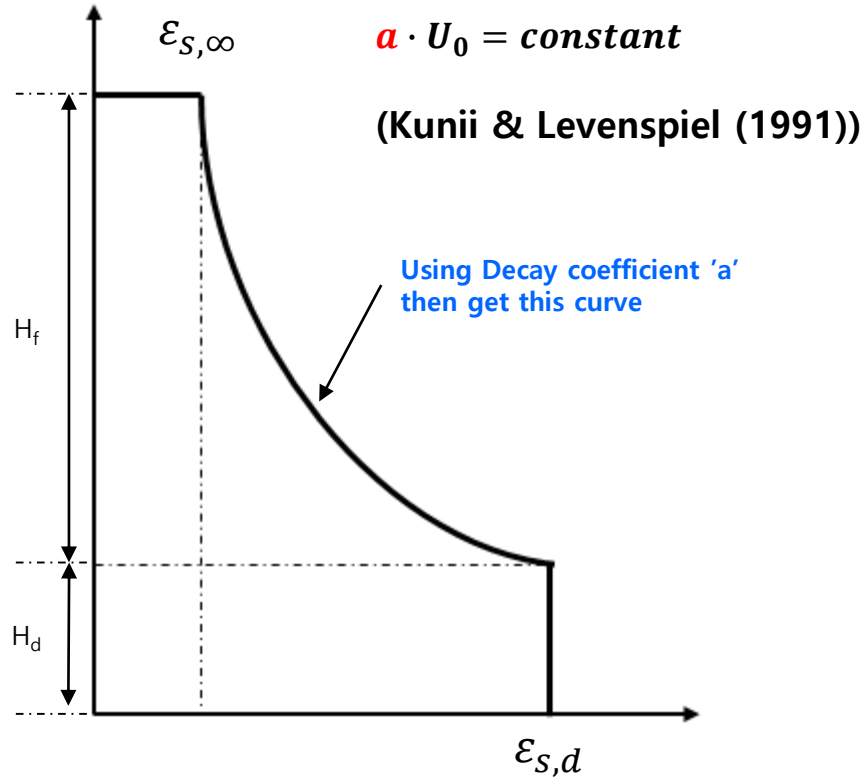
# Prediction of solids volume fraction profile (1D)

- The solids volume fraction in a lower part is constant and the solids volume fraction in the upper part decays exponentially along the height.
- The solids volume fraction profile in transport zone is determined by the slope of curve.

• Axial solids volume profile

$$\epsilon_s = \epsilon_{s,\infty} + (\epsilon_{s,d} - \epsilon_{s,\infty}) \cdot e^{-a \cdot (h - H_d)}$$

Height, z

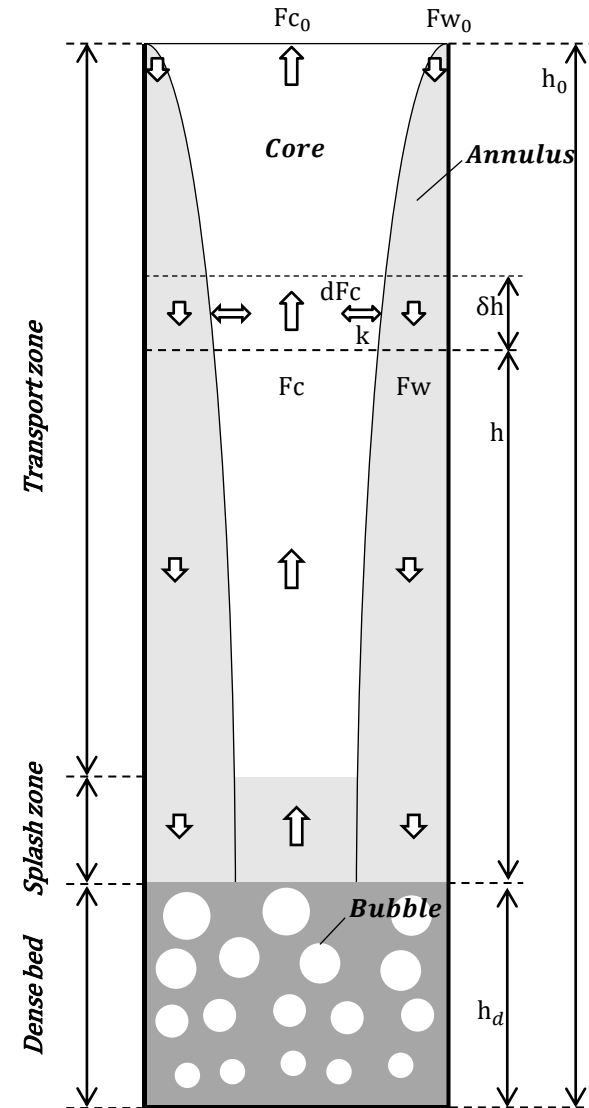
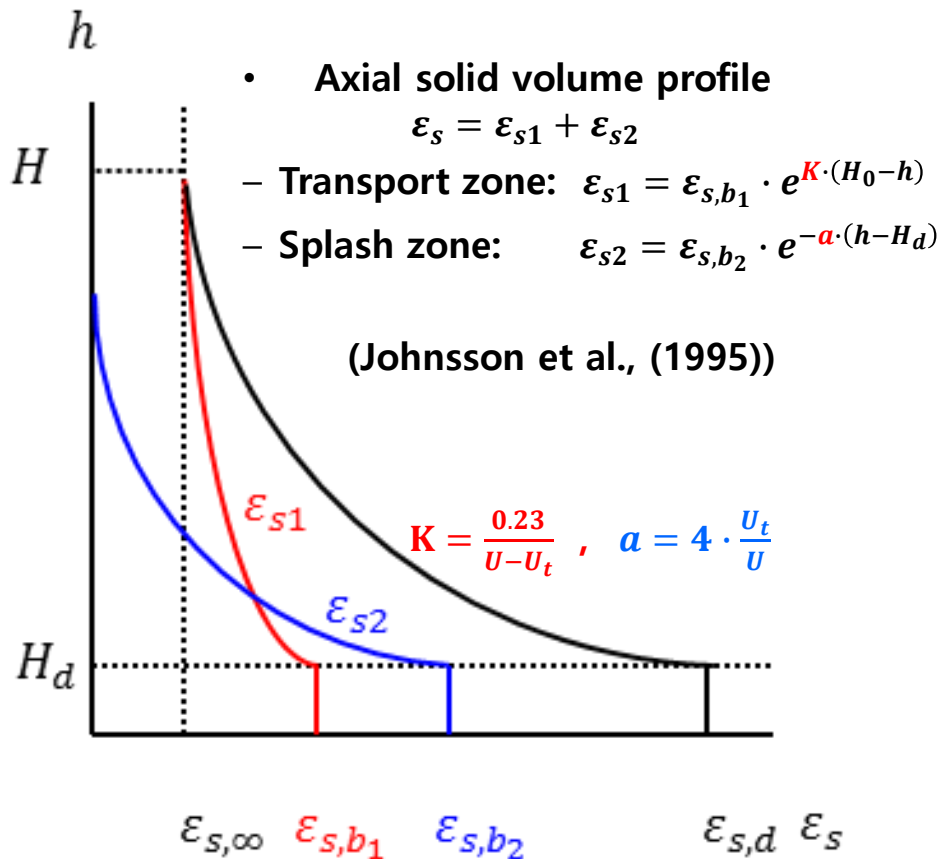


Solids volume fraction profile in fast fluidization

The axial solid volume fraction

# Prediction of solids volume fraction profile (1D)

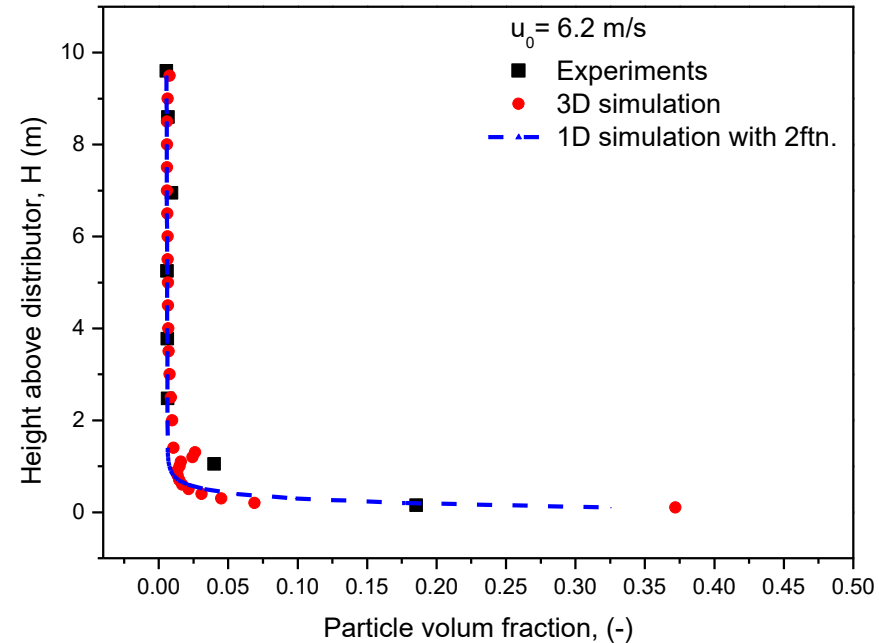
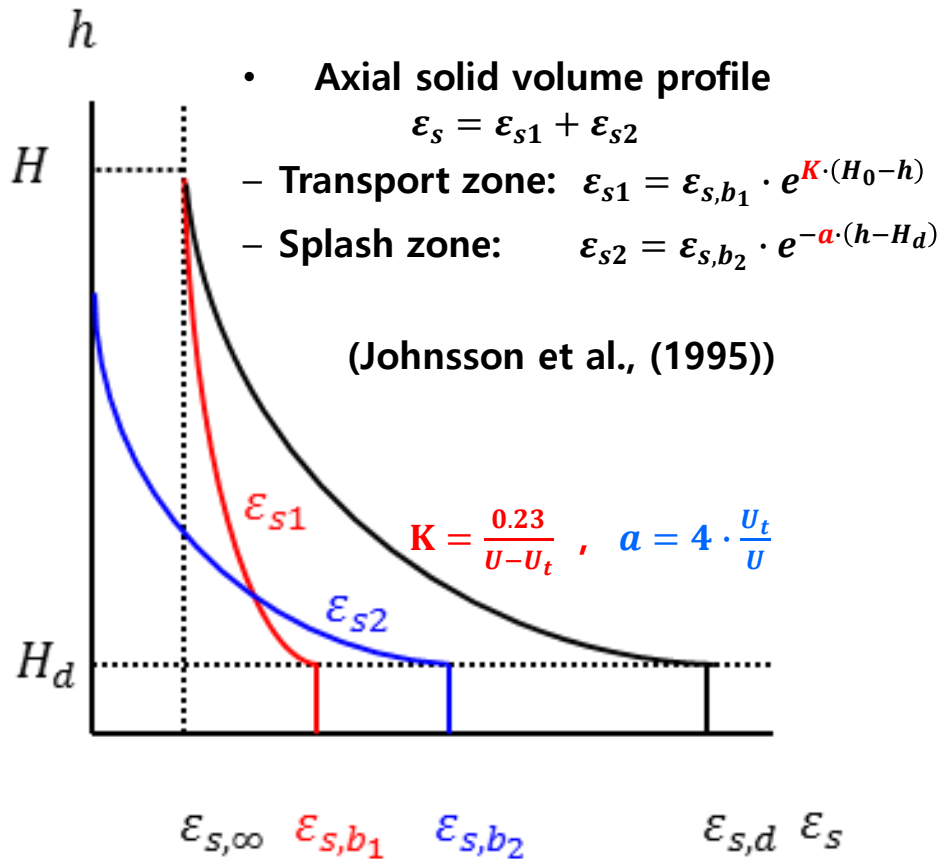
- Two different flow mechanisms for the back mixing in a CFB :
  - A homogeneous particle clustering flow : splash zone (a)
  - A core / annulus flow : transport zone (K)



**Solids volume fraction profile in fast fluidization, from 2curve model**

# Prediction of solids volume fraction profile (1D)

- Two different flow mechanisms for the back mixing in a CFB :
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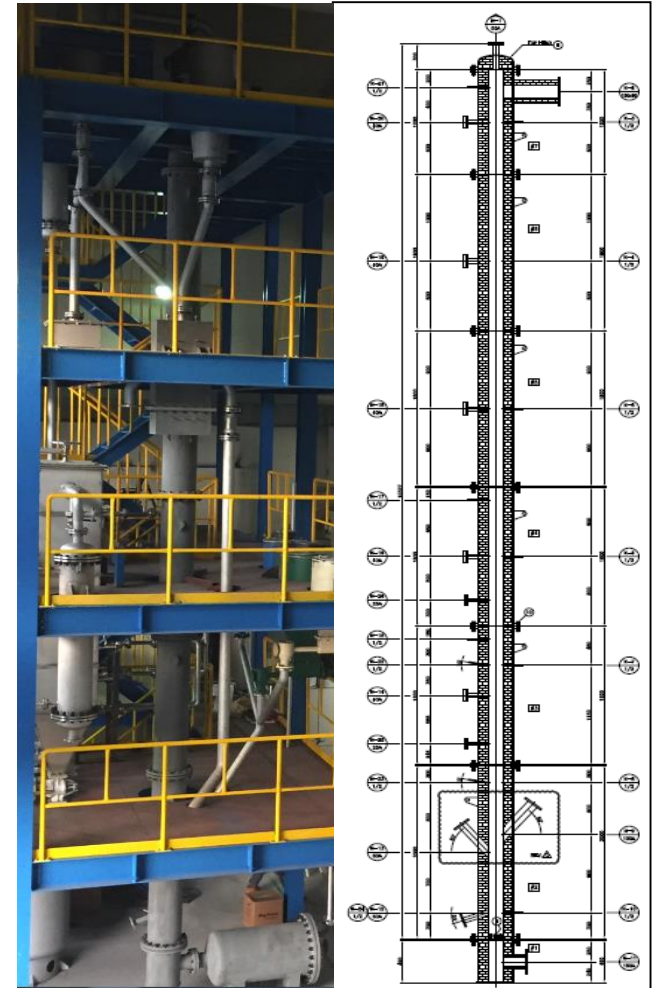


Solids volume fraction profile in fast fluidization, from 2curve model

The axial solid volume fraction

# Objective of study: Air fired CFB test-rig

- 3D simulation of FEP CRC CFB test-rig ( $100\text{kW}_{\text{th}}$ )
- Barracuda-VR® validation with CFB test-rig using the following parameters:
  - Pressure and temperature profiles
  - Gas compositions
- The decay constants  $a$ ,  $K$  obtained from 3D simulation results were used for 1D simulation.
- The performance of 1D simulation was evaluated in comparison with the experiments and 3D simulation results.



100 kW<sub>th</sub> CFBC Test-rig  
(FEP Convergence Research center, KIER)

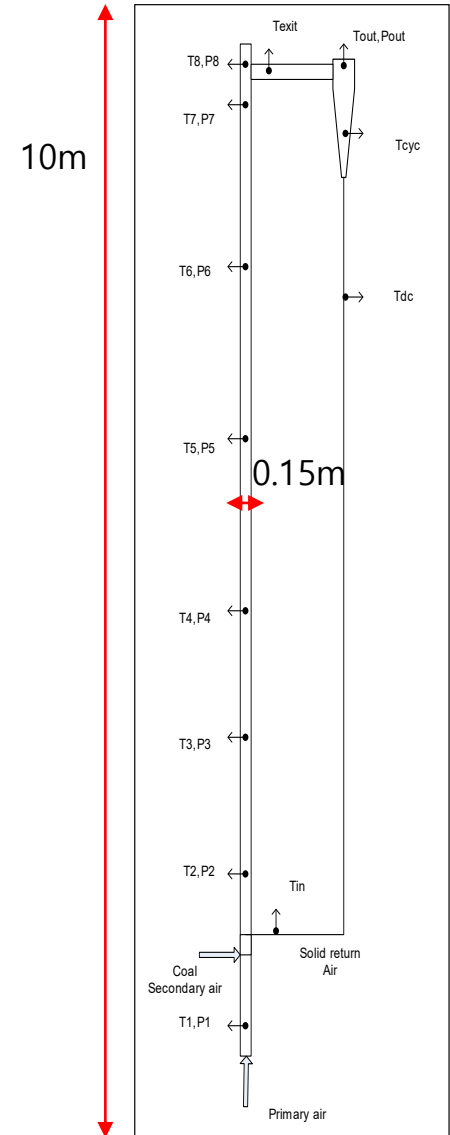
# Operating/Boundary conditions

## Thermal condition (Air fired CFB test-rig)

- CFB test-rig dimensions:  $D = 0.15 \text{ m}$ ,  $H = 10 \text{ m}$

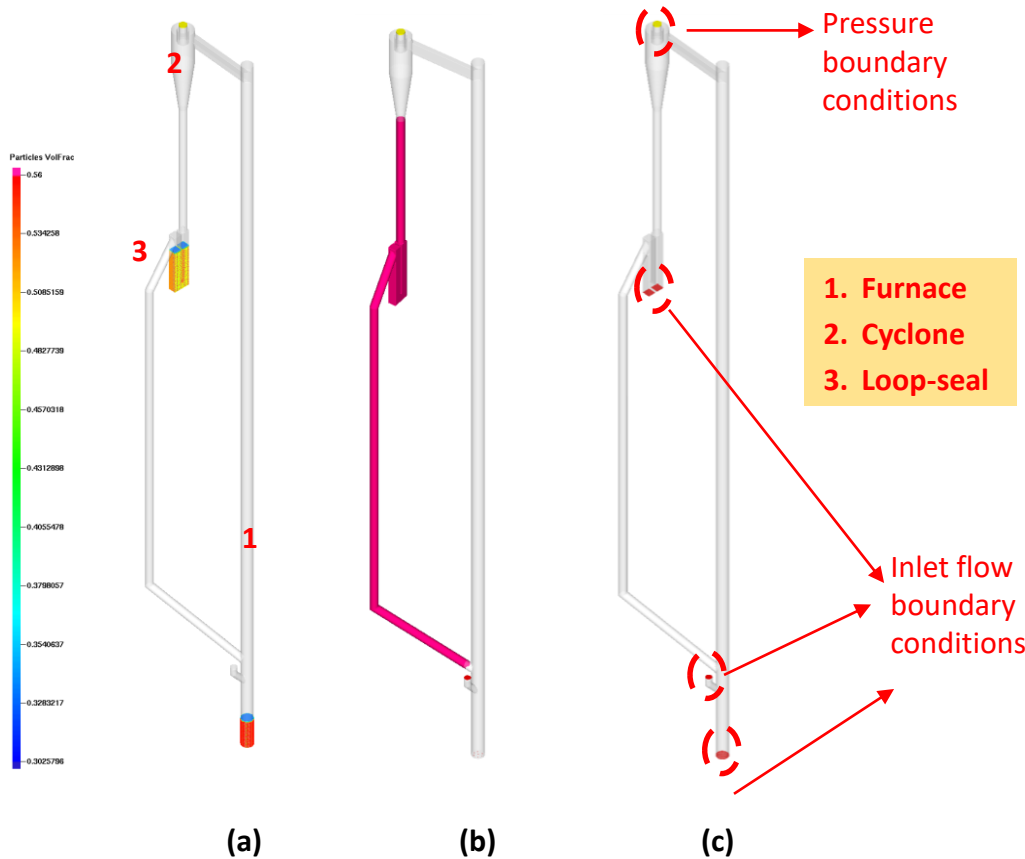
Operating conditions	Run 1	Run 2	Run 3
Fuel	Subbituminous coal/Lignite (70%/30%)		
Coal feeding rate (kg/h)	5	9.5	15.2
Primary air (Nm <sup>3</sup> /h)	19	49	74.5
Secondary air (Nm <sup>3</sup> /h)	11	11	11
Loop-seal air (Nm <sup>3</sup> /h)	8.6	8.6	10.8
Superficial velocity (m/s)	2.5	3.9	6.2

Operating conditions of the 100kW<sub>th</sub> CFB test-rig



# Operating/Boundary conditions

## Thermal condition (Air fired CFB test-rig)



(a) Initial particle volume fraction, (b) Thermal wall BC, (c) Pressure and flow boundary conditions



Hole type

### Input parameters for the calculation

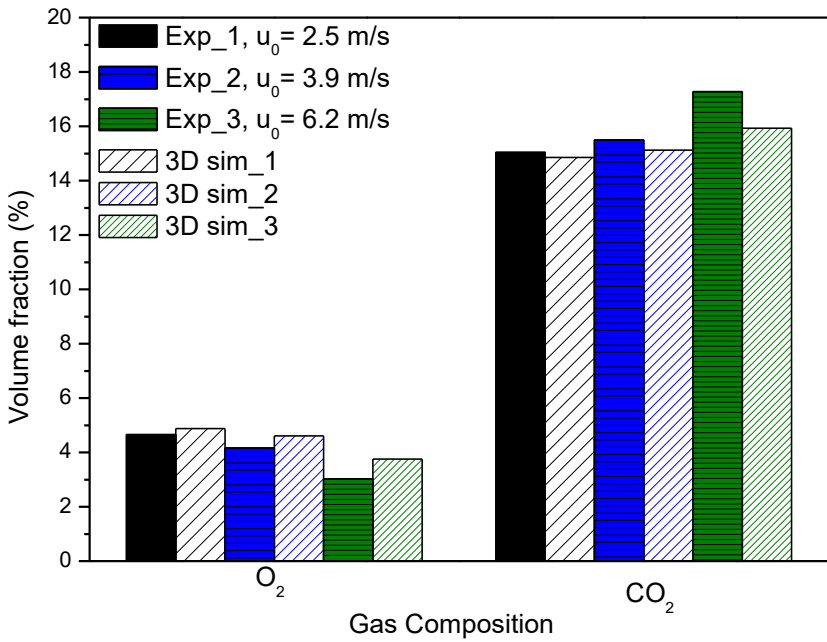
Total number of real cells	274,817
Solid volume fraction at closest packing	0.56
Total mass of particles, kg	22.13
Particle mean diameter, $\mu\text{m}$	320
Particle density, $\text{kg}/\text{m}^3$	2,400
Drag model	Wen-Yu/Ergun
Initial bed temperature	816, 848, 866 °C
Reentered temperature	593, 676, 711 °C
Simulation time, s	60

# Chemical kinetic parameter

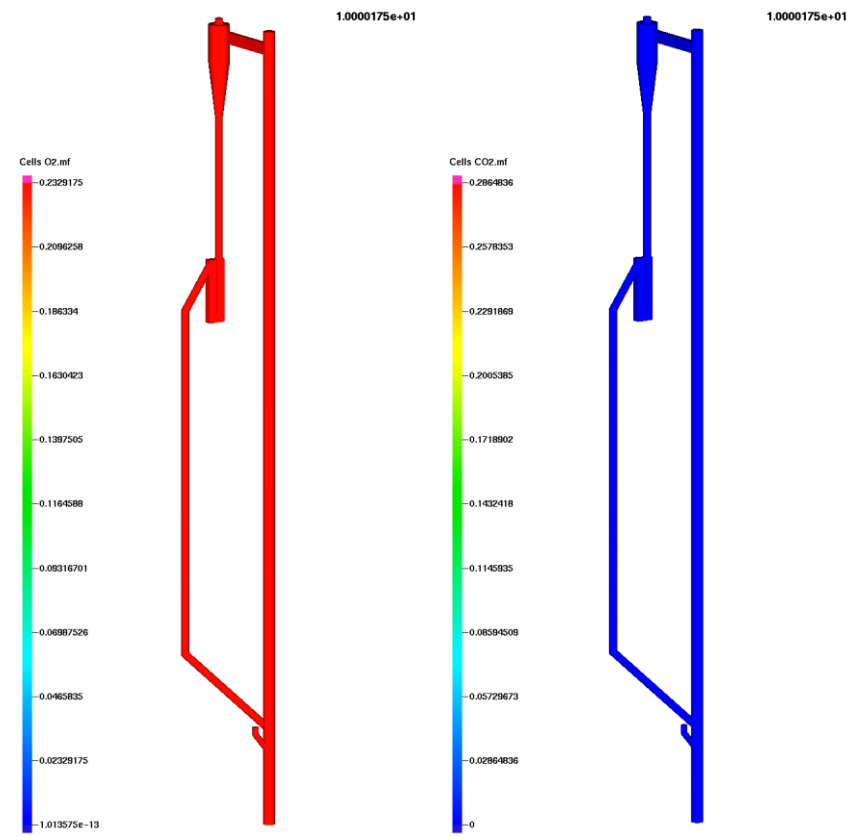
ID	Reaction	Reaction Rate Function
1	VM(s) -> 0.182124 Tar + 0.166835 CO + 0.077459 CO <sub>2</sub> + 0.19103 CH <sub>4</sub> + 0.325458 H <sub>2</sub> + 0.869927 H <sub>2</sub> O + 0.016854 H <sub>2</sub> S + 0.101283 NH <sub>3</sub>	Devolatilization
	R1 = 910.714 exp(-9410.73/T) m <sub>vm</sub>	
2	Tar -> 7.752829 C(S) + 0.180008 CO + 2.857328 CH <sub>4</sub>	Tar cracking
	R2 = 625000 exp(-13965.1/T) [Tar]	
3	C(s) + H <sub>2</sub> O -> CO + H <sub>2</sub>	Char steam gasification_f
	R3 = 0.0265443 T θ <sub>f</sub> <sup>-1</sup> m <sub>c</sub> [H <sub>2</sub> O] / ( exp(15097.4/T) )	
4	CO + H <sub>2</sub> -> C(s) + H <sub>2</sub> O	Char steam gasification_r
	R4 = 2.15263e-11 T <sup>2</sup> θ <sub>f</sub> <sup>-2</sup> exp(1228.57/T) m <sub>c</sub> [H <sub>2</sub> ][CO]	
5	C(s) + CO <sub>2</sub> -> 2CO	Char CO <sub>2</sub> gasification_f
	R5 = 0.0108658 T θ <sub>f</sub> <sup>-1</sup> m <sub>c</sub> [CO <sub>2</sub> ] / ( exp(15097.4/T) )	
6	2CO -> C(s) + CO <sub>2</sub>	Char CO <sub>2</sub> gasification_r
	R6 = 4.10796e-14 T <sup>2</sup> θ <sub>f</sub> <sup>-2</sup> exp(55184.57/T) m <sub>c</sub> [CO <sub>2</sub> ] <sup>2</sup>	
7	C(s) + 2H <sub>2</sub> -> CH <sub>4</sub>	Char h <sub>2</sub> gasification_f
	R7 = 2.83273e-6 T θ <sub>f</sub> <sup>-1</sup> m <sub>c</sub> [H <sub>2</sub> ] / ( exp(8078/T) )	
8	CH <sub>4</sub> -> C(s) + 2H <sub>2</sub>	Char h <sub>2</sub> gasification_r
	R8 = 0.00410463 T <sup>0.5</sup> θ <sub>f</sub> <sup>-0.5</sup> m <sub>c</sub> [CH <sub>4</sub> ] <sup>0.5</sup> / ( exp(13577/T) )	
9	CO + H <sub>2</sub> O -> CO <sub>2</sub> + H <sub>2</sub>	Water gas shift reaction
	R9 = 8.04621e-5 p <sup>0.496</sup> ρ <sub>f</sub> <sup>-2</sup> θ <sub>f</sub> exp(-8425.71/T) m <sub>all</sub> Θ <sub>all</sub> <sup>-1</sup> [H <sub>2</sub> O][CO] - 8.04621e-5 p <sup>0.496</sup> ρ <sub>f</sub> <sup>-2</sup> θ <sub>f</sub> <sup>2</sup> exp(-8425.71/T) m <sub>all</sub> Θ <sub>all</sub> <sup>-1</sup> [H <sub>2</sub> O][CO]	
10	Tar + 13.5574O <sub>2</sub> -> 10.7901CO <sub>2</sub> + 5.71463H <sub>2</sub> O	Tar oxidation
	R10 = 3.40794e+6 θ <sub>f</sub> <sup>-0.75</sup> exp(-15097.1/T) [O <sub>2</sub> ] <sup>1.5</sup> [Tar] <sup>0.25</sup>	
11	CO + 0.5O <sub>2</sub> -> CO <sub>2</sub>	CO combustion
	R11 = 7.91516e+9 θ <sub>f</sub> <sup>-0.75</sup> exp(-20128.8/T) [H <sub>2</sub> O] <sup>0.5</sup> [O <sub>2</sub> ] <sup>0.25</sup> [CO]	
12	H <sub>2</sub> + 0.5O <sub>2</sub> -> H <sub>2</sub> O	H <sub>2</sub> combustion
	R12 = 1.67427e+11 θ <sub>f</sub> <sup>-1</sup> exp(-15096.6/T) [H <sub>2</sub> ][O <sub>2</sub> ]	
13	CH <sub>4</sub> + 2O <sub>2</sub> -> CO <sub>2</sub> + 2H <sub>2</sub> O	CH <sub>4</sub> combustion
	R13 = 1.34384e+9 θ <sub>f</sub> <sup>-0.5</sup> exp(-24355.9/T) [O <sub>2</sub> ] <sup>1.3</sup> [CH <sub>4</sub> ] <sup>0.2</sup>	
14	2C + O <sub>2</sub> -> 2CO	Char oxidation
	R14 = 4.34e+7 T exp(-13590/T) Θ <sub>c</sub> <sup>-1</sup> [O <sub>2</sub> ]	
15	H <sub>2</sub> O(s) -> H <sub>2</sub> O	Moisture release
	R15 = 2830.93 exp(-9410.73/T) m <sub>H<sub>2</sub>O</sub>	

# Exit gas compositions

- The 3D results are in good agreement with experiments, with the relative error of less than 20%
- The average relative errors of the gas composition increase with gas flow rate.



Comparison of exit gas compositions between simulation and experiments

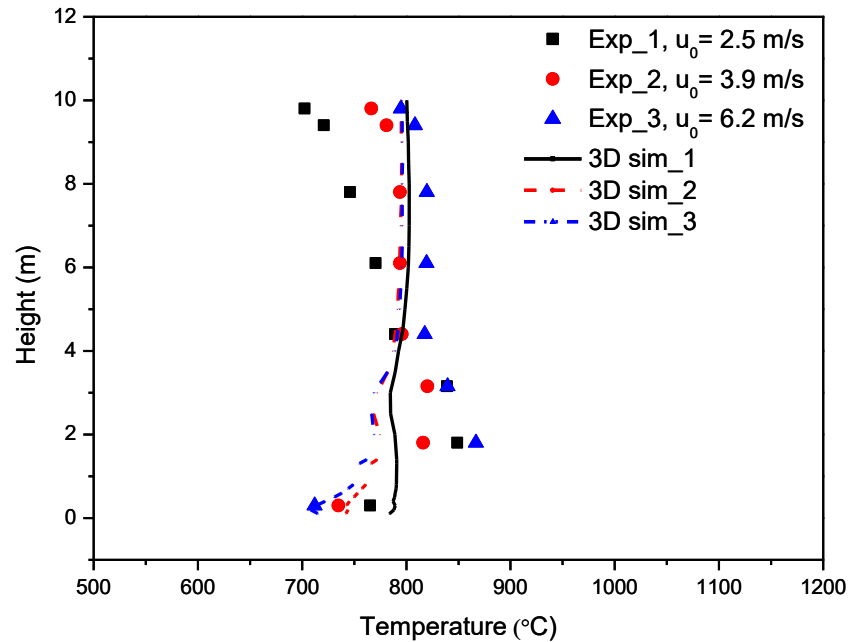


O<sub>2</sub> mass fraction (wt.%)  
3D sim\_3 u<sub>0</sub> = 6.2 m/s

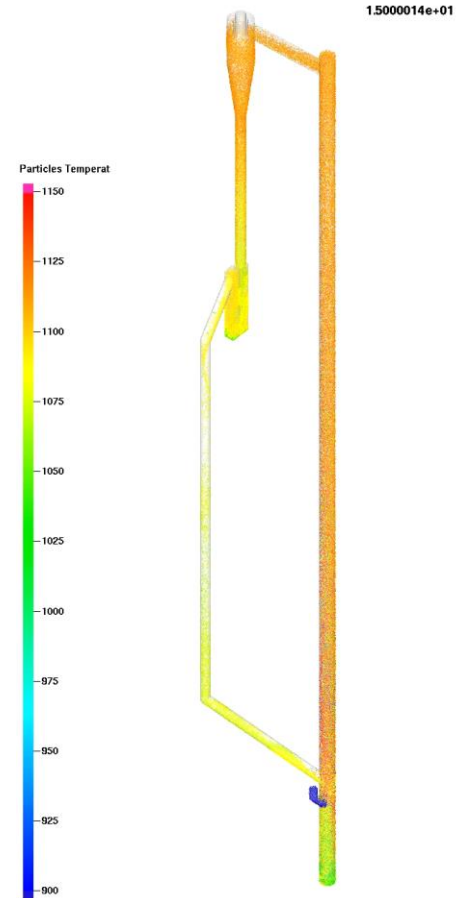
CO<sub>2</sub> mass fraction (wt.%)  
3D sim\_3 u<sub>0</sub> = 6.2 m/s

# CFB test-rig temperature profile

- From the experimental results, the temperature increased as the gas velocity increased.



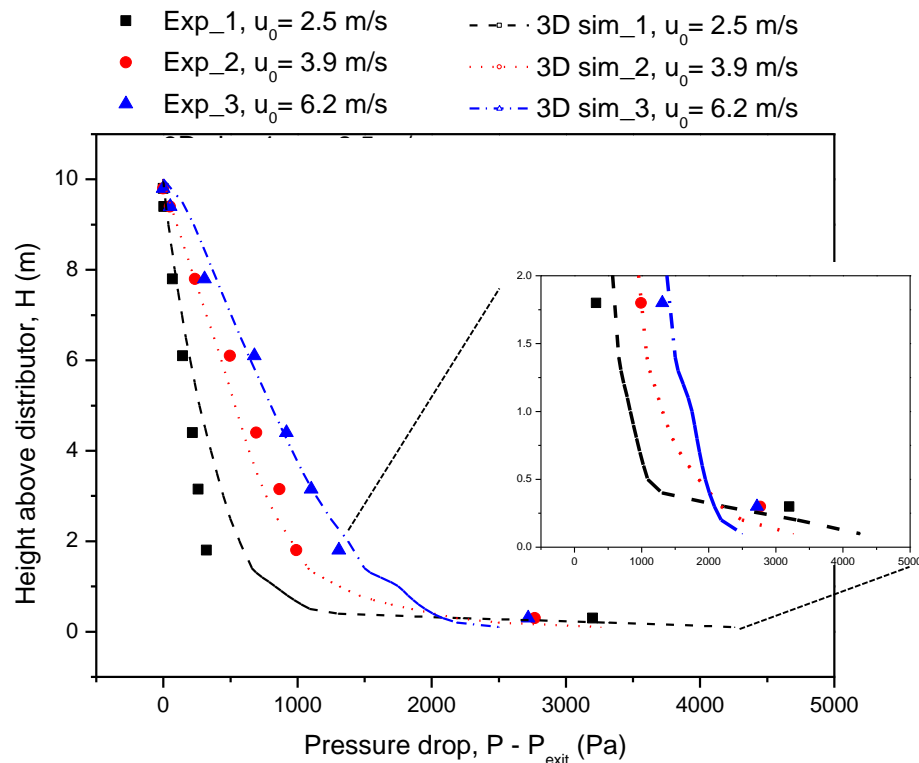
Comparison of axial temperature profile between simulation and experiments



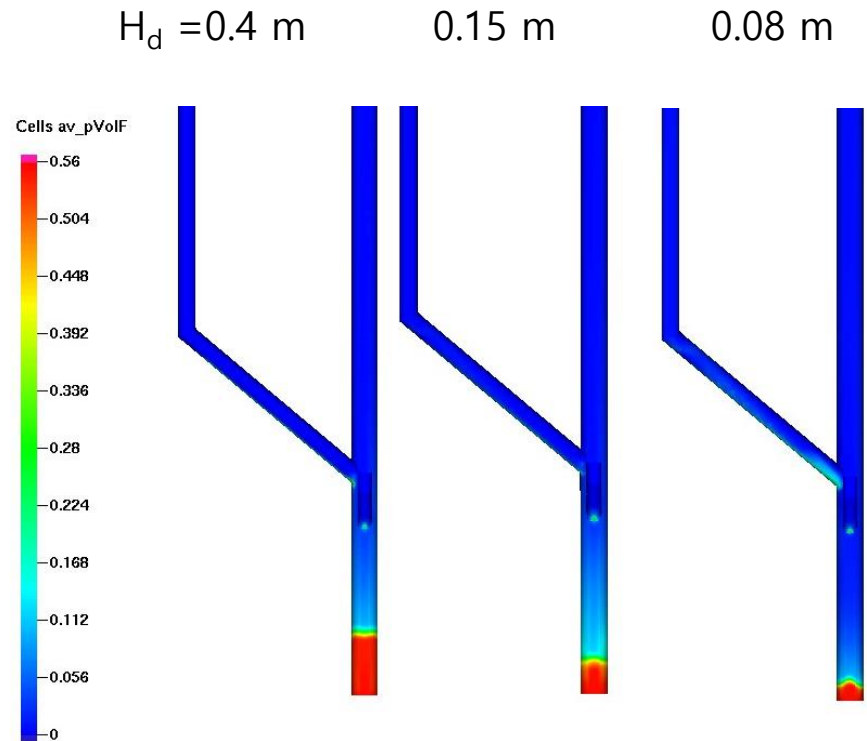
Particle temperature (K)  
3D sim\_3  $u_0 = 6.2$  m/s

# CFB test-rig pressure profile

- Due to the decrease in bed mass as the gas flow rate increase, there is a decrease in lower part pressure.



Comparison of axial pressure profile between simulation and experiments

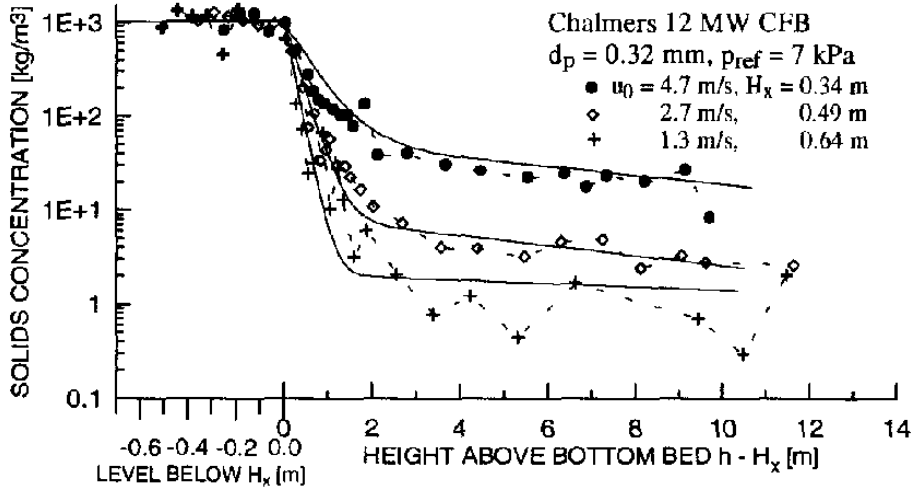
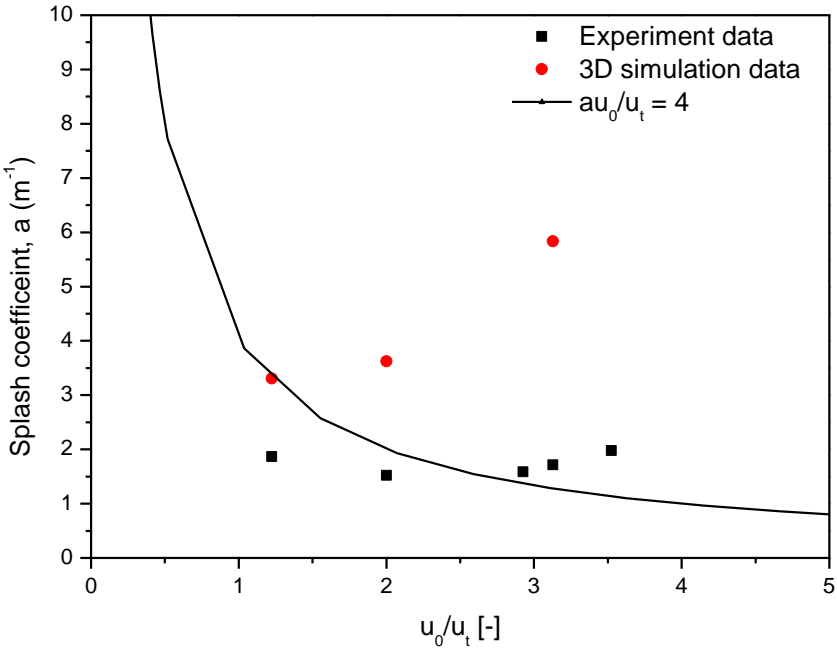


Cell average particle volume fraction (3D simu\_1, 2, and 3)

# Prediction of splash coefficient 'a'

- The splash coefficient 'a' increases as the gas flow rate increases in 3D results.
- Comparing to this 3D results, it is the opposite trend in reference results.

$$\epsilon_s = \epsilon_{s,b1} \cdot e^{K \cdot (H_0 - h)} + \epsilon_{s,b2} \cdot e^{-a \cdot (h - H_d)}$$



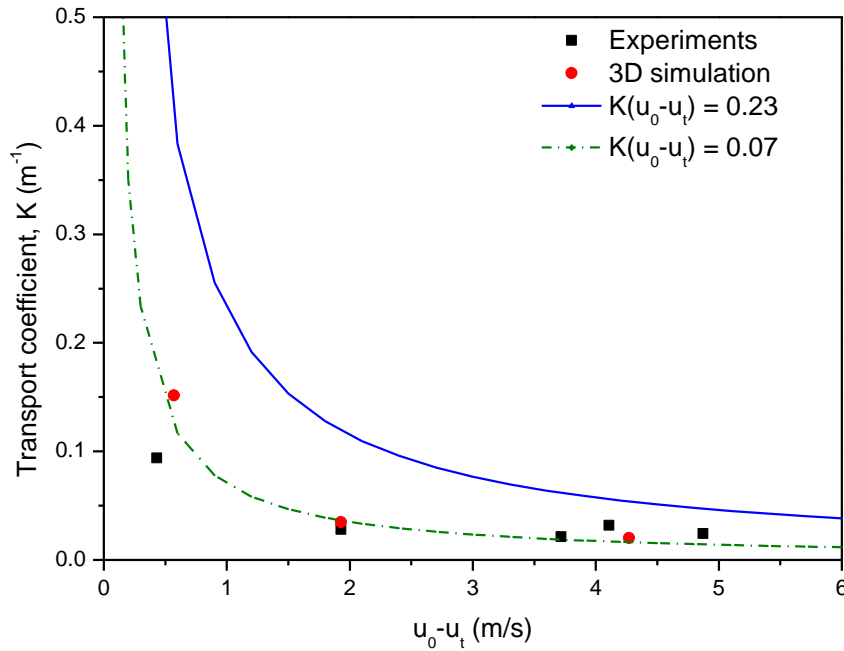
Vertical profiles of solids concentration

The decay constant for the splash zone, a, vs gas velocity  $u_0/u_t$

# Prediction of transport coefficient 'K'

- The solids volume fraction was affected by the splash coefficient 'a' more than the transport coefficient 'K' in the pilot scale reactor.

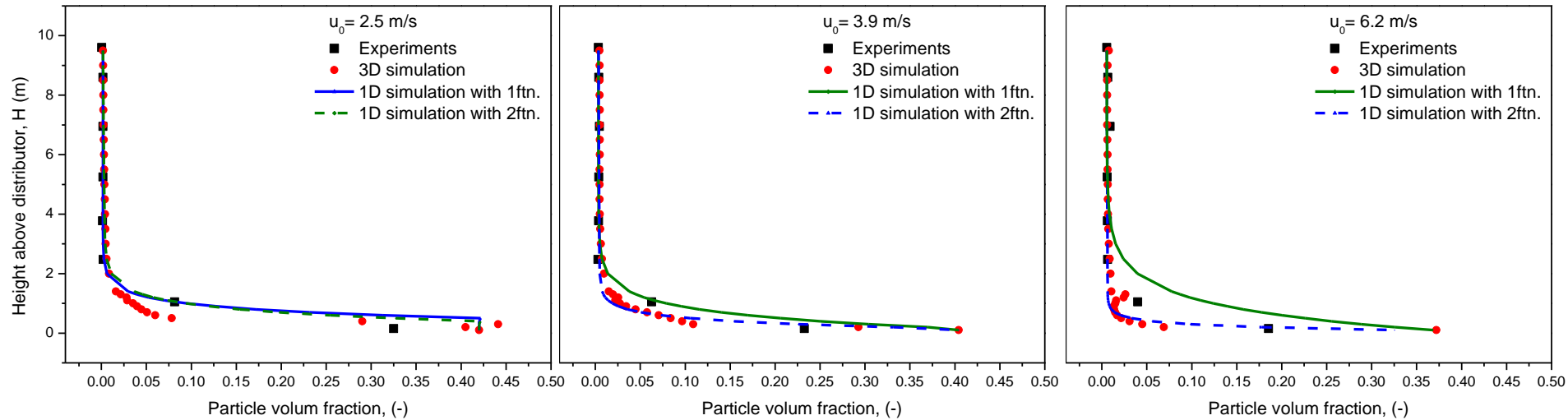
$$\varepsilon_s = \varepsilon_{s,b_1} \cdot e^{K \cdot (H_0 - h)} + \varepsilon_{s,b_2} \cdot e^{-a \cdot (h - H_d)}$$



The decay constant for the transport zone,  
K, vs gas velocity  $u_0 - u_t$

# Effect of decay coefficient on particle volume fraction

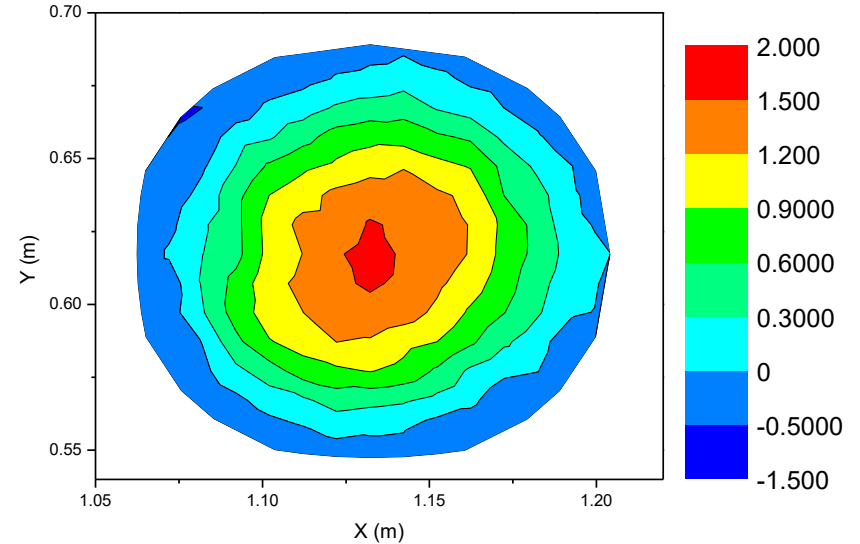
- 1 function model,  $a = 4 \cdot \frac{U_t}{U}$
- 2 function model,  $a = 1.9333 \cdot \frac{U}{U_t}$ ,  $K = \frac{0.15}{U - U_t}$



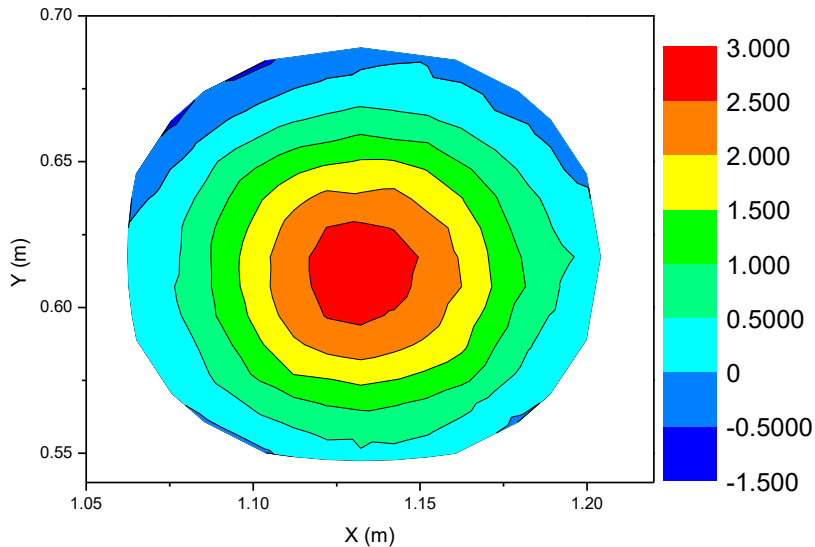
Comparison of axial solid volume fraction between simulation and experiments

# A core / annulus flow : transport zone

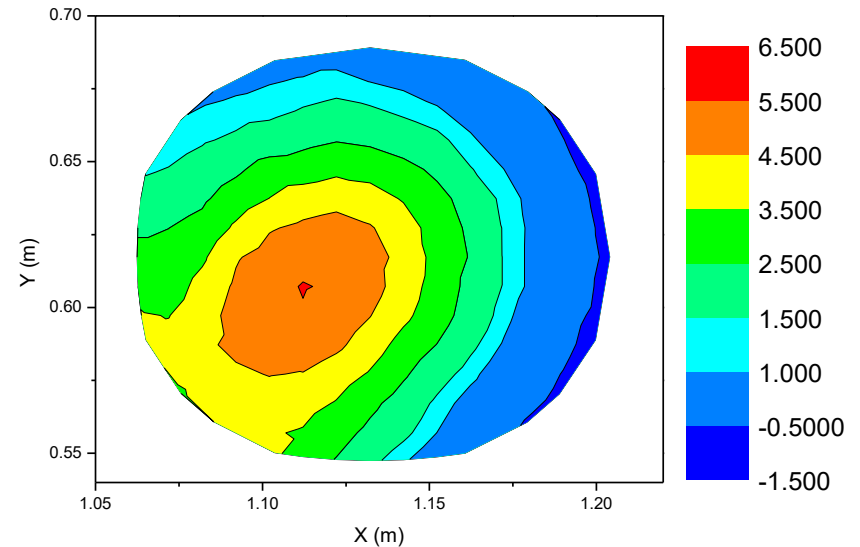
- The particles are biased in one direction as a flow rate increases.



3D\_result\_case\_1,  $u_0 = 2.5$  (9m)



3D\_result\_case\_2,  $u_0 = 3.9$  (9m)



3D\_result\_case\_3,  $u_0 = 6.2$  (9m)

Particle velocity, m/s

# Conclusions

- 3D simulation results show proper trends of gas compositions, pressure and temperature profiles.
- The solids volume fraction was affected by the splash coefficient 'a' more than the transport coefficient 'K' in the pilot scale reactor.
- Addition needed for literature de SO<sub>x</sub> and de NO<sub>x</sub> reactions.
- Further works – The effect of decay coefficient 'a' and 'K' with various size of CFB boiler.

Thank you for your  
attention!!!!