Three-dimensional simulation of sorbent enhanced gasification

July 2020

Kari Myöhänen

LUT University

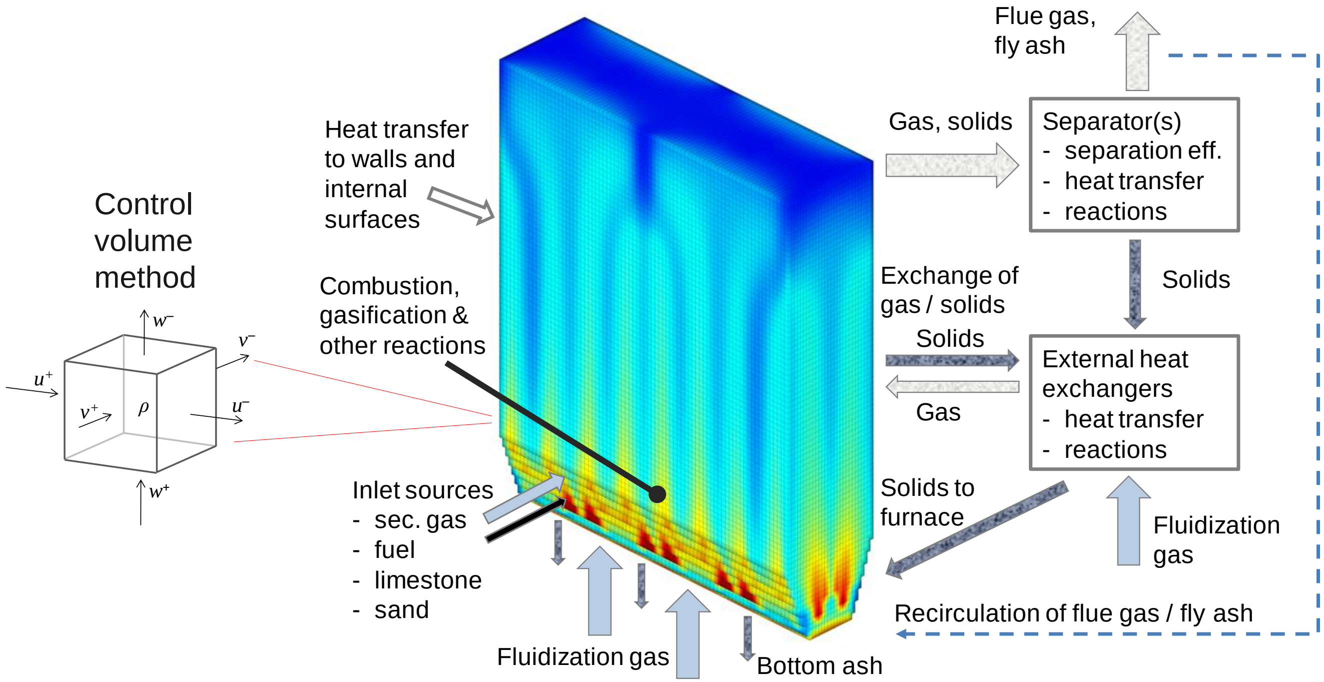
Introduction

- In the FLEDGED project, models at different scales have been developed for sorbent enhanced gasification (SEG).
  - 0D-model => fast
  - 1D-model => more detailed
  - 3D-model => mixing in large scale
- The following presents 3D model results of a 100 MWth SEG unit in a reference point (OP1).
  - Fuel: wood pellets, LHV_{af} 16 MJ/kg,
    feed 6.58 kg/s (gasifier) / 0.07 kg/s (combustor)
  - Molar C/S-ratio 1.50.
  - Fluidization velocity approx. 4.5 m/s.
  - Module M = 2.

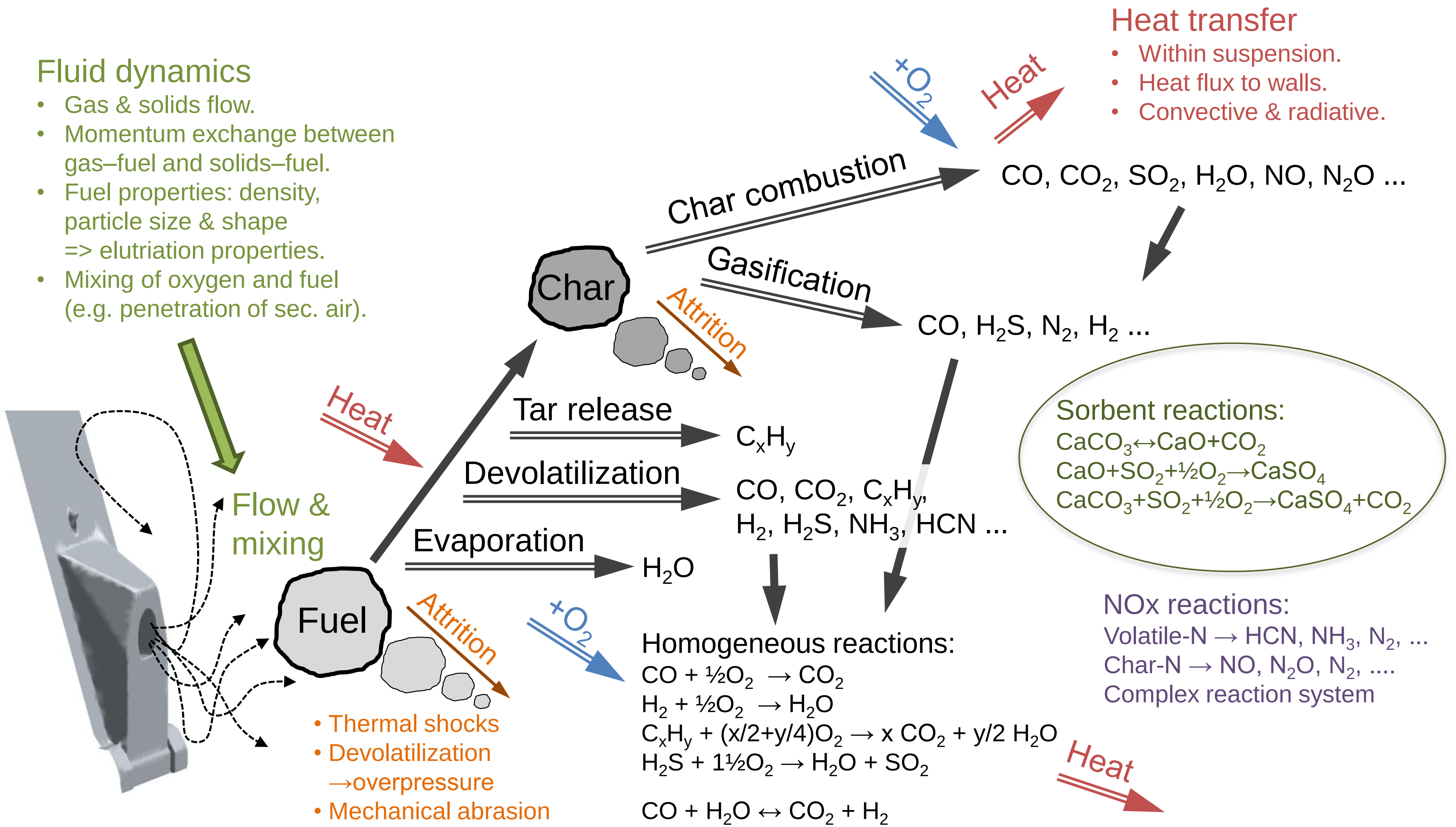
$$M = \frac{H_2 - CO_2}{CO + CO_2}$$

3D model frame

- In-house Fortran-code, steady-state, semi-empirical model.
- Initially for circulating fluidized bed combustion.
- Later developed and applied for various multiphase systems
  - Air/oxygen fired combustion, gasification, calcium looping, bubbling fluidized bed, and even for entrained flow.



Modelled phenomena in multiphase reactors (simplified version)



Main updated model features during the FLEDGED project

- New fuel component: tar
  - Proximate analysis: char + volatiles + moisture + tar + ash.
- New gas component: toluene C_7H_8
  - Gases: O_2, CO_2, H_2O, SO_2, CO, H_2, CH_4, C_2H_4, Cg, H_2S, NO, N_2O, HCN, NH_3, Ar, N_2, C_7H_8
- Modelling of tar release
  - Liquid/solid tar component in fuel released as gaseous toluene.
    - Release rate (1/s) determined as:

$$k_{tar,i} = a_{tar}\left(\frac{d_{p,i}}{d_{ref}}\right)^{b_{tar}}\left(1 - w_{H2O,i}\right)^{c_{tar}}\exp\left(\frac{-E_{tar}}{RT}\right) \qquad \text{(1/s)}$$

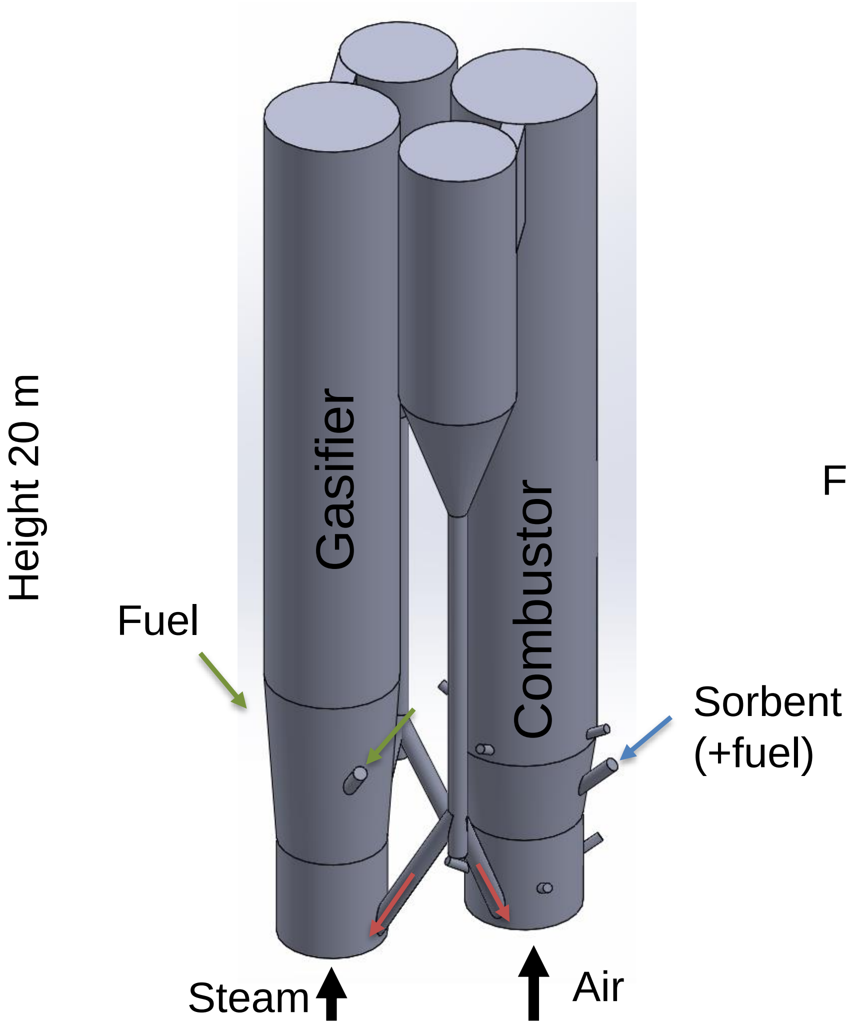
Effects: particle size, moisture, temperature

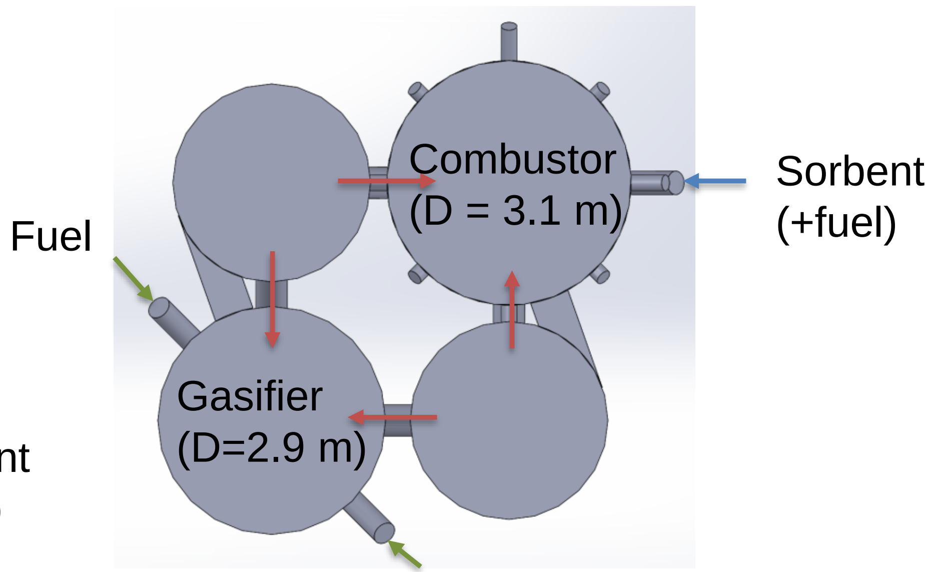
- Combustion of tar: $C_7H_8 + 3.5\ O_2 \rightarrow 7\ CO + 4\ H_2$
  - Combustion rate defined by similar Arrhenius expression as with other gases.

$$r'''_{\mathrm{C7H8}} = k_{C7H8}A_{0,C7H8}\, C_{\mathrm{C7H8}}C_{\mathrm{O_2}}^{b_{O2}}C_{\mathrm{H_2O}}^{b_{H2O}}\exp\left(\frac{-E_{C7H8}}{RT}\right) \qquad (\mathrm{mol/m_3s})$$

- Composition of volatiles updated according to experimental data.

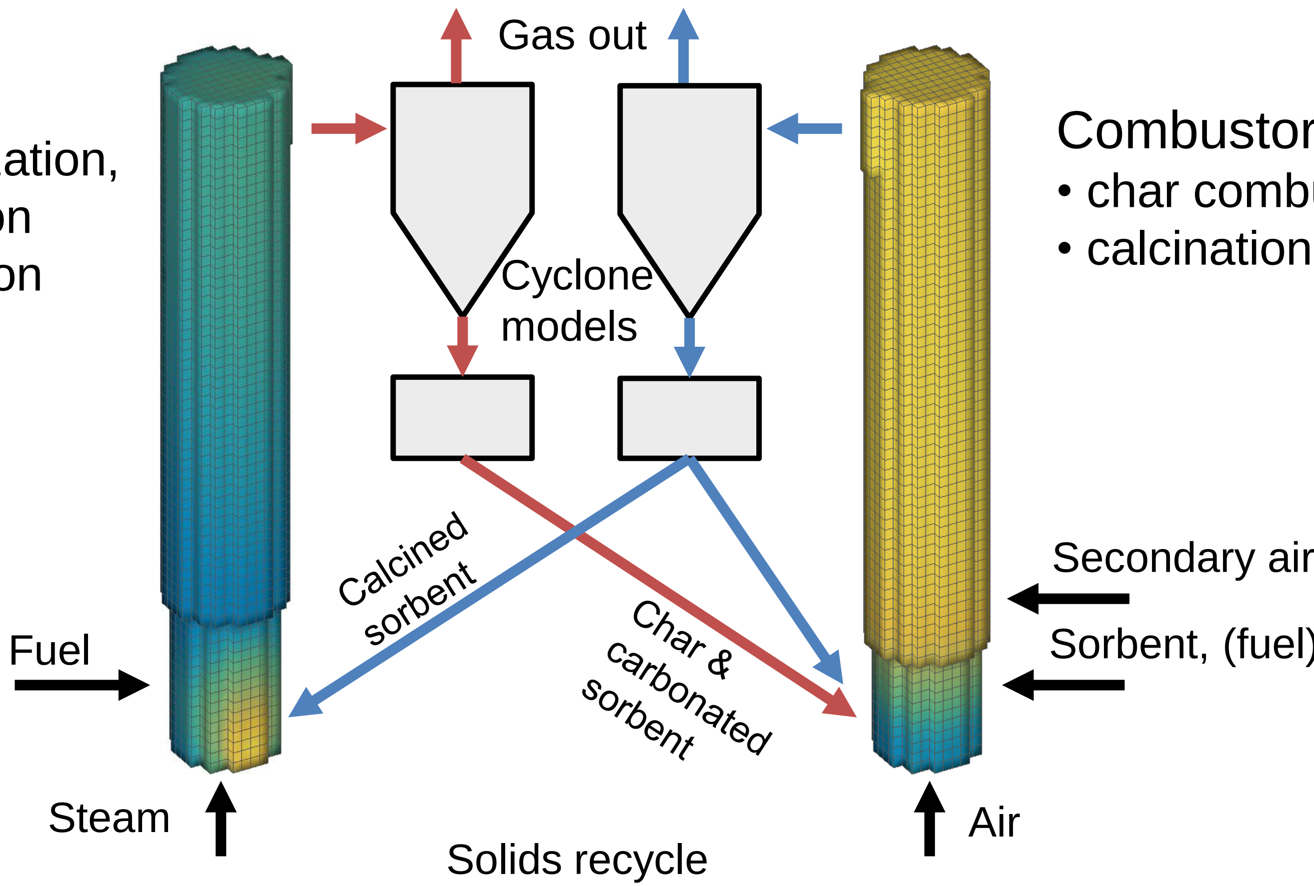
Simplified layout of the coupled reactors





3D modelling of the sorbent enhanced gasification

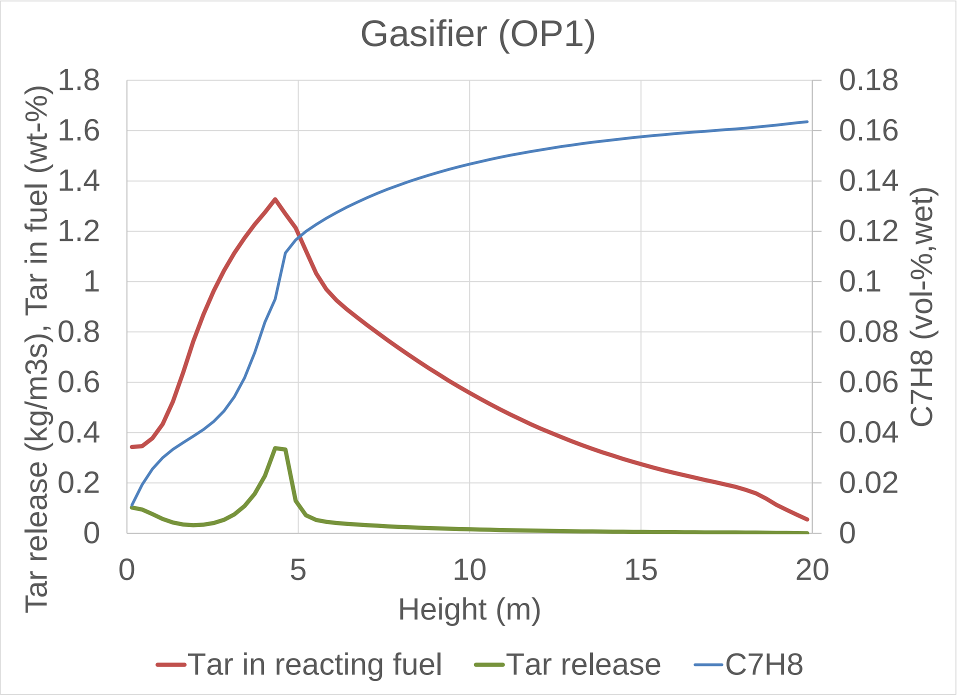
Gasifier
- devolatilization, gasification
- carbonation



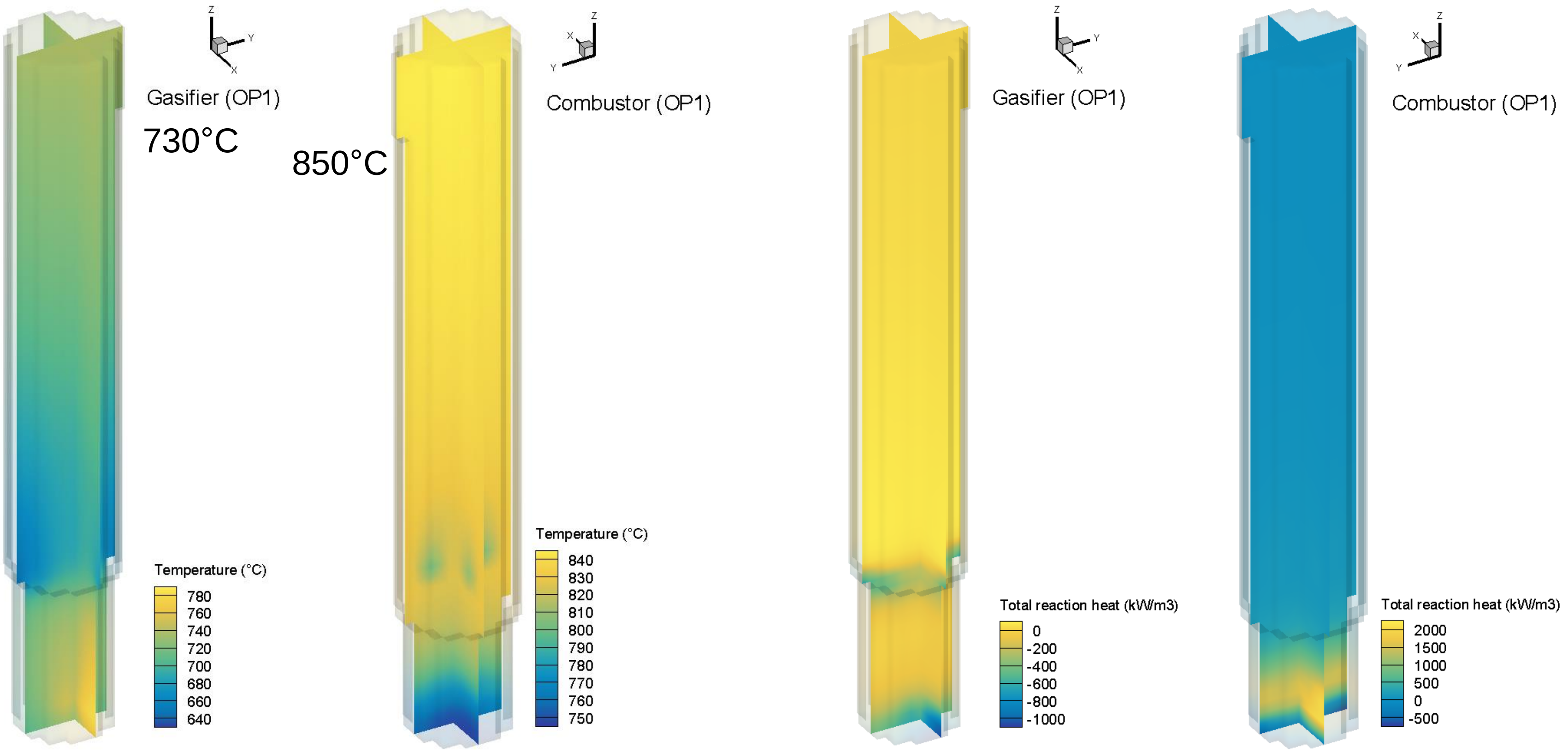
Combustor
- char combustion
- calcination

Modelling of tar

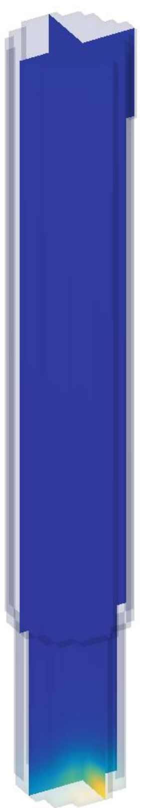
- Tar released to gas phase mainly at the bottom of the gasifier
  - Local maximum at the feeding point.
- At top of the reactor, the reacting fuel is mainly char.



Temperature and total reaction heat profiles

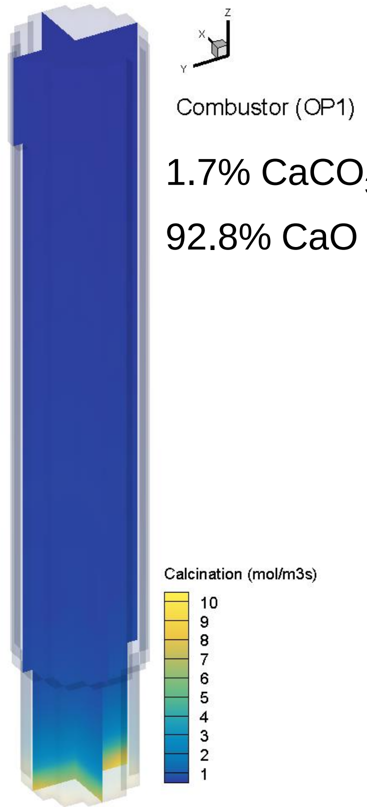


Calcination and carbonation profiles



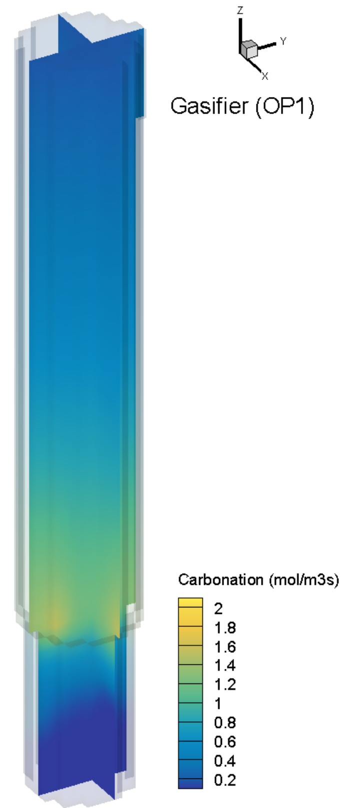
7.9% $CaCO_3$

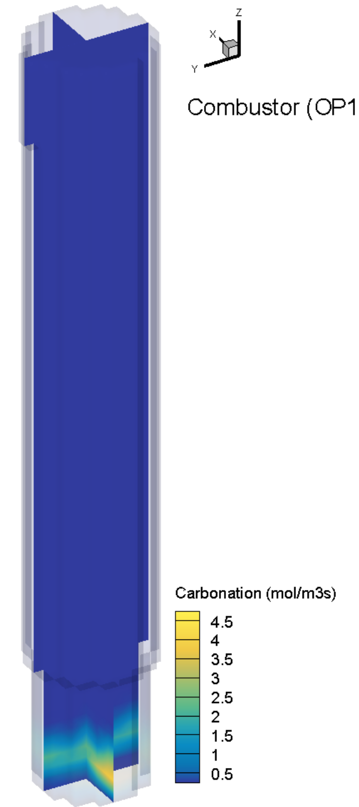
85.5% CaO



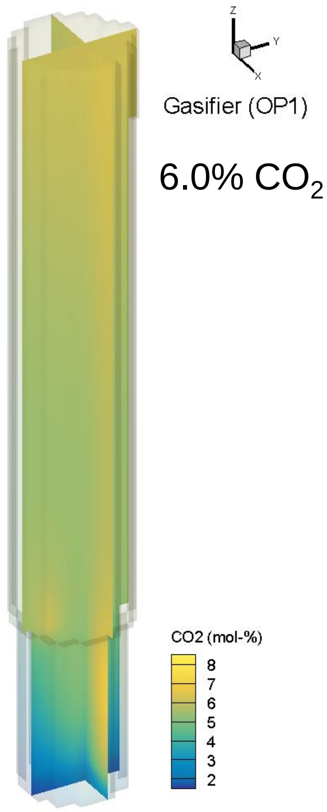
1.7% $CaCO_3$

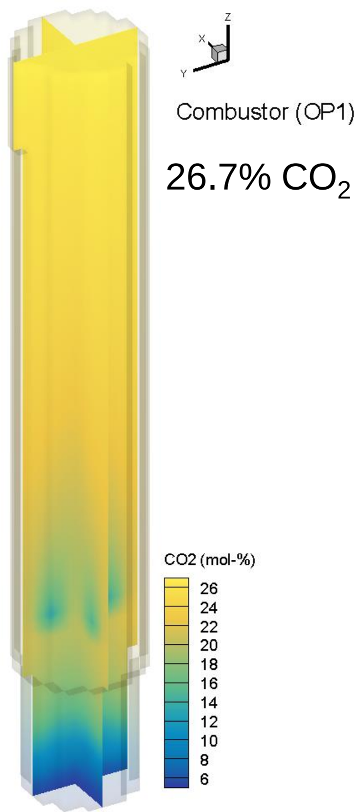
92.8% CaO

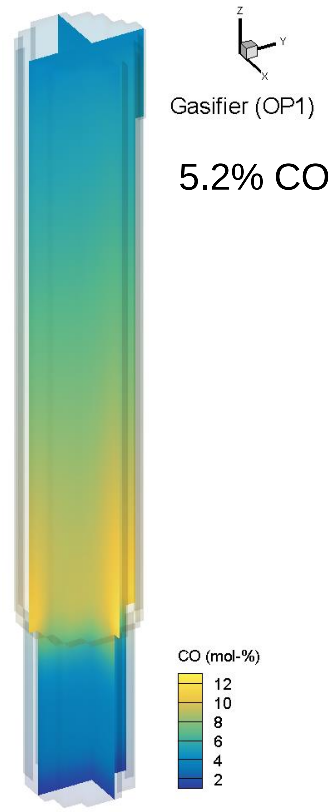




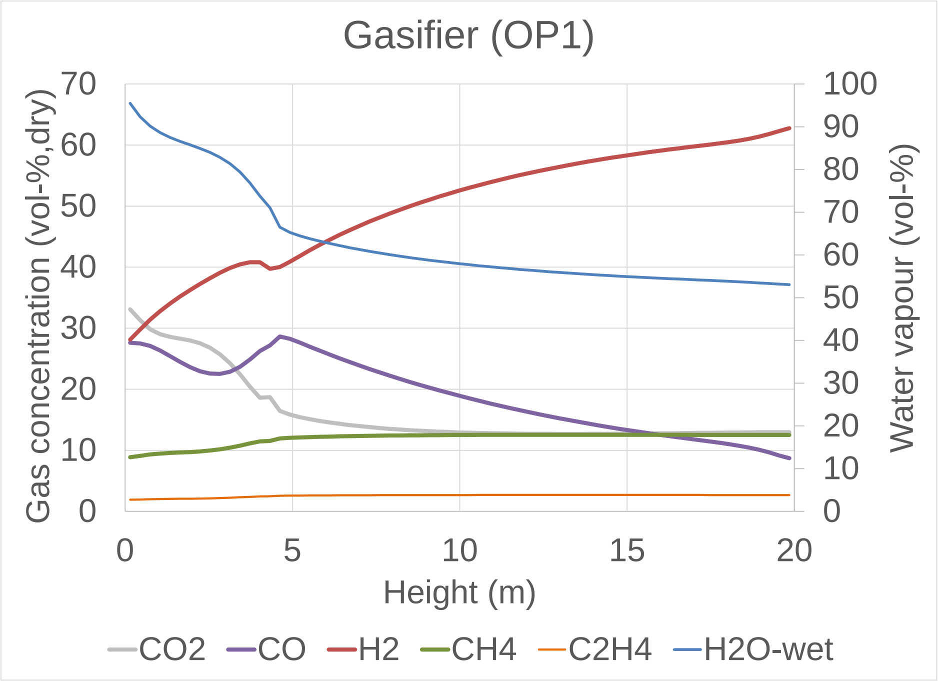
CO_2, CO (gasifier) and O_2 (combustor) profiles

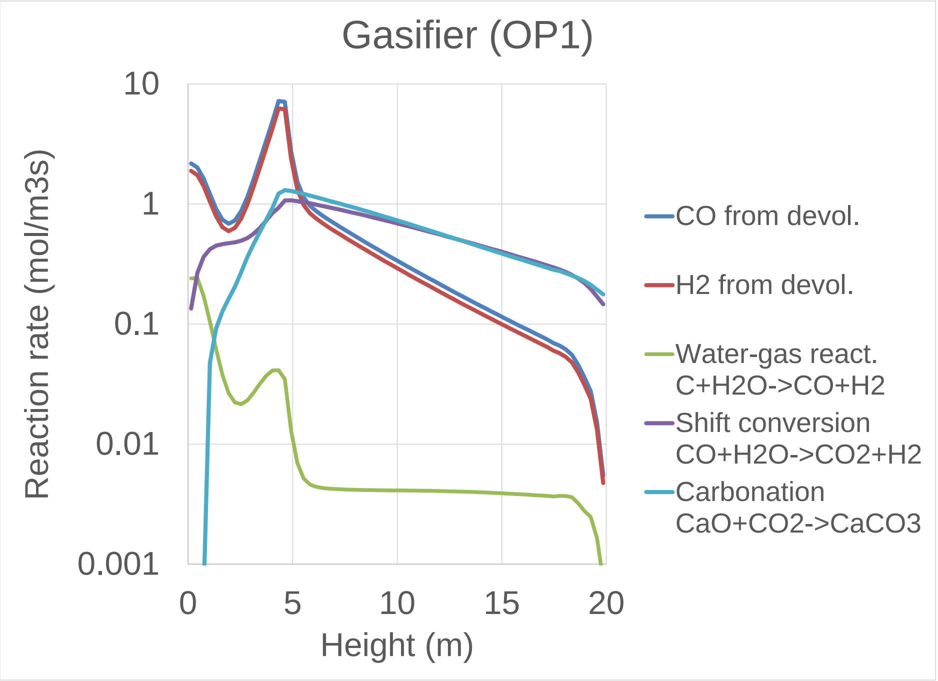






Gas composition and main reaction profiles of gasifier





- In product gas module M = $\frac{H_2 - CO_2}{CO + CO_2} = \frac{60.6 - 12.9}{11.0 + 12.9} = 2.0$

Summary

- A 3D-model developed for sorbent enhanced gasification.
  - Solution of coupled gasifier-combustor system.
- The 3D-model can be used to study local mixing phenomena inside the reactors.
- The global results were satisfactory:
  desired M-module reached.
- The entry points of circulating flow from the adjacent reactor cause local re-calcination and re-carbonation.
- The 3D-model can be utilized for further development of the reactor designs.

Find out more: www.fledged.eu
Contact us: info@fledged.eu
Direct feedback/questions: kari.myohanen@lut.fi

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 727600