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Bio-Flex CLC

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Chemical
Process and
Energy
Resources
Institute

Numerical Modelling of Fuel Reactors in Chemical Looping Combustion Pilot Plants

G Kanellis[1]*, T Lyras[1] and N Nikolopoulos[1]

[1]Chemical Process & Energy Resources Institute, Centre for Research and Technology Hellas (CERTH), 52 Aigialias street, 15125, Athens, Greece

Presenter Mr. Georgios Kanellis
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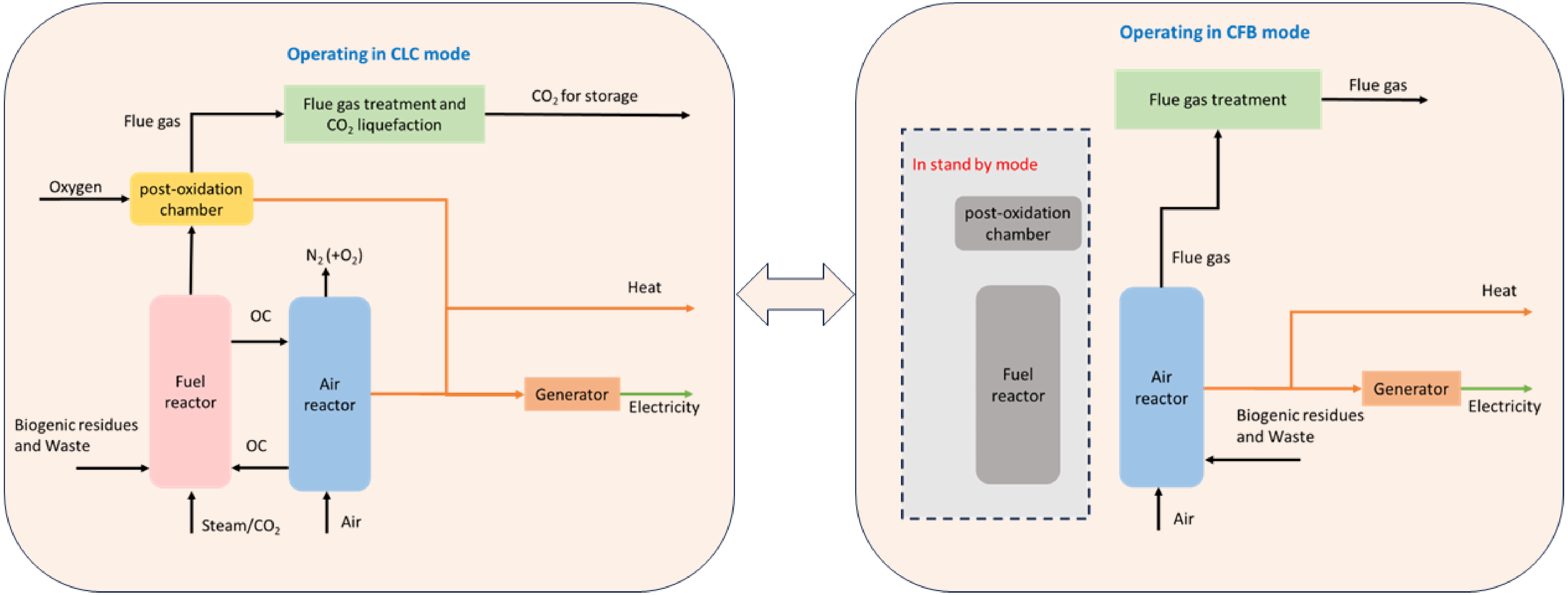
*Contact information Mr. G Kanellis ✉ g.kanellis@certh.gr

The Bio-FlexCLC EU project



Operating in CLC mode

Flue gas

Flue gas treatment and CO_2 liquefaction

CO_2 for storage

Oxygen

post-oxidation chamber

$N_2 (+O_2)$

Heat

OC

Fuel reactor

Air reactor

Generator

Electricity

Biogenic residues and Waste

OC

Steam/CO_2

Air

Operating in CFB mode

Flue gas treatment

Flue gas

In stand by mode

post-oxidation chamber

Fuel reactor

Flue gas

Heat

Air reactor

Generator

Electricity

Biogenic residues and Waste

Air

Figure and more information on Bio-FlexCLC project can be found in:

https://www.bioflexclcproject.eu

Modelling Scope and Objectives

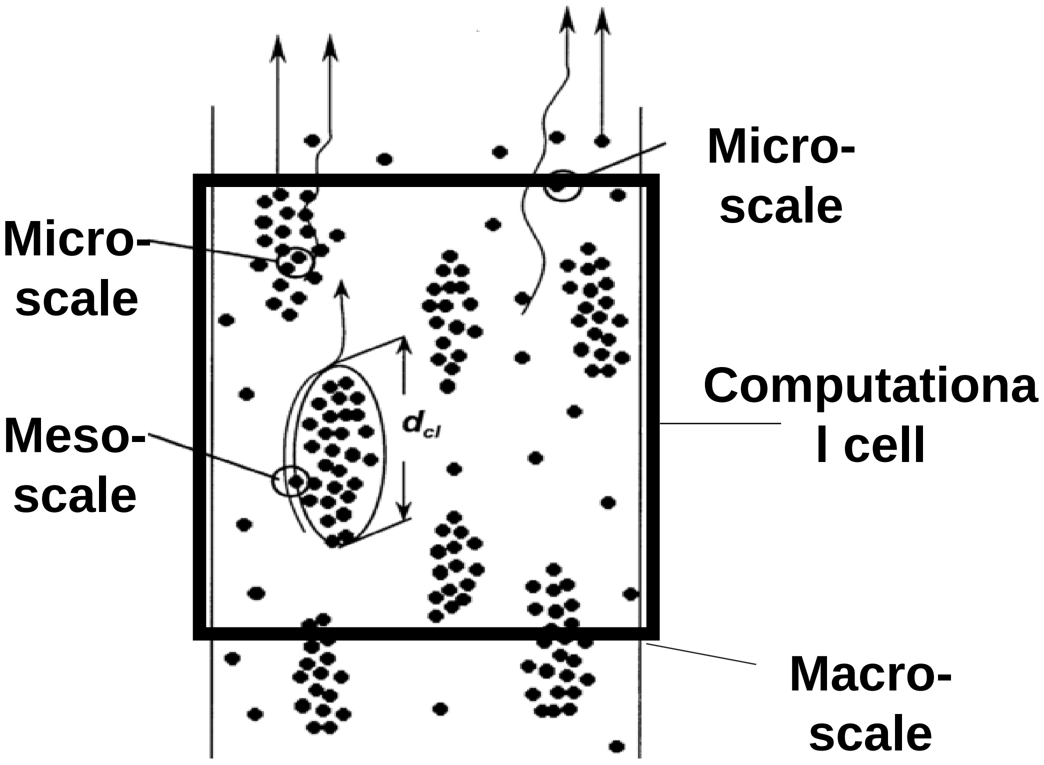
SCOPE: To model fuel reactors of pilot CLC plants of partners

- **CTH** - Chalmers University of Technology (Sweden)
- **CSIC** - Spanish National Research Council (Spain)
- **TUDA** -Technische Universität Darmstadt (Germany)

- Focus here is on the **fuel reactors** of **CTH's 10 kW$_{th}$** and **TUDA's 1 MW$_{th}$** CLC pilot plants.
- Simulations were performed prior to experiments.
- **Goal:** To support the design and operation of the units by exploring design sensitivities and providing qualitative guidance

MODEL DESCRIPTION – General setup

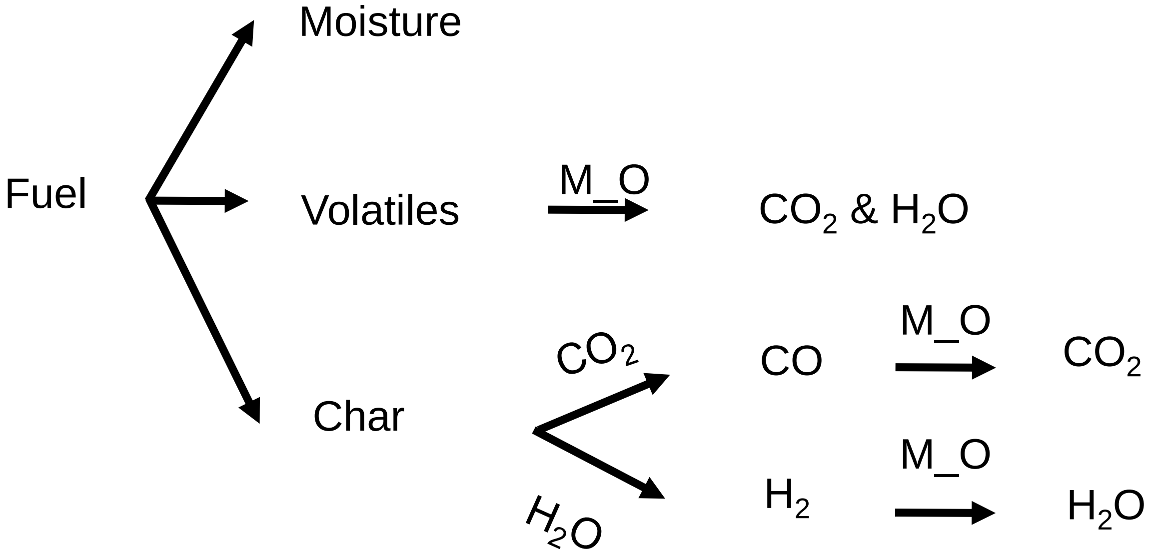
- TFM Eulerian model for gas and OC particles
- DPM Lagrangian model for fuel particles
- Isothermal simulations
- Simulation of ~ 300s of flow time
- Calculated averages over a range of ~50s after equilibrium was achieved
- Selected drag model dependent on the $\frac{D_{cell}}{d_p}$.
- Up to ~20 the **Gidaspow** drag model is considered
- For greater ratios, the **EMMS** model is chosen



When cell-size is relatively big → EMMS

MODEL DESCRIPTION – Reactions

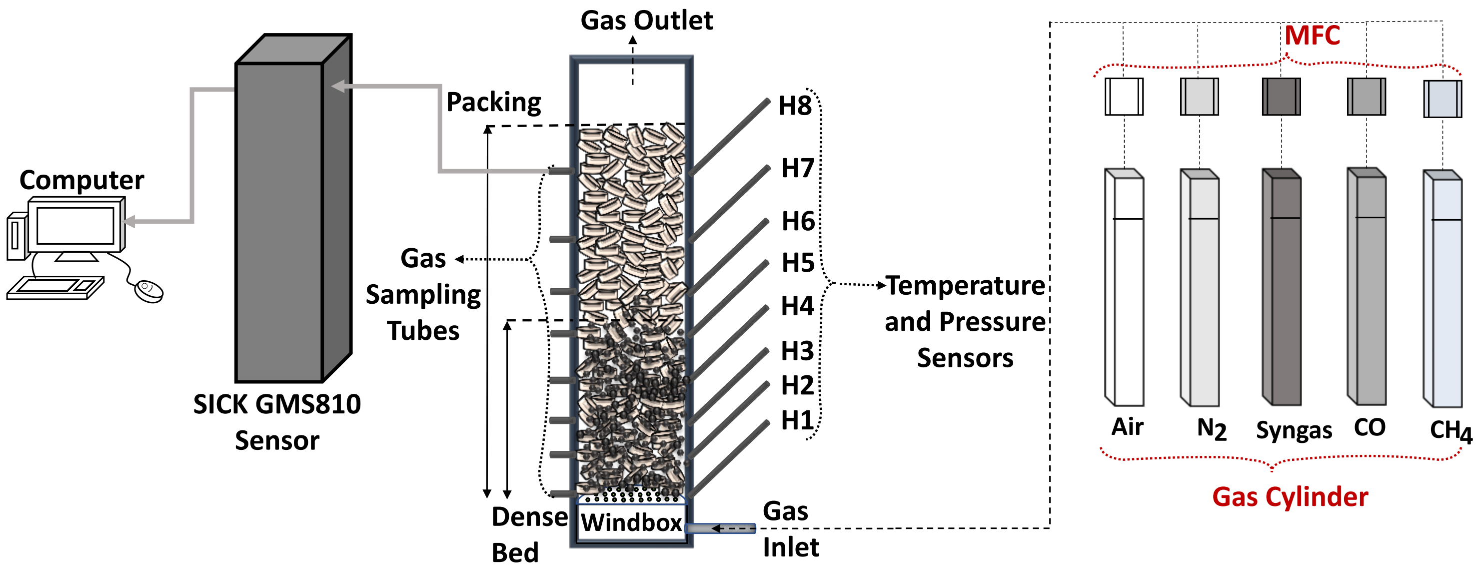
- Fuel volatiles consist (apart from moisture) of: **CH_4, CO, CO_2, H_2, O_2, N_2**.
- The exact volatiles composition is calculated based on elemental and energy balances.
- Fuel char is gasified with H_2O and CO_2.



Reactions	
R_1	$C + CO_2 \rightarrow CO$
R_2	$C + H_2O \rightarrow H_2 + CO$
R_3	$CO + M\_O \rightarrow M + CO_2$
R_4	$H_2 + M\_O \rightarrow M + H_2O$
R_5	$0.25CH_4 + M\_O \rightarrow M + 0.5H_2O + 0.25CO_2$
R_6	$CO + H_2O \rightleftarrows H_2 + CO_2$
R_7	$CO + O_2 \rightarrow CO_2$
R_8	$H_2 + 0.5O_2 \rightarrow H_2O$

Heterogeneous reactions

Reactors with packings - Background

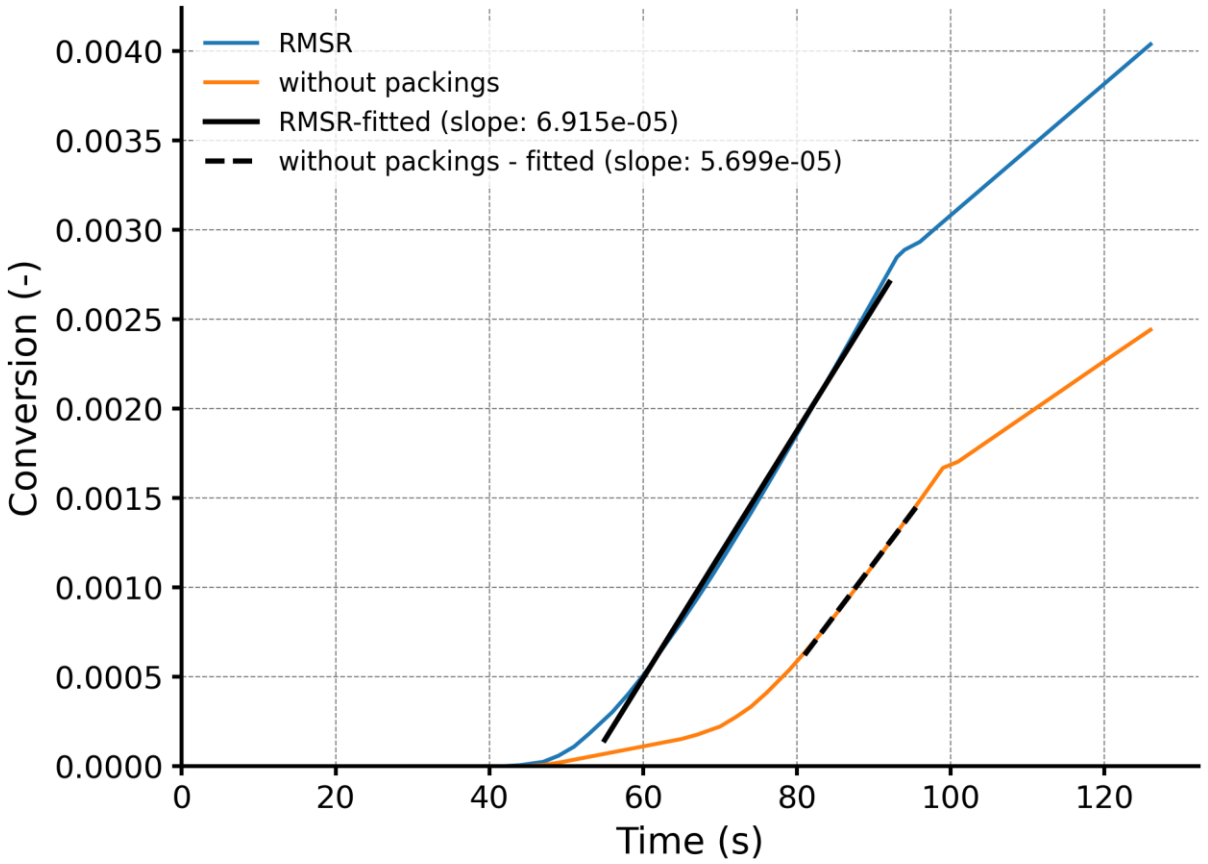


Packing	**Void factor (-)**	Bulk density (kg/m3)
Hiflow	**0.95**	280
RMSR	**0.96**	204

I. Nemati N.; Rydén M.; Chemical-looping combustion in packed-fluidized beds: experiments with random packings in bubbling bed. 2021.

II. Nemati N.; Tsuji Y.; Mattisson T.; Rydén M.; Chemical-looping combustion in packed-fluidized bed reactor – fundamental modelling and batch experiments with random metal packings. 2022.

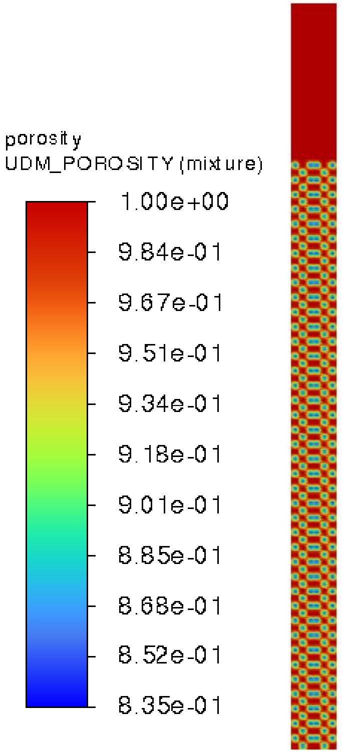
Reactors with packings - Analysis



- ✓ Consideration of the “stable” part of the experiment
- ✓ With packings a clearly higher conversion rate is observed (~20% higher)

Reactors with packings - CFD – pt1

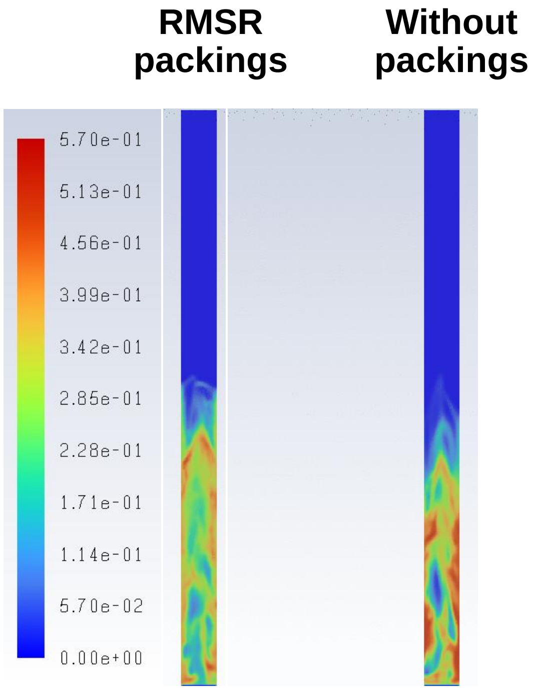
- Initial simulations with a porosity field did not show any difference between the packings and the no packings cases
- The use of non-uniform domain porosity was investigated
- Porosity variation is induced through sine functions in both radial and axial dimension
- According to the results the CFD model **can correctly predict** the fact that the bubble size decreases
- However, according to the CFD model the decrease of the bubble size is not reflected on the increase of the rate. The rate increases only by little (5% vs 20% in the experiment).



Non uniform porosity field - example

Reactors with packings - CFD – pt2

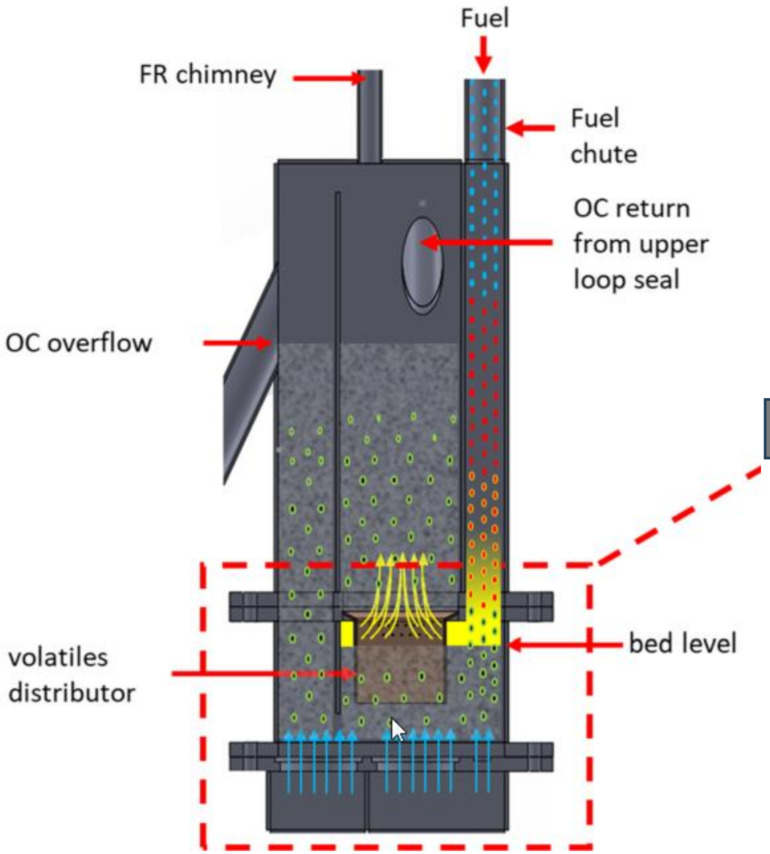
	No packings	RMSR packings
$\delta_{bubbles}$	0.3556	0.462
ε_f	0.6677	0.6988
$d_{b,\delta}$	0.1321	0.079
$d_{b,\varepsilon}$	0.1718	0.1189

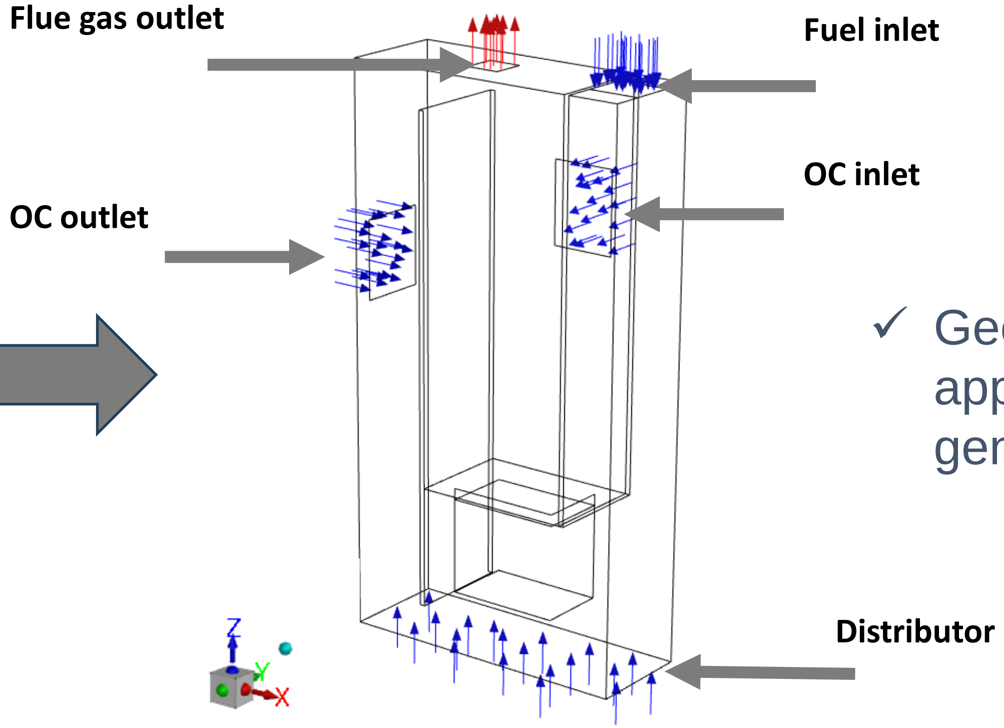


Contour plot of volume fraction of solid phase within the reactor. Average cell value is presented.

Based on the results, when using non-uniform porosity, we can capture the reduction of the average bubble size, but we cannot capture the increase in rate, which comes with the use of packings

10 kW$_{th}$ CTH fuel reactor

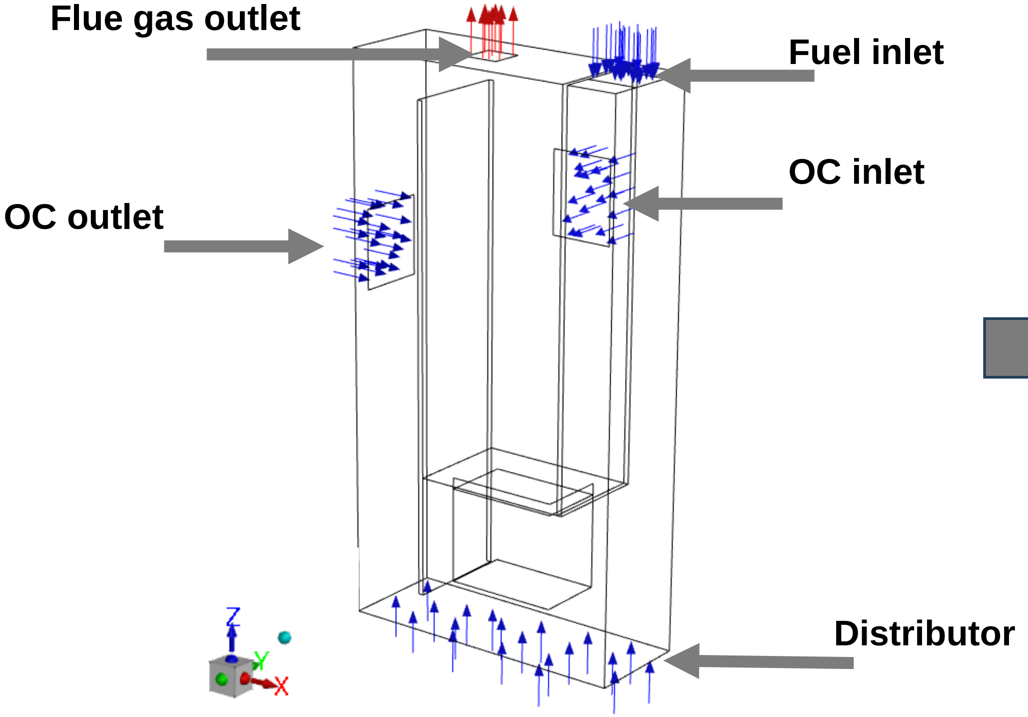


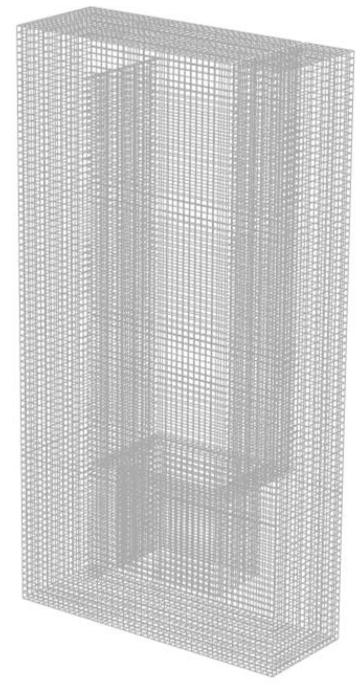


- ✓ Geometry simplifications applied to facilitate grid generation!

10 kW$_{th}$ CTH fuel reactor

Computational grid





- ✓ 70000 hexahedral cells
- ✓ 5 mm average cell length
- ✓ Ratio $\frac{D_{cell}}{d_p} \cong 20$
- ✓ This means that the **Gidaspow** drag model can be used (i.e no need for EMMS)

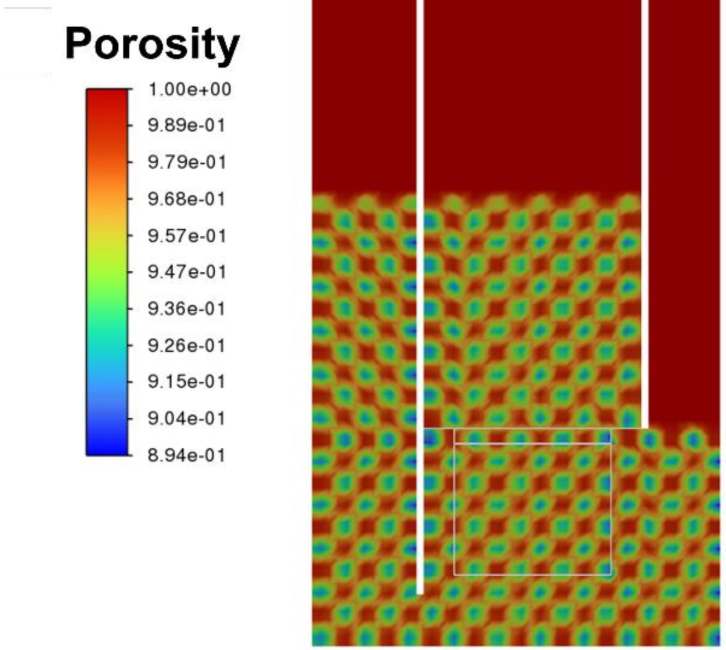
10 kW$_{th}$ CTH fuel reactor

Simulated cases

- ✓ Circulation was unknown and calculated for the “LowCirc” case so that the incoming oxygen suffices to completely “burn” the fuel!

Case ID	Circulation flux (kgh^{-1})	Packings
LowCirc	81.72	No
HighCirc	163.44	No
HighCircPack	163.44	Yes

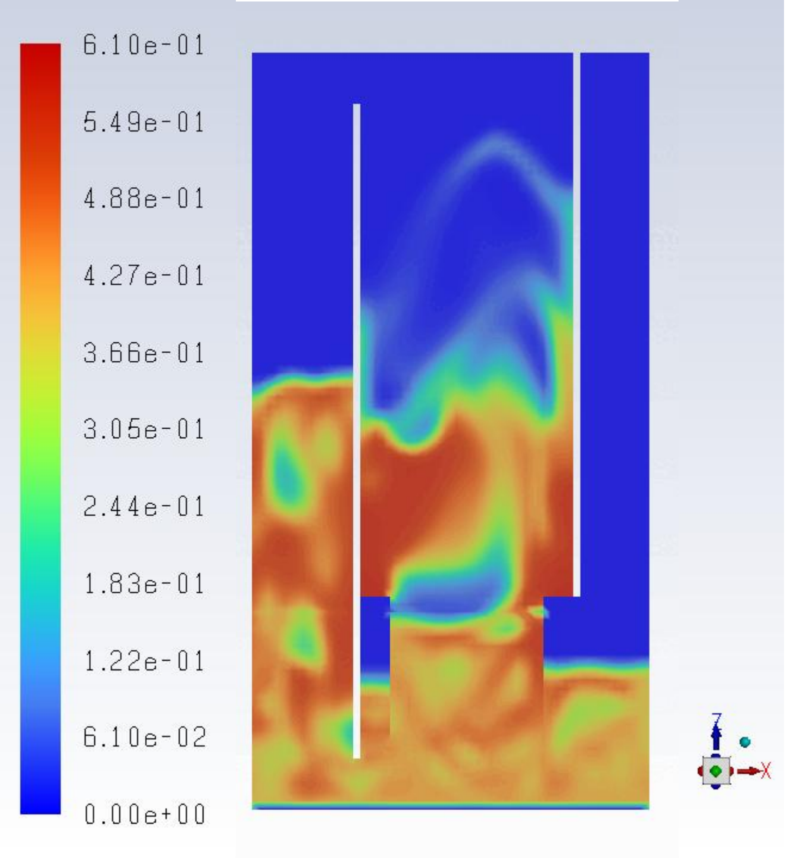
Applied non-uniform porosity field



10 kW$_{th}$ CTH fuel reactor

Results – Fluidization –LowCirc Case

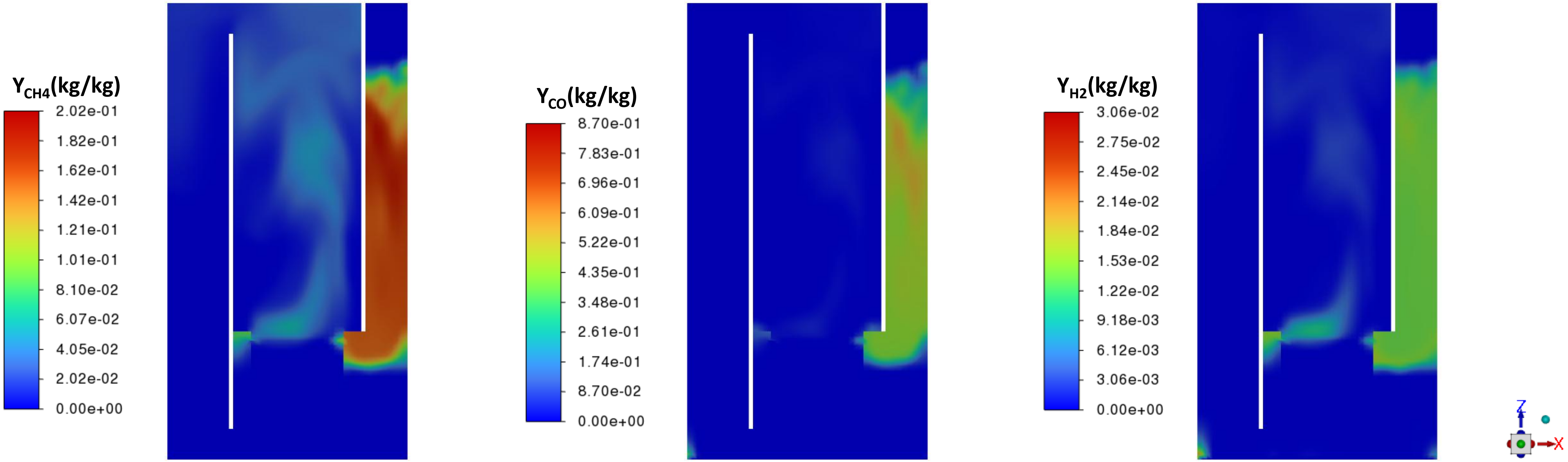
Volume fraction of OC



- ✓ **Average OC inventory: ~4.9kg**

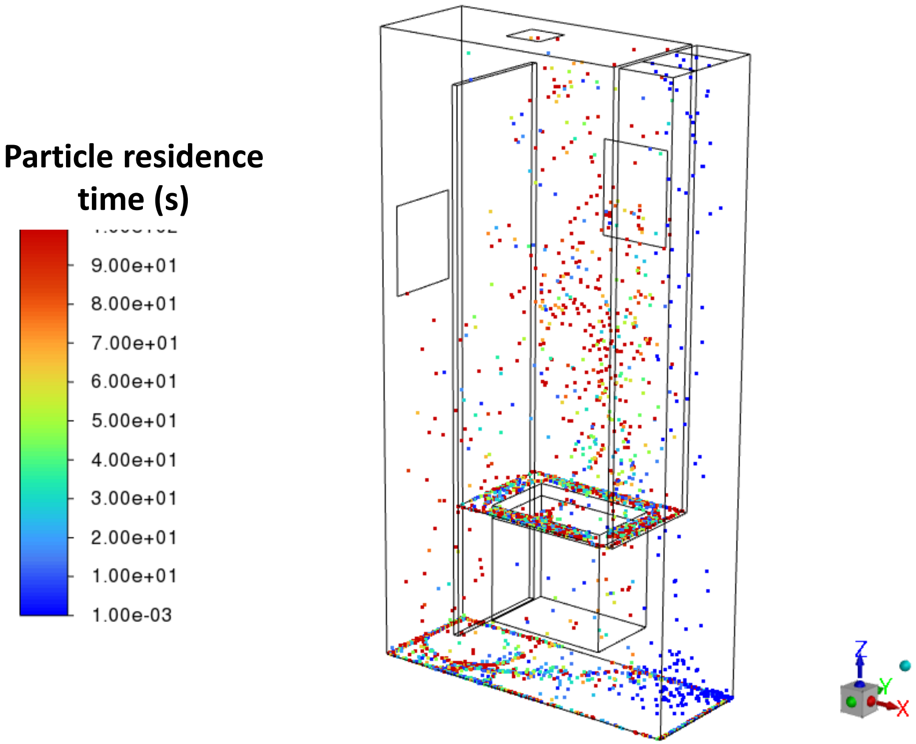
10 kW_{th} CTH fuel reactor

Results – Contours of combustible volatiles for the LowCirc Case



10 kW$_{th}$ CTH fuel reactor

Results – Fuel particles



Instantaneous picture at t = 100s for LowCirc case

Case ID	Avg. Fuel Residence Time (s)	Char Gasified (%)	% of fuel particles exiting via OC outlet
LowCirc	66	72.5	55
HighCirc	40	66	70
HighCircPack	45	66.8	70

10 kW$_{th}$ CTH fuel reactor

Results – Combustion efficiency

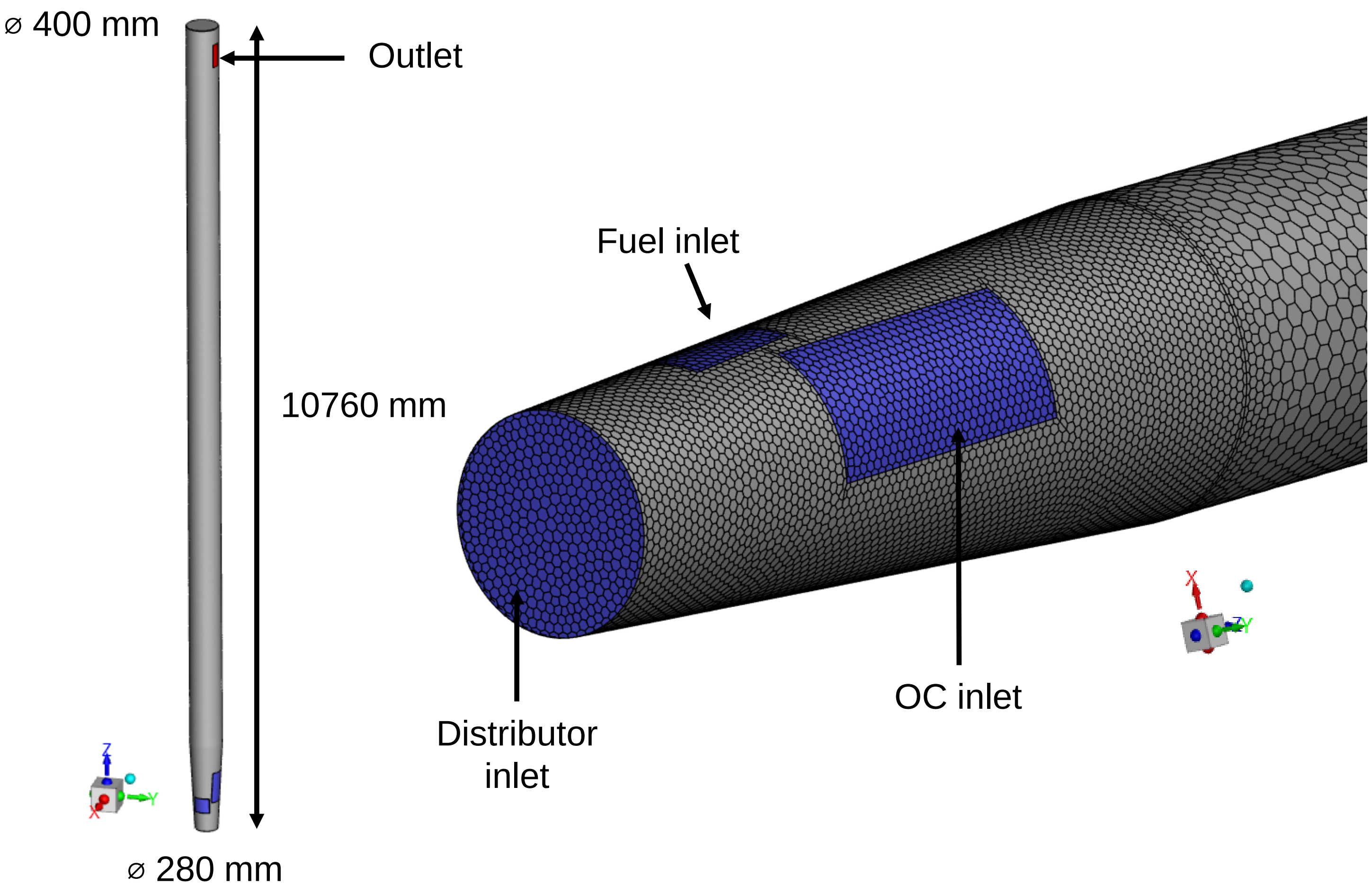
- ✓ O_2 – based efficiency metric defined as:

$$1-\frac{O_{flue-gas}}{O_{fuel}}$$

$\boldsymbol{O_{fuel}}$: stoichiometric O_2 required to fully oxidize the incoming fuel (as fed)
$\boldsymbol{O_{flue-gas}}$: stoichiometric O_2 still required to fully oxidize the *outlet stream* (flue gas plus entrained unburned particles/char

Case ID	Inventory (kg)	O_2-Based Efficiency (%)
LowCirc	4.9	71.7
HighCirc	4.9	73
HighCircPack	4.9	73

1MWth TUDA fuel reactor



Simulated cases:

- **TUDA-85:** Fixed inventory at 85kg
- **TUDA-160:** Fixed inventory at 160 kg

- ✓ 76000 polyhedral cells
- ✓ 5 mm average cell length
- ✓ Ratio $\frac{D_{cell}}{d_p} \cong 330$
- ✓ This means that the **EMMS drag model should be used!!!**

1MWth TUDA fuel reactor

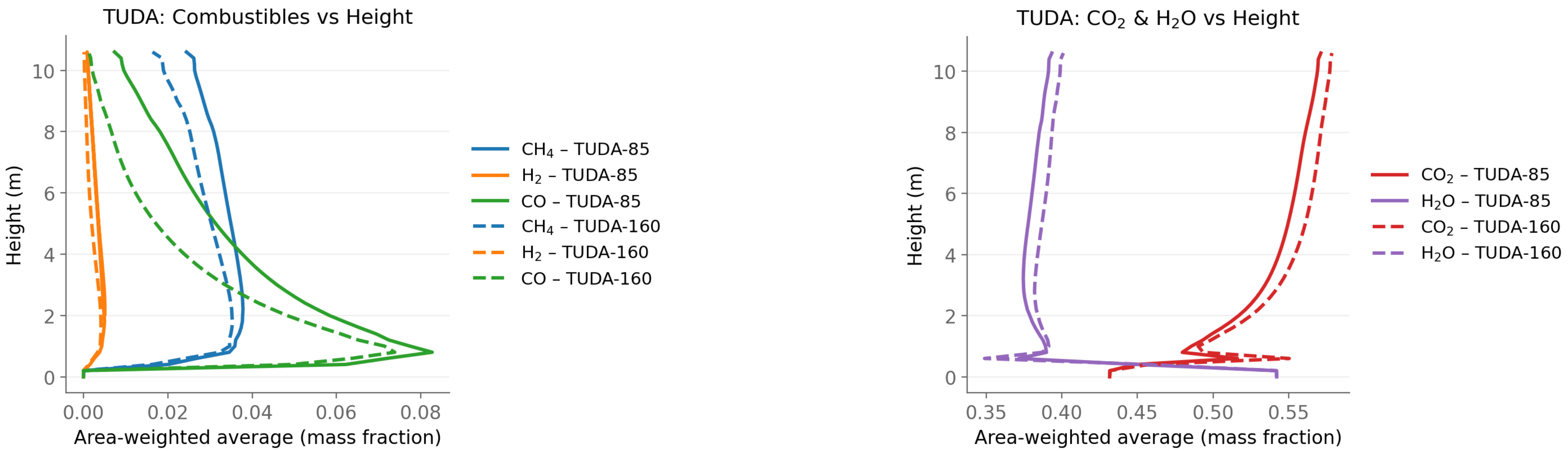
Results – Combustion efficiency

Case ID	Inventory (kg)	Circulation (kg/h)	Avg. OC Residence Time (s)	Avg. OC Conversion (%)	Char Gasified (%)	O_2-Based Efficiency (%)
TUDA-85	85	150000	2	1	92	21
TUDA-160	160	202484	2.9	1	91	71

- ✓ Importance of inventory is highlighted. The case with the higher inventory (TUDA-160) shows best conversion.
- ✓ Reason: Increased inventory → Increased chances of contacting the fuel combustible volatiles

1MWth TUDA fuel reactor

Results – AWA profiles of gas species



✓The higher efficiency with increased inventory is reflected in higher CO_2 and H_2O levels and lower concentrations of combustibles along height.

CONCLUSIONS AND FUTURE WORK

- The bubbling bed CTH reactor simulations have shown that the limiting factor is the residence time of fuel and volatiles.
- In the bubbling bed CTH reactor volatile conversion improved with the increase of the circulation.
- The increased circulation in the CTH reactor reduced the fuel particle's residence time thus reducing char conversion.
- The packings did not show any decrease in bubble size.
- In the circulating bed reactor of TUDA the value of inventory was shown to be a crucial parameter.
- Future work includes verification with the experimental results. The CFD models will be rerun at the exact conditions of the experiments.

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Thank you

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