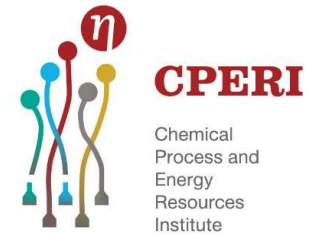




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Numerical Simulation of Industrial-Scale Fluidised Bed Reactors Using an Artificial Neural Network EMMS Drag Model

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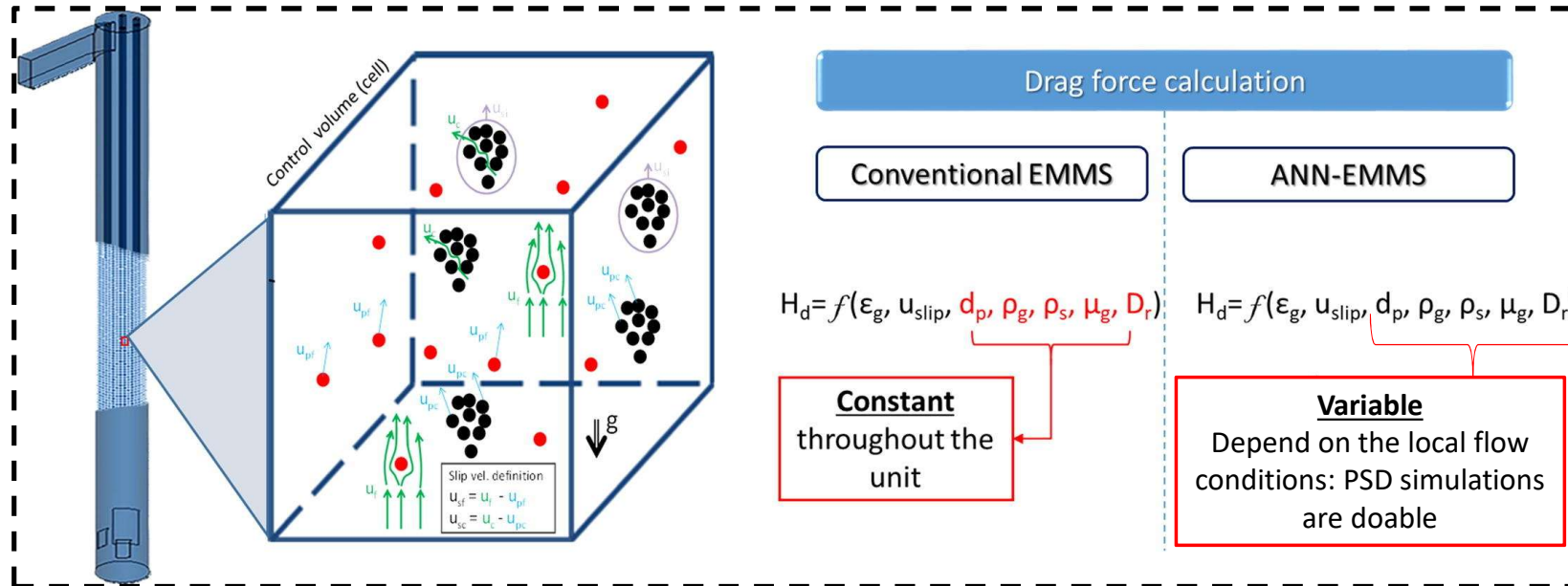
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ANN-EMMS implementation in 3-D DDPM CFD simulations



Scope: Development of an Artificial Neural Network (ANN) to enhance the resolution of meso-scale structures in gas–particle interactions. The ANN-EMMS model was developed, trained, and validated using data generated from a custom-built solver for the EMMS (Energy-Minimization Multi-Scale) equations, covering a broad range of gas–particle mixture properties.

Methodology:

i. Select the **representative range of properties** corresponding to several particle properties and reactor operating conditions (**24 individual cases**).

22 cases have been selected for training of EMMS artificial neural network.

2 extra cases have been used for validation of ANN, which are excluded from the training.

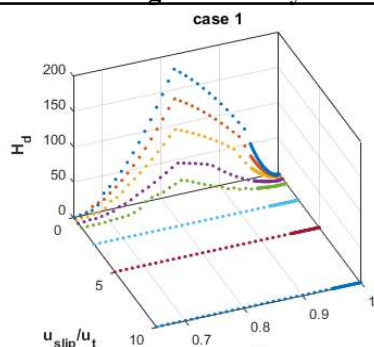
Range of operating properties

$$d_p \in [50-425] \quad \bar{u} \in [0.15-10] \quad \mu_g \in [3.75e-5 - 5e-5] \quad \rho_g \in [0.25 - 0.4] \quad \rho_s \in [3500 - 5300]$$

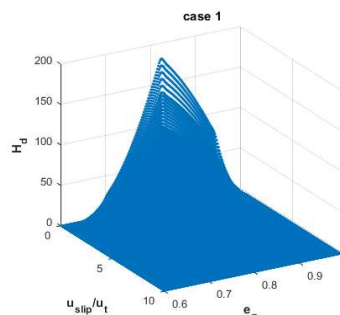
ii. Solve the **EMMS equation** in order to calculate the **heterogeneity index** ($H_d = F_{WenYu} / F_{EMMS}$) for each case.

iii. Additional data have been produced via interpolation schemes based on the generated data in order to have smoother curve of H_d according to u_{slip}/u_t and ϵ_g .

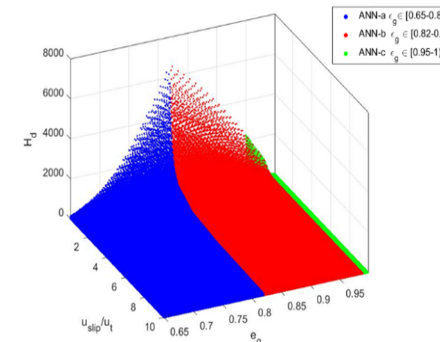
Indicative data generated by the EMMS code



Additional data after interpolation



Dataset for training were divided in three regions



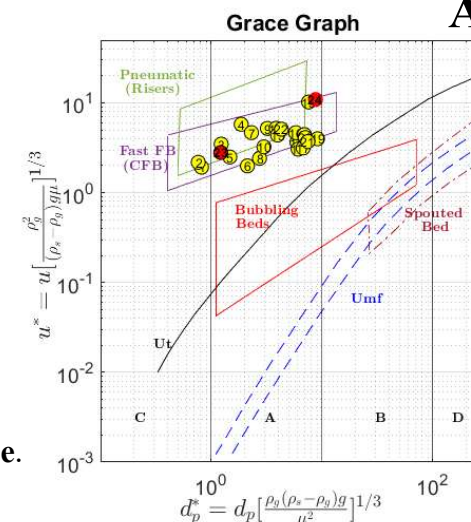
- **Eight** $\bar{u} = u_{slip}/u_t$: 0.15, 0.2, 0.3, 0.6, 1, 2.5, 5 and 10
- ϵ_g : **40 and 50 point** for dense and dilute region
- **720** H_d points for each case.

- Interpolation for u_{slip}/u_t using a step of **0.01**
- Interpolation for ϵ_g using a step of **0.002**
- **310,500** H_d points for each case

- Dense area 1, ϵ_g [0.65-0.82], **ANN-a** (2,353,722 data)
- Dense area 2, ϵ_g [0.82-0.95], **ANN-b** (1,832,922 data)
- Dilute area, ϵ_g [0.95-1), **ANN-c** (2,182,246 data)

iv. Train three ANNs algorithms by dividing the ϵ_g region into three **areas** for better prediction:

v. Validation of the neural network using particle and gas properties which are **excluded from the train data set**.

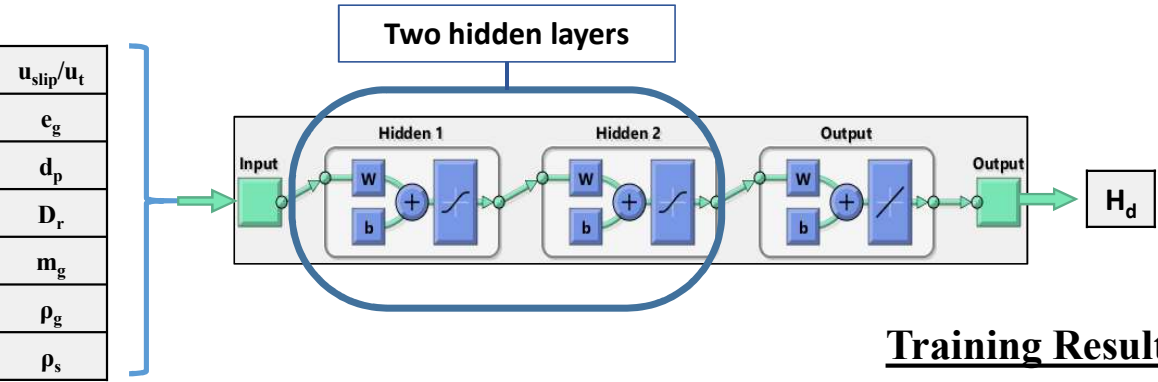




Artificial Neural Network scheme

- Each ANN was trained individually.
- Parametric studies were made in order to define the optimal number of layers and neurons in each region.
- The criterions to select the optimal network was the minimization of **Mean Absolute Percentage Error**:

$$Mape = \frac{1}{n} \sum_{i=1}^n \left| \frac{H_{d_{ANN}} - H_{d_{EMMS}}}{H_{d_{EMMS}}} * 100 \right|$$



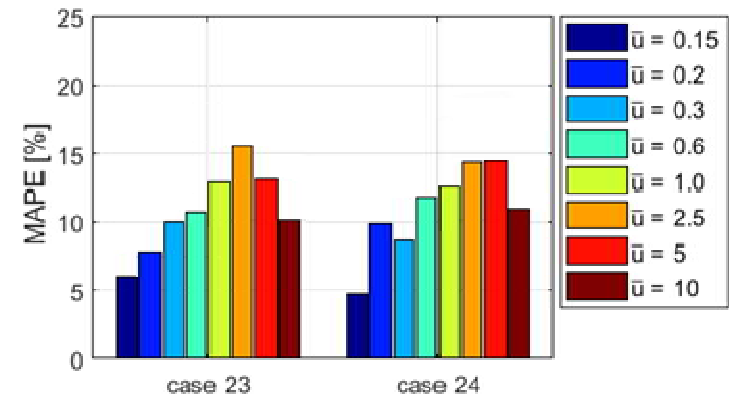
Training Results

ANN	Number of neurons		MAPE [%]	R	y = a·x + b	
	1st layer	2st layer			a	b
ANN-a	17	14	19.32%	0.998	1	0.022
ANN-b	17	8	19.2%	0.999	1	0.03
ANN-c	14	19	14.07%	0.993	1	0.26

Validation Results

Validation of ANN-EMMS model using the operation conditions of the Cases **23** and **24** (*not included in the training data set*)

- Average **MAPE** of case **23** is less than **14.5%**
- Average **MAPE** of case **24** is less than **13.5%**



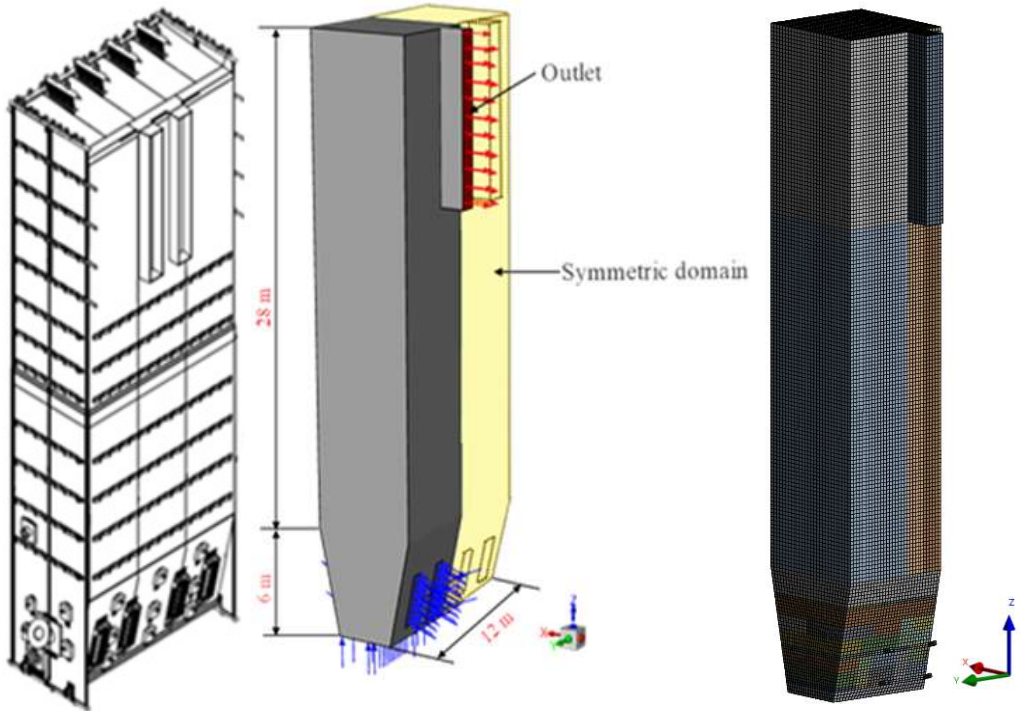


CFD simulations

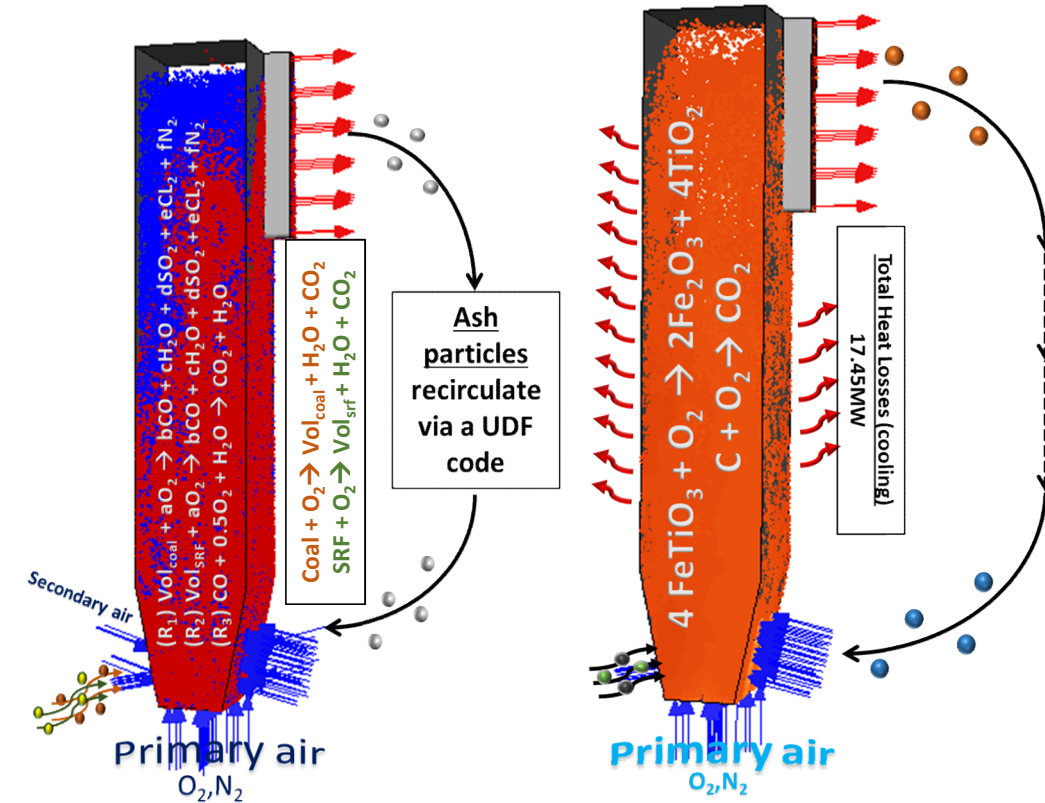
Geometry & Operating modes

Industrial scale fluidized reactor

Operating conditions/modes:



The grid with 259,322 number of elements



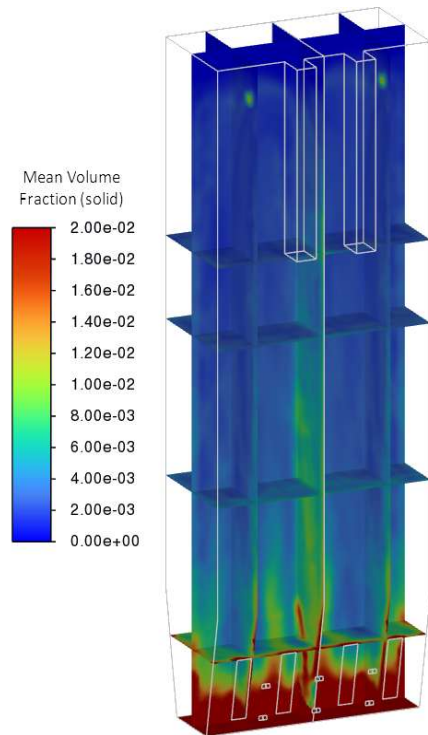
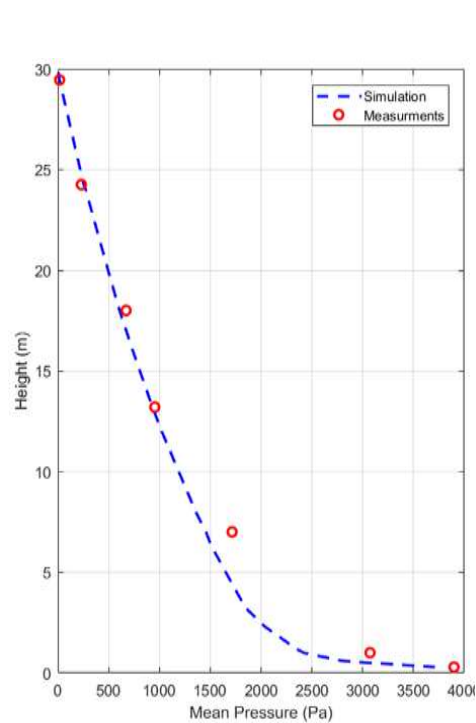
(a) Co-combustion mode

(b) Retrofitted Air reactor mode





ANN-EMMS Accurately Predicts Pressure Drop



z (m)	Pressure drop (Exp.) [Pa]	Pressure drop (CFD) [Pa]	Error [%]
29.46	15	16.37	9.13
24.26	244.33	255.1	4.41
18.01	684.68	610.2	10.88
13.21	967.35	931.4	3.72
7.01	1728.24	1457	15.69
1.01	3285.1	2417	26.43
0.3	3911.19	3709	5.17
AVER.			10.78

The CFD model shows very good agreement with experimental data for pressure drop along the column, with an average deviation of only **10.78%**.

Species	Mean mass fraction [%]
O ₂	4.77 - numerical 5.6 - experimental
H ₂ O	6.67
CO ₂	18.84
SO ₂	0.078
Cl ₂	0.044
CO	1.70E-04
Volatiles SRF	8.35E-05
Volatiles Coal	1.40E-05
N ₂	69.60
SUM	100

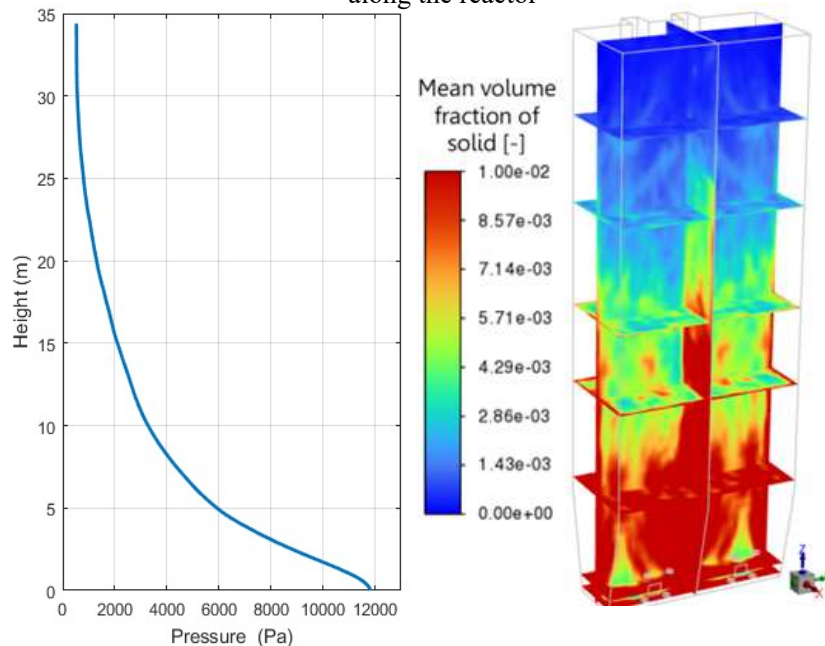
The deviation in O₂ mass fraction at the outlet, comparing simulation results with experimental data, was calculated to be **14.82%**.



z (m)	Pressure drop [Pa]
29.46	449.13
24.26	640.35
18.01	1606.98
13.21	2479.06
7.01	4761.69
1.01	11147.17
0.3	12686.85

Average Pressure Drop is approximately 12,600 Pa which corresponds to 37,280kg of fuel inside the reactor.

Time-averaged pressure drop and Mean volume fraction of solid phase along the reactor



Outlet solid phase

	1D simulation	CFD	ERROR [%]
Mass flow rate [kg/s]	721.74	837.56	16.05%
FeTiO ₃ [%]	6.2	7.16	15.4%
Fe ₂ O ₃ [%]	46.9	46.42	1.02%
TiO ₂ [%]	46.9	46.42	1.02%

A discrepancy can be observed at the mass flow rate of the solid at the outlet, which is reasonable since Ansys CFD simulation takes in to account the full physics of a 3D transient approach in contrast to aspen 1D steady state approach.

Outlet gas phase

	1D simulation	CFD	ERROR [%]
Mass flow rate [kg/s]	100.307	102.076	1.8%
Temp [K]	1273.15	1283.45	0.8%
O ₂ [%]	10.60	11.31	6.7%
CO ₂ [%]	0.30	0.25	6.8%
N ₂ [%]	89.10	88.44	0.7%

Co-combustion reactor

- ✓ The ANN-EMMS model accurately predicts the pressure profile, showing strong agreement with experimental data.
- ✓ Full-scale CFD simulation of the Co-Combustion reactor achieved:
 - Average pressure drop prediction error: **10.85%**
 - Outlet O₂ mole fraction prediction error: **14.82%**

Retrofitted Air reactor

- ✓ The model predictions show excellent agreement with the 1D steady-state simulation results.
Average prediction errors at the outlet:
 - Gas temperature: **0.8%**
 - Gas mass flow rate: **1.8%**
 - Gas species concentrations: **< 10%**
 - Solid species concentrations: **< 5%**



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