Detailed Numerical Three-dimensional and Transient Analysis of a Grate Firing Combustion Process by Innovative High Performance Computing

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1. CFD-XDEM coupling
2. Biomass furnace design and setup
3. Chemical reactions
4. Preliminary results
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6. Summary

XDEM = Extended Discrete Element Method

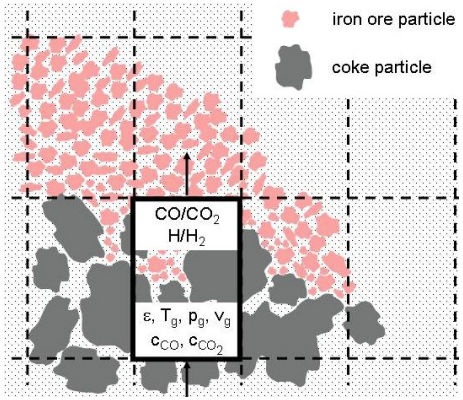
Multi-physics simulation toolbox

Dynamics (particle motion)

Snow, Sand, Wood, …

Thermodynamics

Coke, Iron, Biomass, …



\+ coupling with external libraries: CFD with OpenFOAM, FEM with Diffpack

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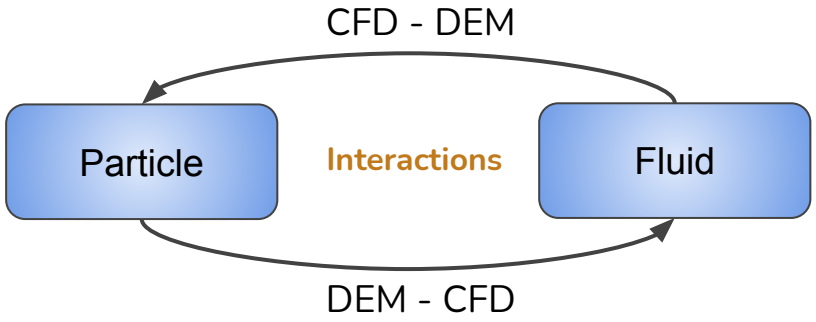
DEM-CFD coupling

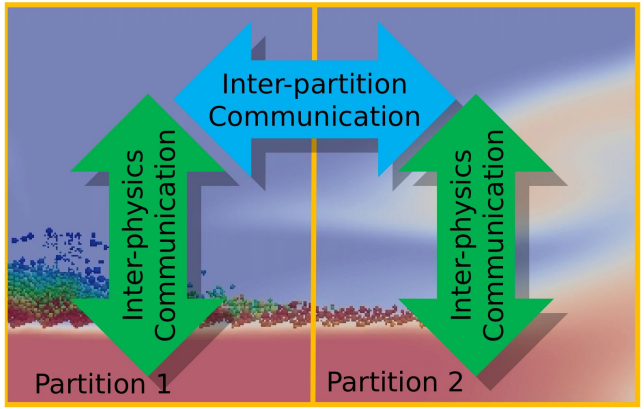


2-way coupling approach

(X)DEM for:

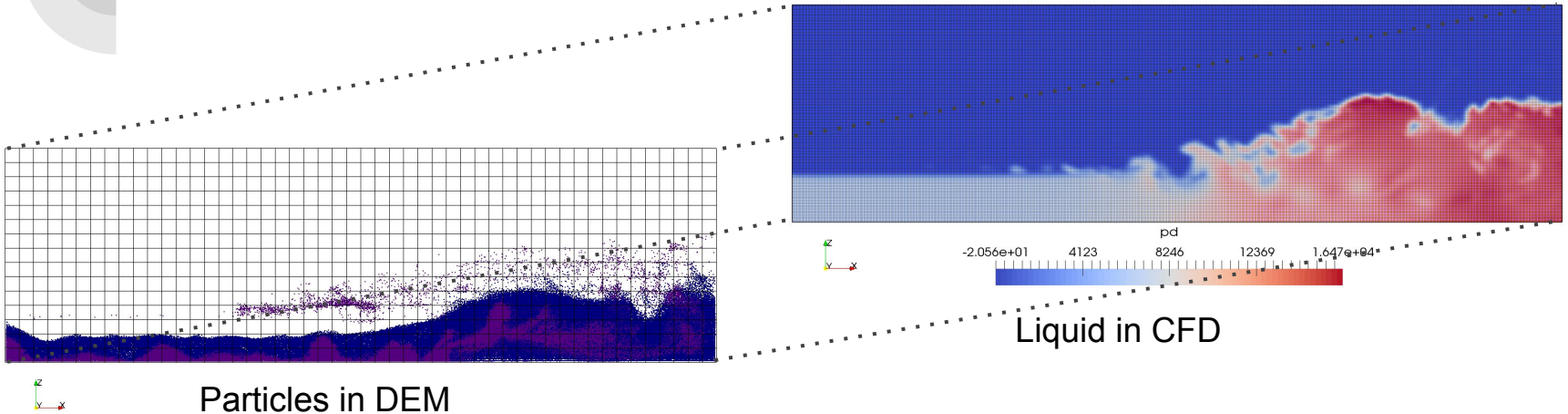
- wood particles motion (Lagrangian approach)
- Conversion (thermodynamics state)

OpenFOAM for gas phase (Eulerian approach)



CFD-(X)DEM Coupling

Moving particles interacting with fluid (gas+liquid)



From CFD to DEM

- Lift force (buoyancy)
- Drag force
- Heat and mass transfer

From DEM to CFD

- Porosity
- Particle source of momentum
- Heat and mass transfer

Biomass furnace design

Enel Green Power ”Cornia 2” power plant

16MW combustion chamber

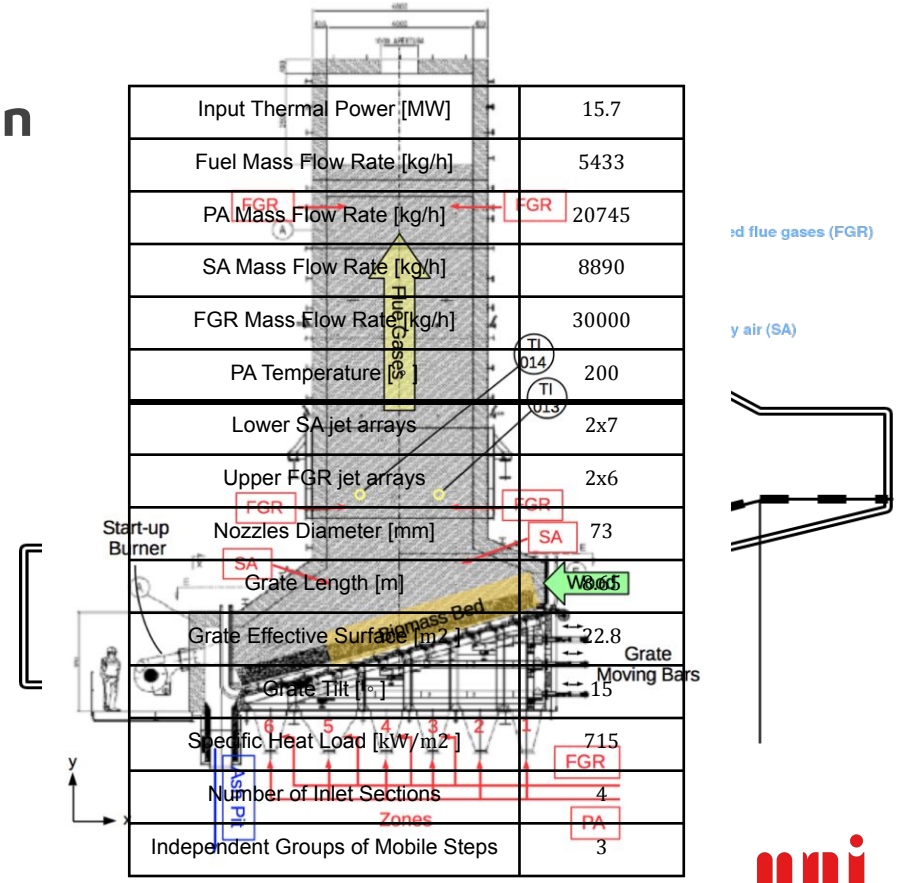
Three different moving grates

Primary Air injection (PA)

Secondary Air injection (SA)

Flue Gas Recirculation (FGR)

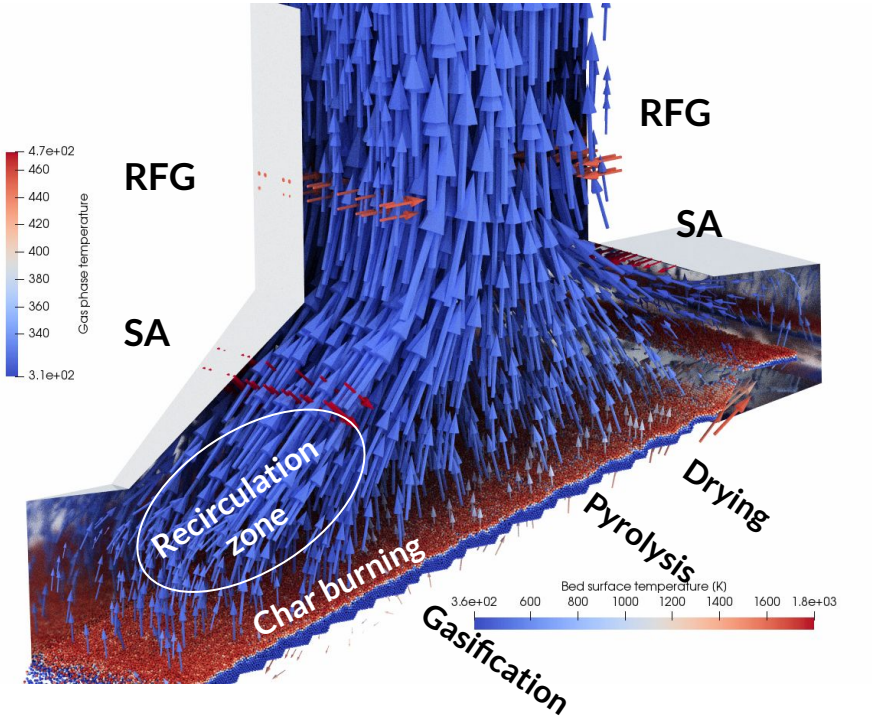
Ash pit



Chemical reactions

- **Biomass conversion**
  - **Drying:** evaporation of bound water
  - **Pyrolysis**(3 reactions): Wood ⇒ Char, tar, H2, CH4
  - **Gasification**: Char ⇒ CO, CO2
- **Freeboard conversion**
  - Tar → light gases (CO, H2O)
  - CH4 ⇒ CO2, H2O
  - CO ⇒ CO2
  - H2 ⇒ H2O
- Arrhenius approach chemical kinetics

- **Energy conservative** scheme from solid to gas phase reactions



Numerical approach

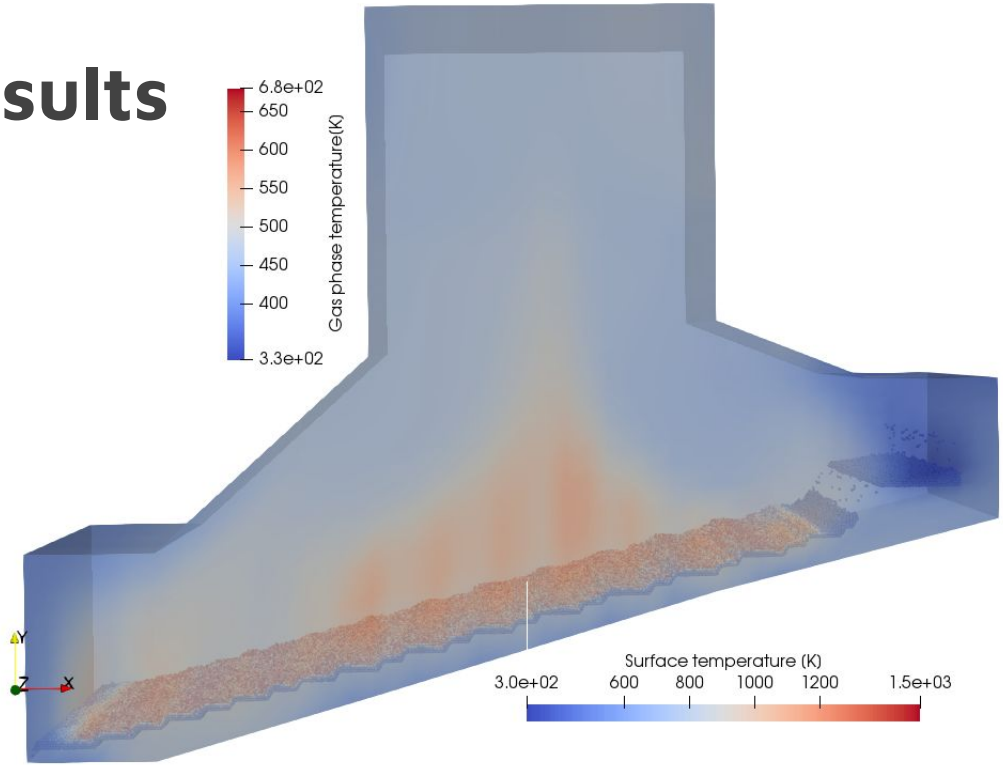
- Coupling of XDEM-OpenFOAM
- Multi-phase, multi-scale and multi-species approach
- DEM for particles motion on forward acting grates
- XDEM → thermal conversion(Radiation + Conduction + Conversion)
- CFD for gas flow in void space of moving bed
- Interaction between solid and gas phase through
  - Heat transfer
  - Mass transfer
  - Momentum transfer
- Simultaneous coupling between solid and fluid phase

- ~300.000 particles
- 100.000 DEM cells
- 88470 CFD cells

Preliminary results

Bed surface average temperature

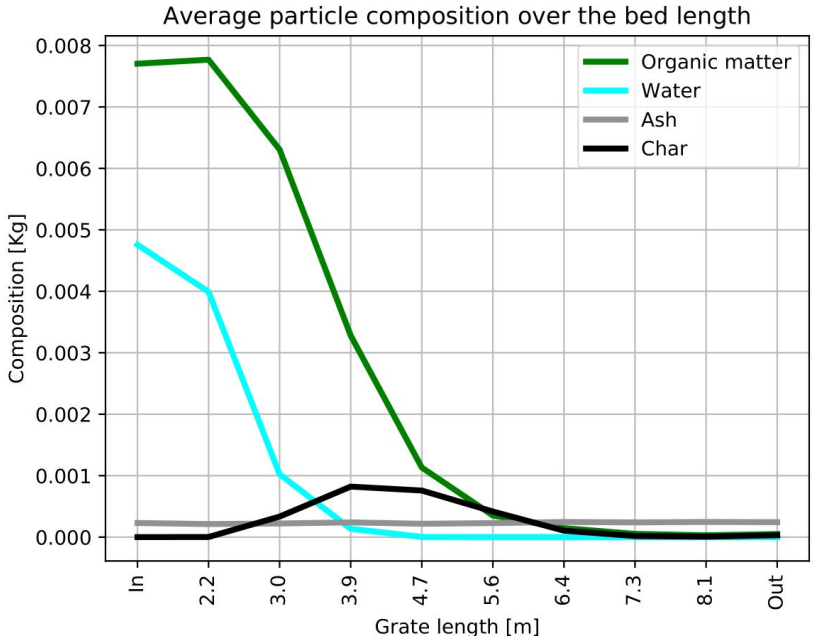
1. Heat up
2. Pseudo-steady state
3. Gas streaks oscillation
4. Unpredictable gas streaks with freeboard-only approach



Preliminary results

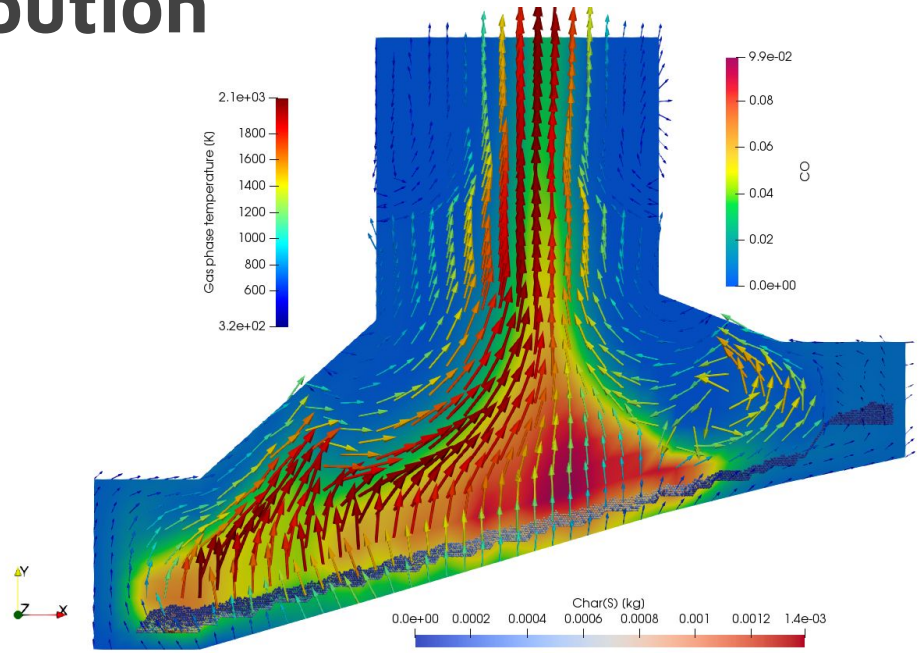
Particle average composition

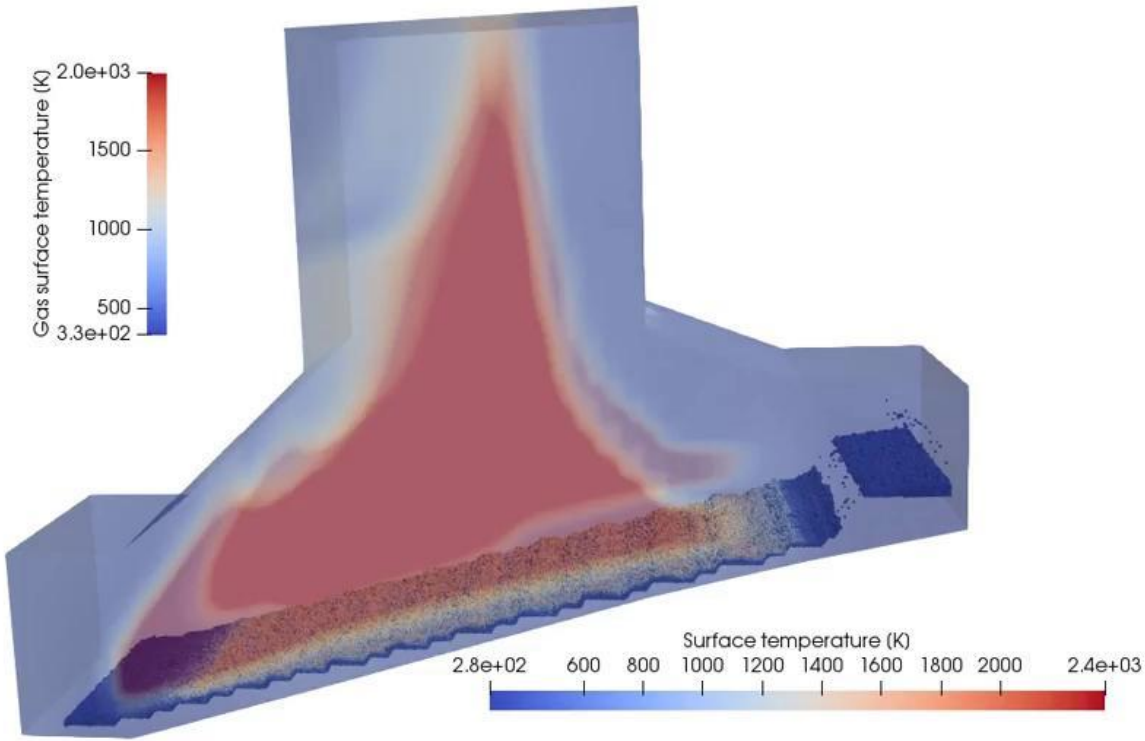
- Drying process (complete)
- Combustion
- Char production+burning



Species distribution

- ➔ Gas phase temperature
- ➔ CH4[Kg] and Tar
- ➔ C02[Kg] and Char
- ➔ CO2[Kg] and Organic matter
- ➔ C0[Kg] and Char




Gas surface temperature (K)
2.0e+03
1500
1000
500
3.3e+02
Surface temperature (K)
2.8e+02
600
800
1000
1200
1400
1600
1800
2000
2.4e+03

Parallelization: Direct coupling approach

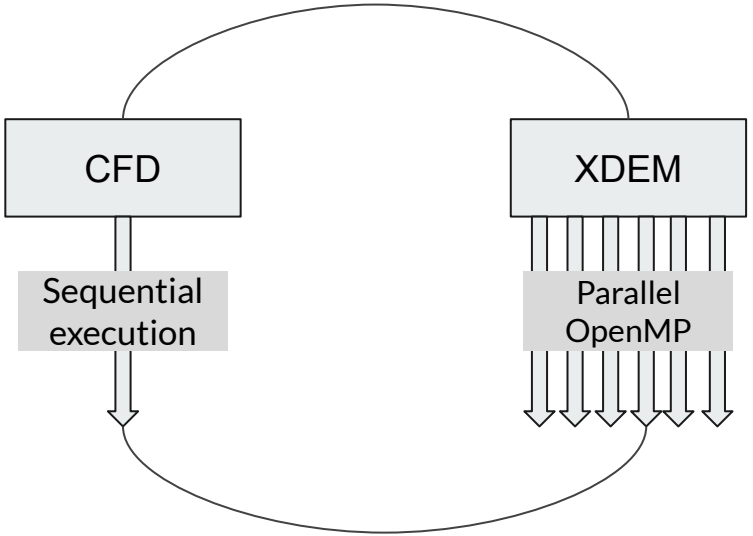
XDEM+OpenFOAM linked in shared memory

XDEM ⇒ Multi-threaded approach

OpenFoam ⇒ Sequential

Work in progress:

- Hybrid (MPI+OpenMP) XDEM
- MPI OpenFOAM

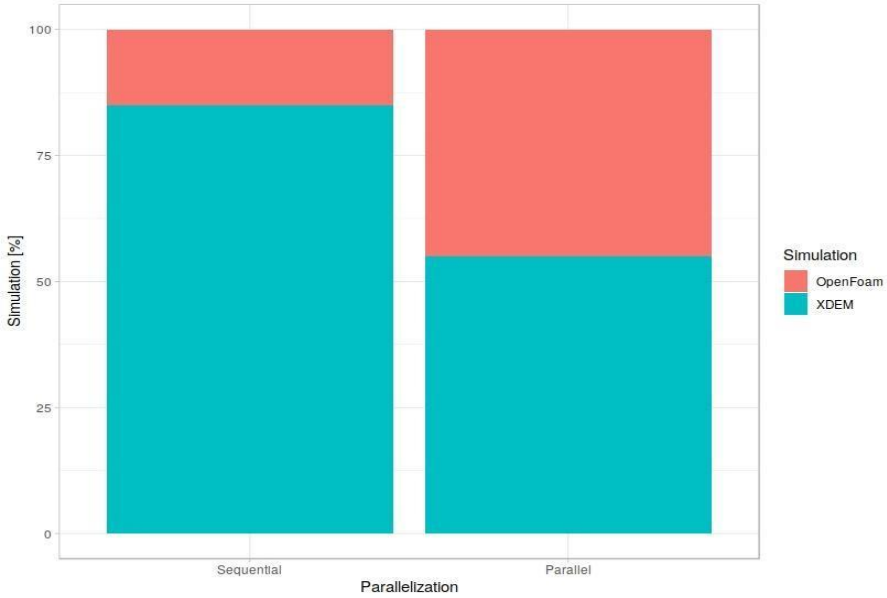


Performance analysis

Sequential vs parallel simulations

UL HPC facilities ⇒ 1 node = 28 cores

- Seq: 80% XDEM vs 20% Openfoam
- Multi-threading: 55% XDEM vs 45% Openfoam



https://hpc.uni.lu/

Conclusion

Average of 58% of char and 42% of ashes by wt.

Unburnt carbon (5% of dried biomass)

Consistent with sampling data from industrial plant

Ability to predict gas flux behaviour (recirculation) and thermal field

3D real plant scale for practical use

Runs in parallel

Heavy in computational time (multi-scale, phase and species)

23 days for a complete simulation (2500 sec)

Parallel implementation and flexibility (MPI+OpenMP)

Thank you for your attention

Chemical reactions

- **Pyrolysis** in three different reactions:

$$\text{wood} \longrightarrow \text{char} \qquad \text{wood} \longrightarrow \text{tar}$$

$$\text{wood} \longrightarrow \nu\text{CO} + \nu\text{CO2} + \nu\text{H2O} + \nu\text{H2} + \nu\text{CH4}$$

$$wood \longrightarrow \nu_{CO} CO + \nu_{CO2} CO2 + \nu_{H20} H2O + \nu_{H2} H2 + \nu_{CH4} CH4$$

- Tar subjected to a **crack reaction** → light gases

$$tar \longrightarrow \gamma_{tar_{inert}} tar_{inert} + \gamma_{CO} CO + \gamma_{CO2} CO2 + \gamma_{H2} H2 + \gamma_{CH4} CH4$$

- **Combustion**:

$$\text{CO} + 0.5\text{O2} \longrightarrow \text{O2} \qquad \text{CH4} + 2\text{O2} \longrightarrow \text{CO2} + 2\text{H2O}$$

$$2\text{H2} + \text{O2} + \text{H2O} \qquad \text{tar} + 2.9\text{O2} \longrightarrow 6\text{CO} + 3.1\text{H2}$$

- **Gasification** and **combustion**:

$$\text{C(s)} + \text{O2} \longrightarrow 2(\Omega\text{ -1})\text{CO} + (2\text{-}\Omega)\text{CO2} \qquad \text{C(s)} + \text{H2O} \longrightarrow \text{CO} + \text{H2}$$

$$\text{C(s)} + \text{CO2} \longrightarrow 2\text{CO}$$

Operating conditions

ar = as received
daf = dry ash free

80% of woodships
20% of agricultural residuals

Properties	Woodchips	Residues	Mixture
Mix fraction [%wt,ar]	80	20	100
LHV [MJ/kgar]	11.3	7.4	7.4
Granulometry range [mm]	-	-	5400
Average particle size [mm]	-	-	15
Moisture [%wt, ar]	34.0	51.0	37.4
Volatiles [%wt, ar]	53.7	35.6	50.1
Fixed carbon [%wt, ar]	11.3	8.3	10.7
Ashes [%wt, ar]	1.0	5.1	1.8
Carbon [%wt, daf]	49.60	51.15	49.82
Hydrogen [%wt, daf]	5.95	6.23	5.99
Oxygen [%wt, daf]	44.23	41.67	43.86
Nitrogen [%wt, daf]	0.22	0.95	0.33