CFD-DEM modeling of the formation of producer gas contaminants during biomass gasification

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Biomass gasification overview

Biomass Gasification: the thermal decomposition of biological materials at sub-stoichiometric oxygen levels, generating producer gas (CO, H_2, CO_2, and CH_4).

Downstream applications

- Fischer–Tropsch synthesis
- Methanol synthesis
- Internal combustion engines
- Steam turbines
- Gas turbines

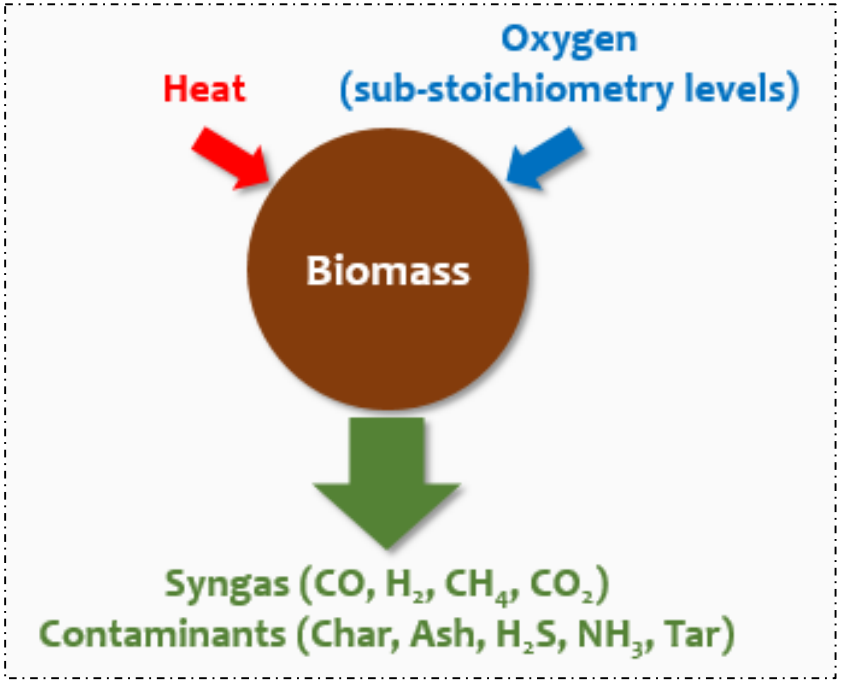


Fig. 1: Biomass gasification process.

Biomass gasification mechanism

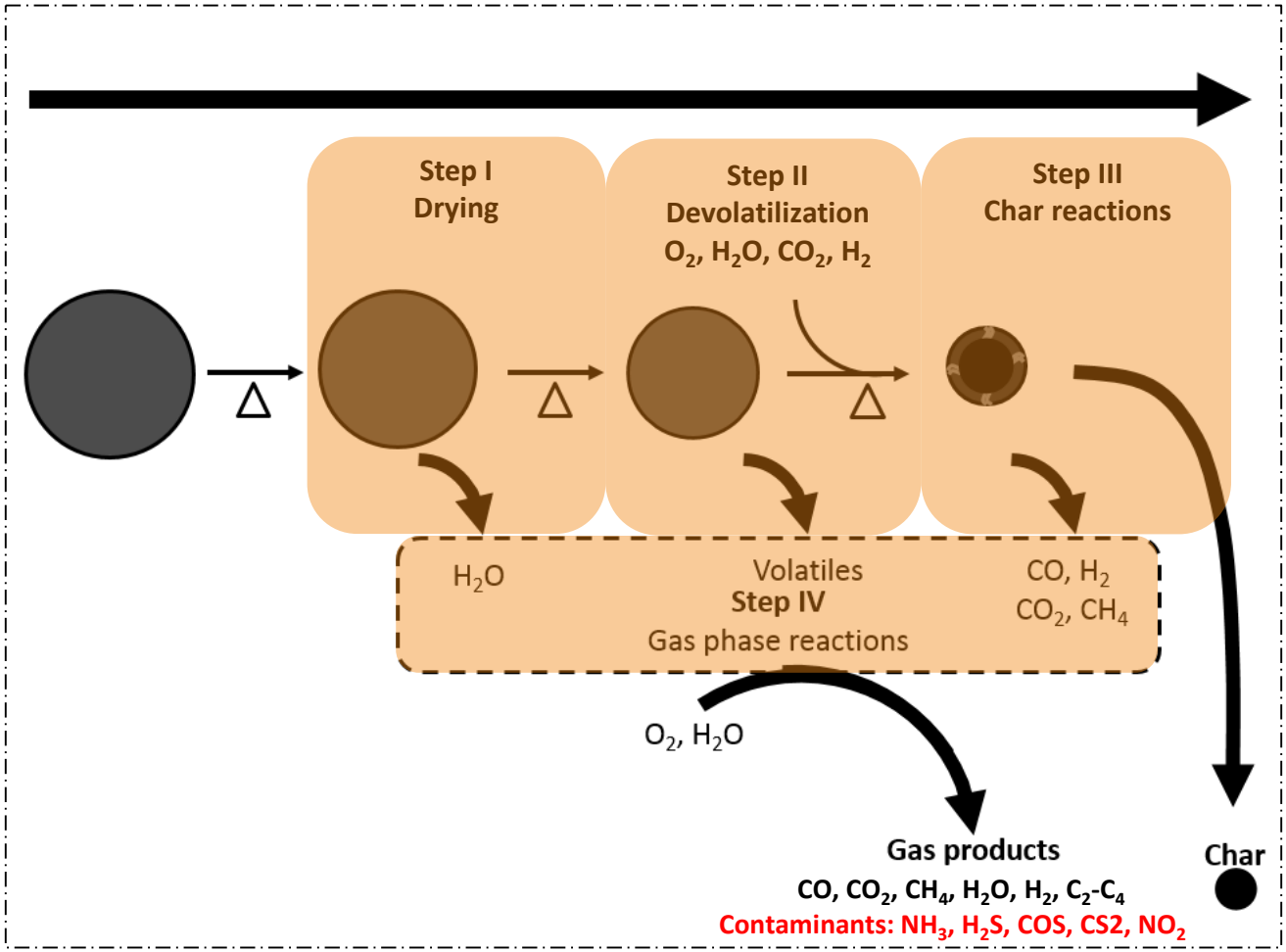


Fig. 2: Gasification flow diagram.

Basu, 2010
Abdoulmoumine et al., 2015

Problem statement

Contaminants present in producer gas reduce its usefulness.

- Foremost challenge for biomass gasification projects
- Downstream catalyst deactivation concerns and air pollution issues
- Additional cost for producer gas cleanup process

Objective: Develop a CFD-DEM numerical model to simulate the formation of producer gas and nitrogen contaminants (HCN and NH_3) during biomass gasification.

Simulation approach

OpenFOAM was used in this work.

Methodology was based on Eulerian-Lagrangian framework

Materials simulated were gas, biomass particles, and sand particles

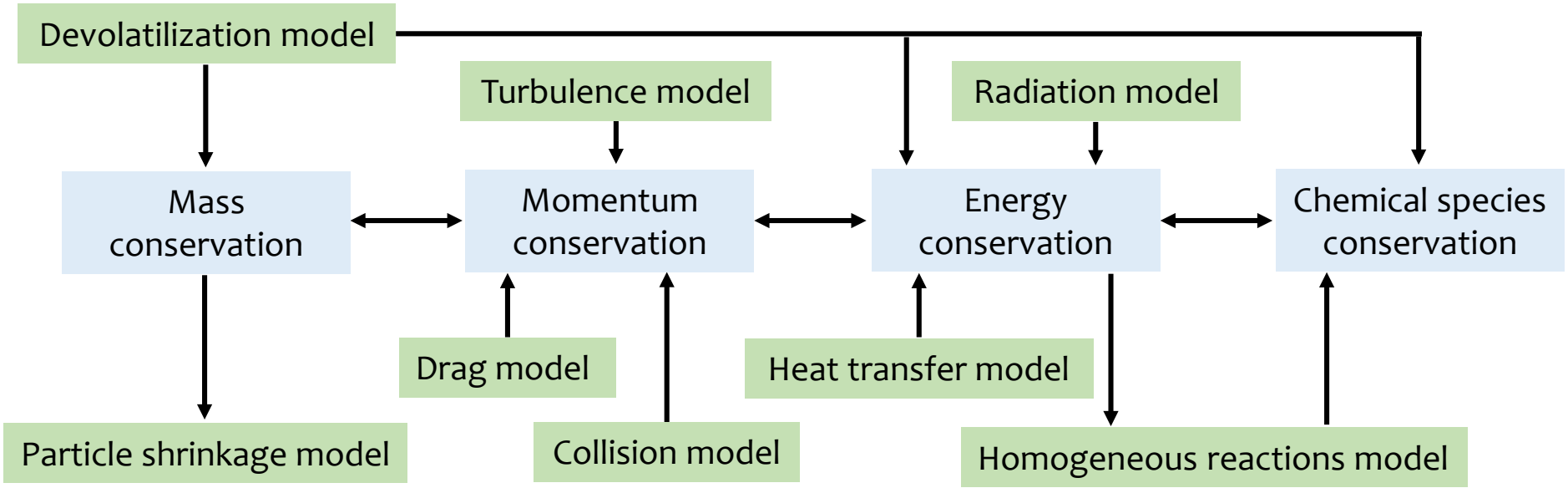


Fig. 3: Models and sub-models needed in the CFD framework

Method: Gas phase equations

Mass conservation

$$\frac{\delta}{\delta t}\left(\varepsilon_g \rho_g\right) + \nabla \cdot \left(\varepsilon_g \rho_g \mathbf{U}_g\right) = S_\rho$$

Energy conservation

$$\frac{\delta}{\delta t}\left(\varepsilon_g \rho_g E\right) + \nabla \cdot \left(\varepsilon_g \mathbf{U}_g (\rho_g E + p)\right) = \nabla \cdot \left(\varepsilon_g \alpha_{eff} \nabla h_s\right) + S_h + S_{p,h} + S_{rad}$$

Momentum conservation

$$\frac{\delta}{\delta t}\left(\varepsilon_g \rho_g \mathbf{U}_g\right) + \nabla \cdot \left(\varepsilon_g \rho_g \mathbf{U}_g \mathbf{U}_g\right) = -\nabla p + \nabla \cdot \left(\varepsilon_g \boldsymbol{\tau}\right) + \varepsilon_g \rho_g \mathbf{g} + S_m$$

Chemical species conservation

$$\frac{\delta}{\delta t}\left(\varepsilon_g \rho_g Y_i\right) + \nabla \cdot \left(\varepsilon_g \rho_g \mathbf{U}_g Y_i\right) = \nabla \cdot \left(\varepsilon_g \rho_g D_{eff} \nabla Y_i\right) + S_{p,Y_i} + S_{Y_i}$$

ε_g	Gas volume fraction
ρ_g	Gas density
$\mathbf{U}_g$	Gas velocity
S_p	Mass source
$\boldsymbol{\tau}$	Stress tensor
S_m	Momentum source
E	Energy
p	Pressure
α_{eff}	Thermal diffusivity
S_h source	Reaction enthalpy
$S_{p,h}$	Particle enthalpy source
S_{rad}	Radiation source
Y_i	Species mass fraction
D_{eff}	Mass diffusion constant
S_{p,Y_i}	Particle species source
S_{Y_i}	Reaction species source

Method: Particle and reaction models

Table 3. Models used to describe particles and chemical reactions behaviors.

Behavior	Model used
Turbulence mixing	k-ε turbulence model
Heat transfer	Nusselt model
Particle collision	Spring-slider-damper model
Particle drag force	Gidaspow model
Homogenous reactions	Arrhenius model
Heterogeneous reactions	Diffusion limited Arrhenius model
Particle shrinking	Mass-proportional shrinkage model

Heterogeneous reaction

$$C + H_2O \rightarrow CO + H_2$$

$$C + CO_2 \rightarrow 2CO$$

Homogenous reaction

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

$$H_2 + O_2 \rightarrow H_2O$$

$$CH_4 + H_2O \rightarrow CO + 3H_2$$

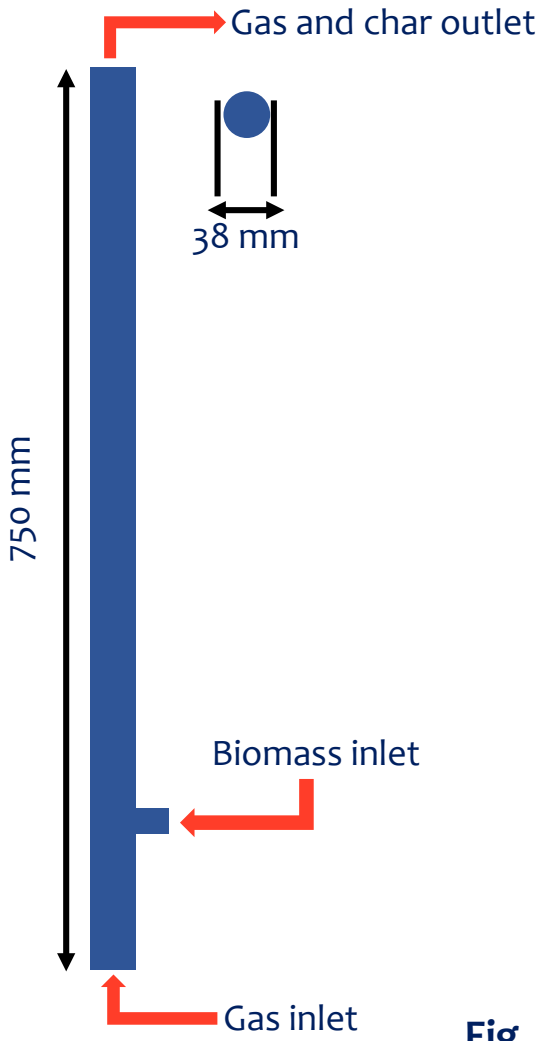
$$2CO + O_2 \rightarrow 2CO_2$$

$$CO_2 + H_2 \rightarrow CO + H_2O$$

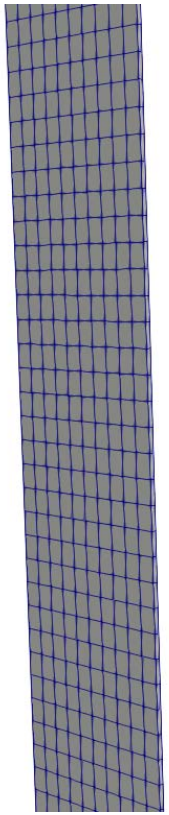
$$HCN + H_2O \rightarrow NH_3 + CO$$

$$2NH_3 \rightarrow N_2 + 3H_2$$

Method: Meshing



Mesh statistics:



Number of points	= 3300
Number of faces	= 6119
Max aspect ratio	= 5.765
Min. face area	= 3.81e-06 m^2
Max. face area	= 1.94e-05 m^2
Min. volume	= 1.91e-08 m^3
Max. volume	= 1.94e-08 m^3
Max. non-orthogonality	= 0.000
Max. skewness	= 1.33e-13

Fig. 4: Reactor geometry and meshing.

Method: CFD parameters settings

Table 6. Proximate Analysis of Biomass

Component	Mass percent
Moisture Content	12.00
Ash Content	4.31
Volatile Matter Content	82.27
Fixed Carbon Content	13.42

*Moisture content values are on wet basis and all other values are on dry basis.

Table 7. Gas composition of volatile gas

Gas component	Mass fraction
CH_4	0.100
H_2	0.024
CO_2	0.198
CO	0.619
H_2O	0.050
HCN	0.005
NH_3	0.003

Oevermann et al. 2010
Abdoulmoumine et al., 2014

Results: Gas phase physical variable

https://www.youtube.com/watch?v=KkT1gvxtbY0

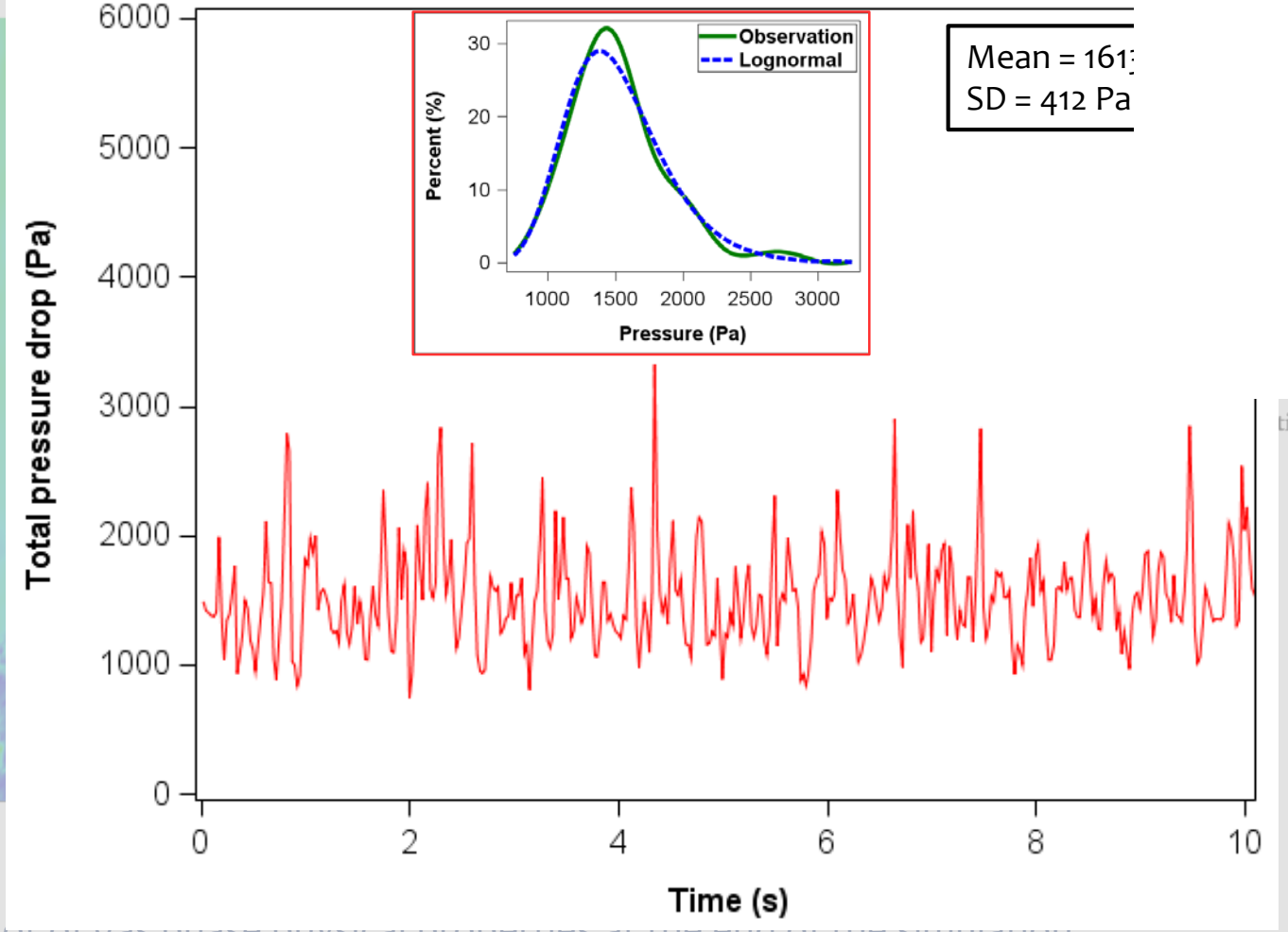


Fig. 5: Snapshot of gas phase physical properties at the end of the simulation.

Results: Gas phase chemical variables

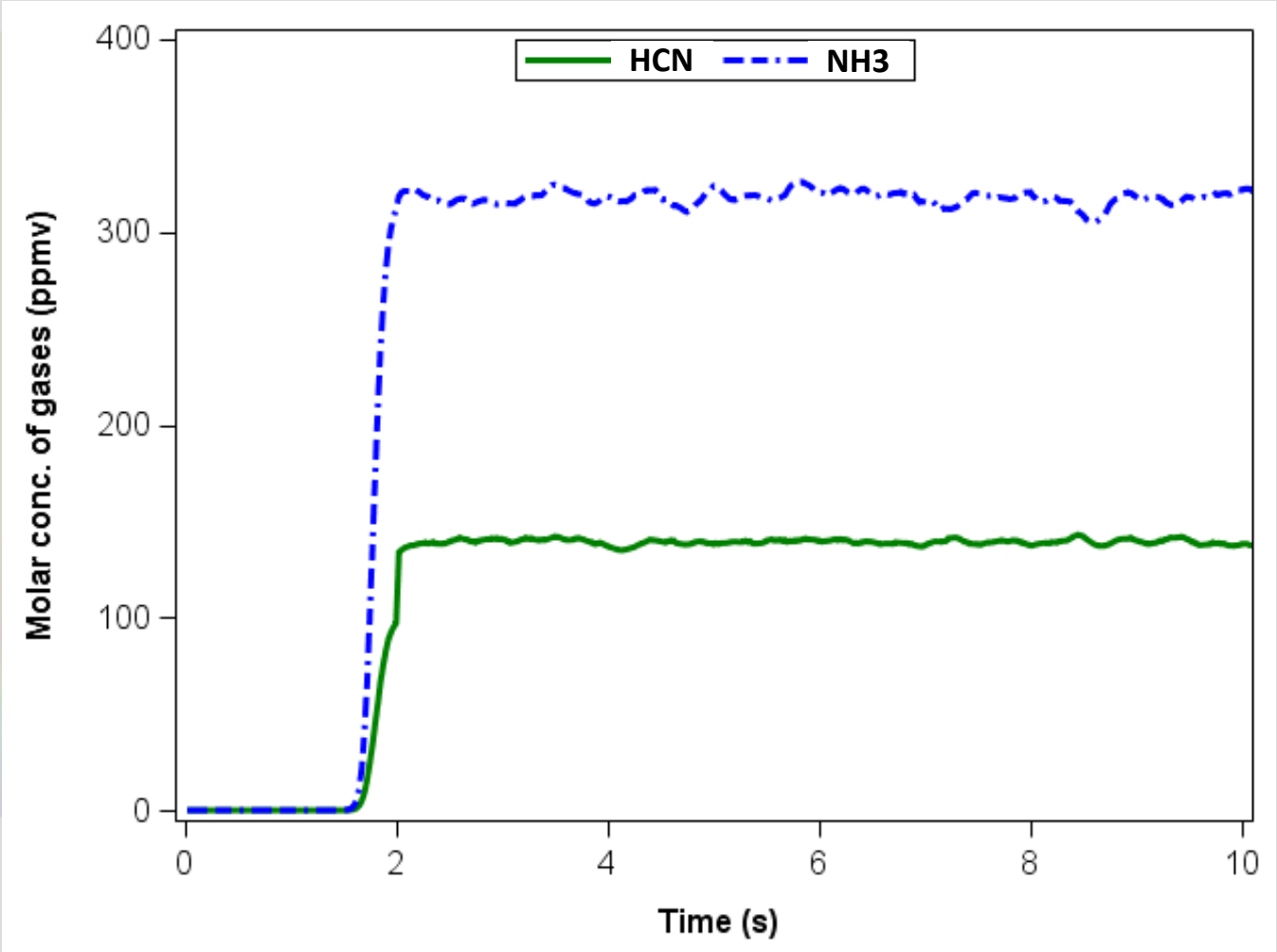


Fig. 6: Snapsh

Results: Biomass particle tracking

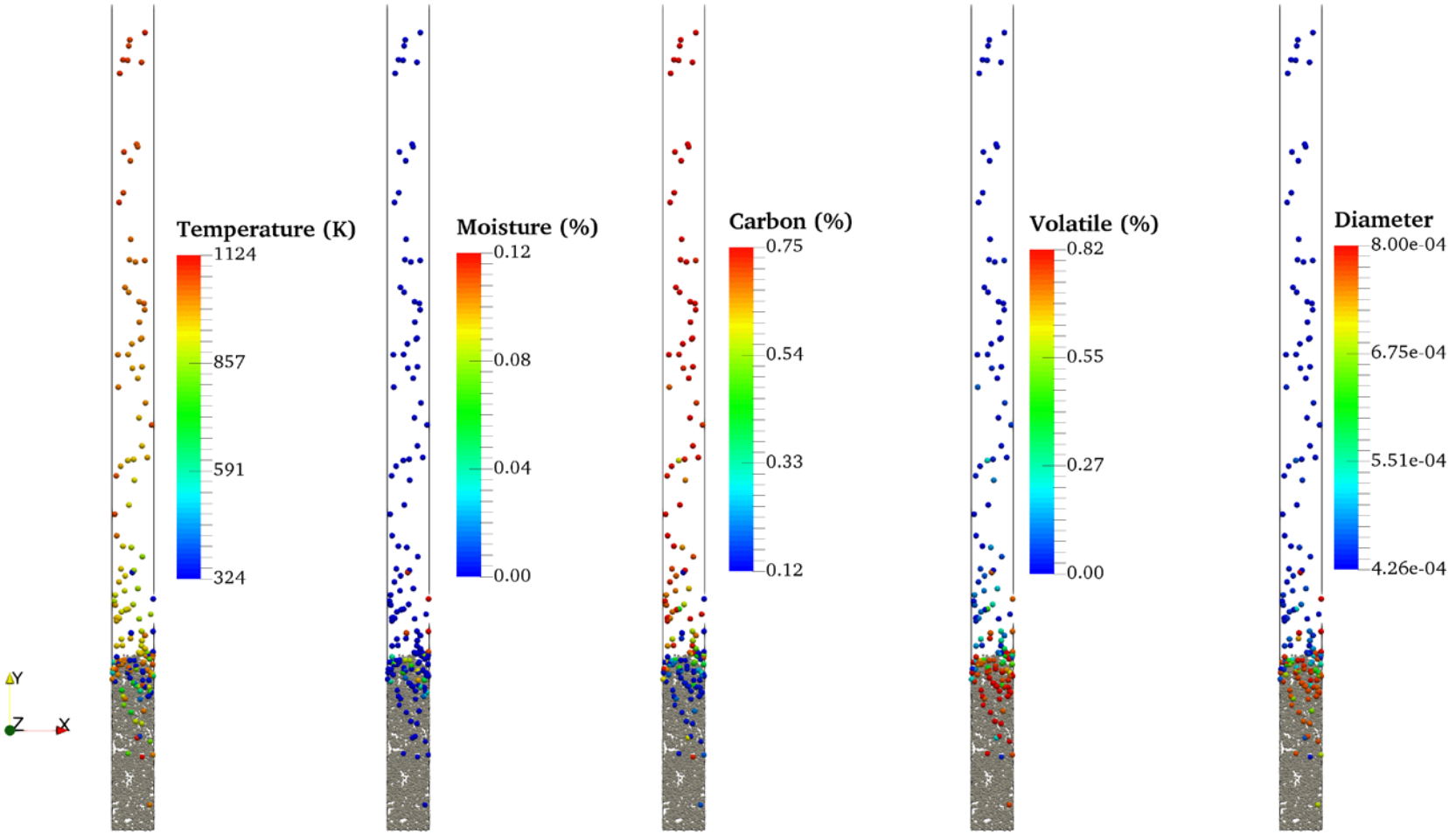


Fig. 7: Snapshot of biomass properties at the end of the simulation.

Conclusions

- Biomass gasification was simulated in an Eulerian-Lagrangian framework using OpenFOAM.
- Biomass particle properties and positions were tracked.
- Steady-state was achieved at approximately 2 s.
- The average pressure drop along the reactor height was approximately 1613 Pa at 0.5 m/s superficial air velocity.
- NH_3 and HCN concentrations were obtained. NH_3 concentration was higher than HCN concentration.
- In future works, different operating conditions will be simulated to established trends and validated.

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THANK YOU!

QUESTIONS?