Towards high-fidelity CFD simulations of coal gasification

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Outlook

- **Motivations and background**
- Chemistry tabulation strategies for coal gasification
- Results
- Conclusions and future remarks

Motivations and background

- Today CFD is valuable tool for developing, improving, and optimizing fluid-dynamics industrial processes
- A previous work[1] showed that accurate modeling of industrial-scale gasifiers may be achieved using detailed kinetics of coal thermo-conversion reactions
- However, global results are also influenced by the accurate modeling of the turbulent flows in the reactors
- High-fidelity simulations can improve the global accuracy of the numerical simulations

1. Vascellari et al. (2015). From laboratory-scale experiments to industrial-scale CFD simulations of entrained flow coal gasification. *Fuel*, *152*, 58–73.

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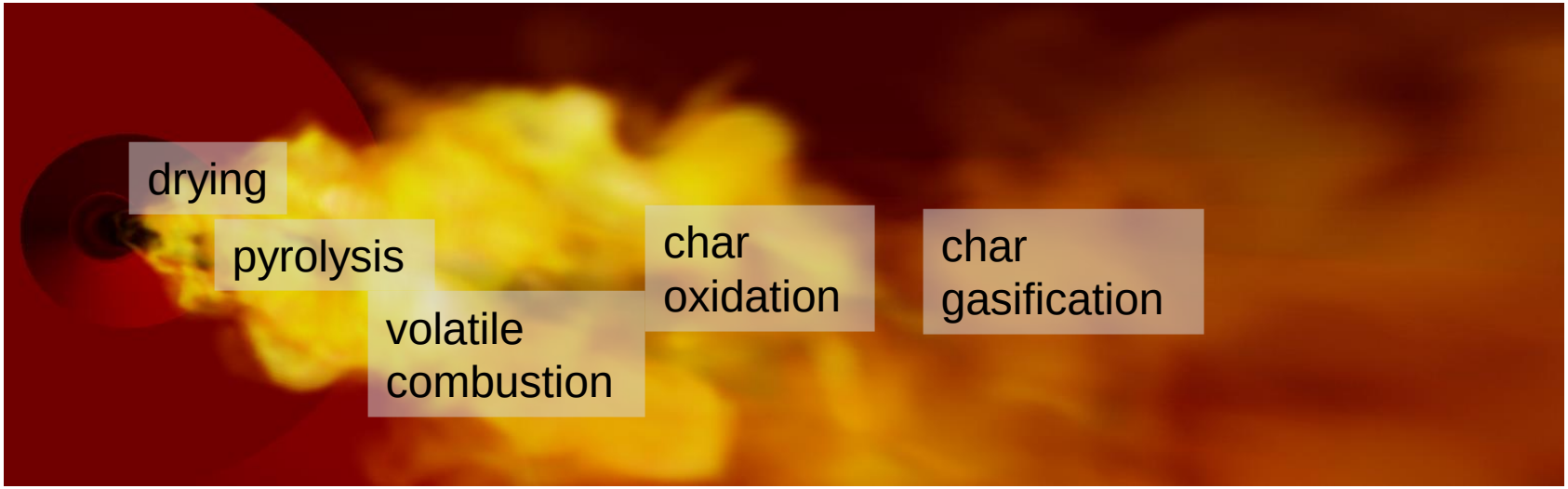
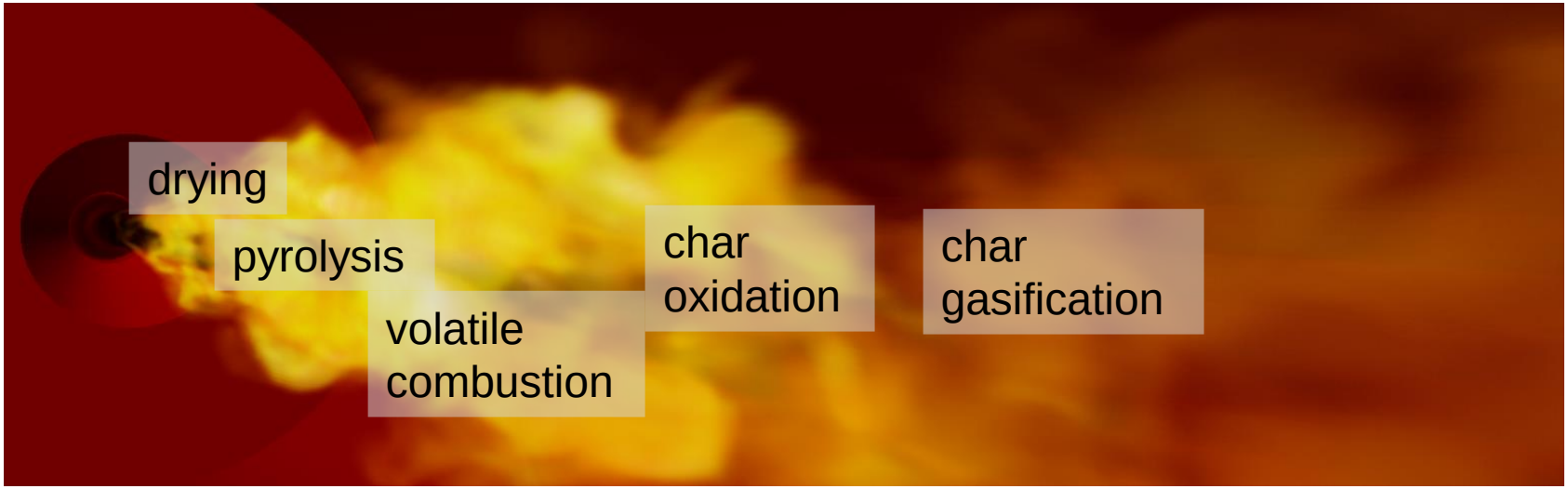
Thermal conversion of coal



- In entrained-flow gasification char gasification is the governing step in coal conversion
- Large residence times are necessary to achieve high conversion of the carbon
- Strong recirculation necessary for increasing residence time of coal particles

Thermal conversion of coal

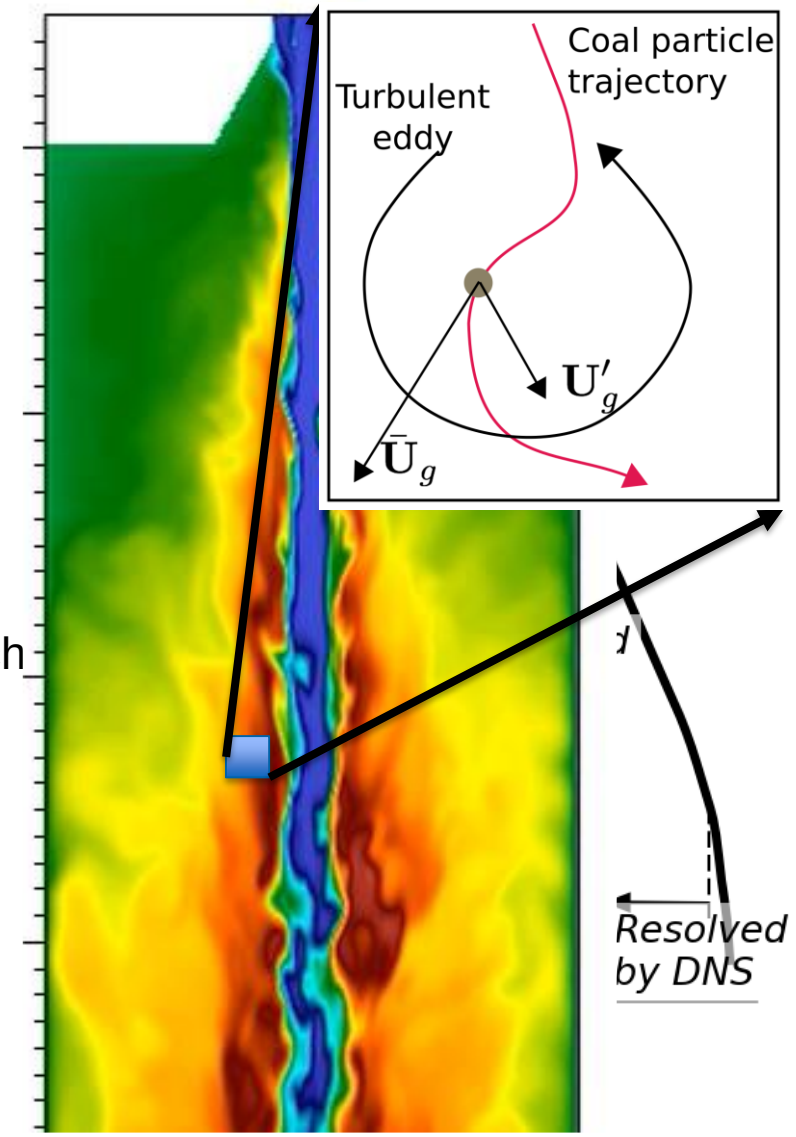


The following phenomena require accurate modeling

- Detailed estimation of coal conversion rates
- **Estimation of the particle residence time**
- Radiation heat transfer
- Slag flow on the reactor walls

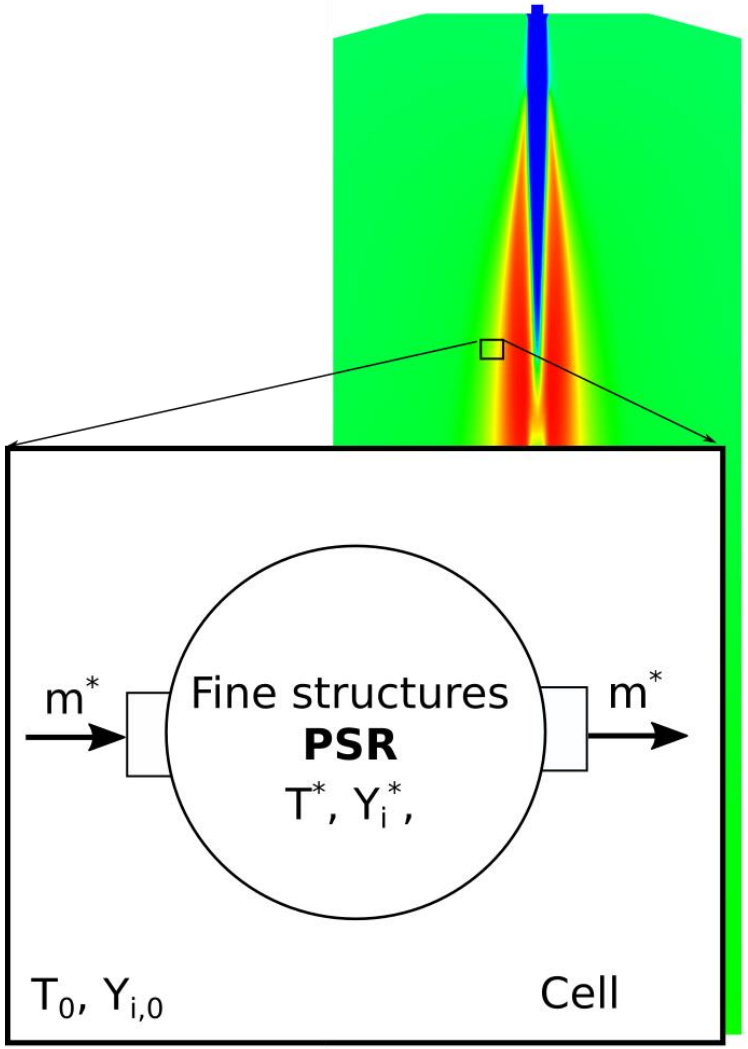
RANS vs LES

- RANS is normally used for modeling entrained-flow coal gasification
- Flow turbulent fluctuations are modeled in RANS
- Coal particle trajectories are influenced by the turbulent fluctuations
  - Stochastic component of the gas velocity is added to the drag forces
  - Model constant should require calibration for each specific problem
- LES resolves most of the turbulent fluctuations
  - Better estimation of the particle trajectories
  - More accurate estimation of the **residence time**



Gas phase chemistry – Eddy Dissipation Concept

- In gasification the slow endothermic gasification (mainly WGS) needs an accurate modeling of the kinetics and the interaction with the turbulent flows
- The **Eddy Dissipation Concept** (EDC) is used as standard model for CFD simulations
- Flexible approach allows to obtain accurate results including finite-rate chemistry
- Based on the solution of an homogeneous reactor for each cell
- Computationally very **demanding!** Not usable for LES

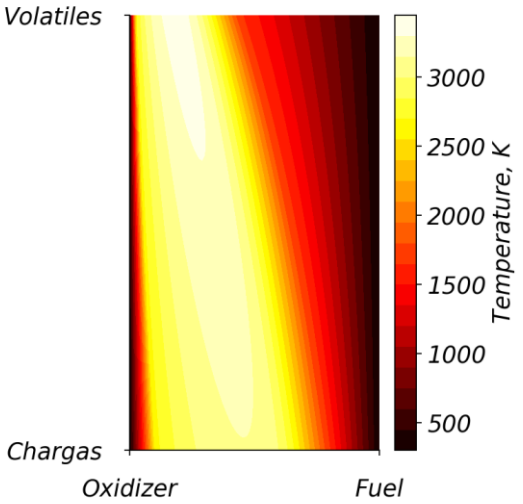


Tabulation methods for reacting flows

- Tabulation methods use a simplified representation of the flow conditions with a limited numbers of representative variables (i.e. mixture fraction, progress variable)

$$\mathbf{\Phi} = \mathbf{\Phi}_{\mathrm{FLUT}}\left(Z, C\right)$$

- Gas conditions are obtained by solving reference 0D/1D flames and stored in **flamelet look-up tables** (FLUT)



Diffusion/premix/equilibrium Flamelet

CFD

$$\rho\frac{\partial Z}{\partial t} + \nabla\cdot\left(\rho\mathbf{U}Z\right) = \nabla\cdot\left(\rho D\nabla Z\right)$$

$$\rho\frac{\partial y_c}{\partial t} + \nabla\cdot\left(\rho\mathbf{U}y_c\right) = \nabla\cdot\left(\rho D\nabla y_c\right) + \dot{\omega}_c$$

$\rho, H, T, \nu, \lambda, D, \dot{\omega}_c$

Flamelet Look-Up Table (FLUT)

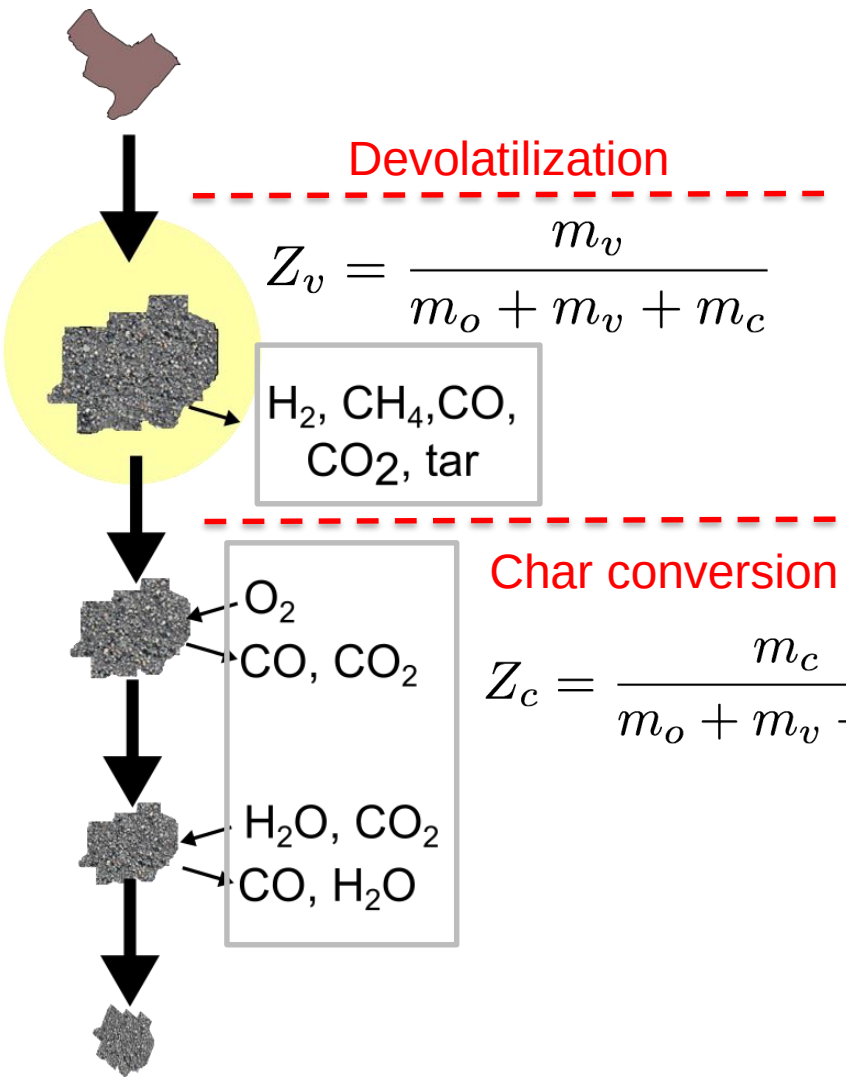
Z, y_c, Z_s, χ_s

Implementation of new PDF-equilibrium model in Ansys-Fluent

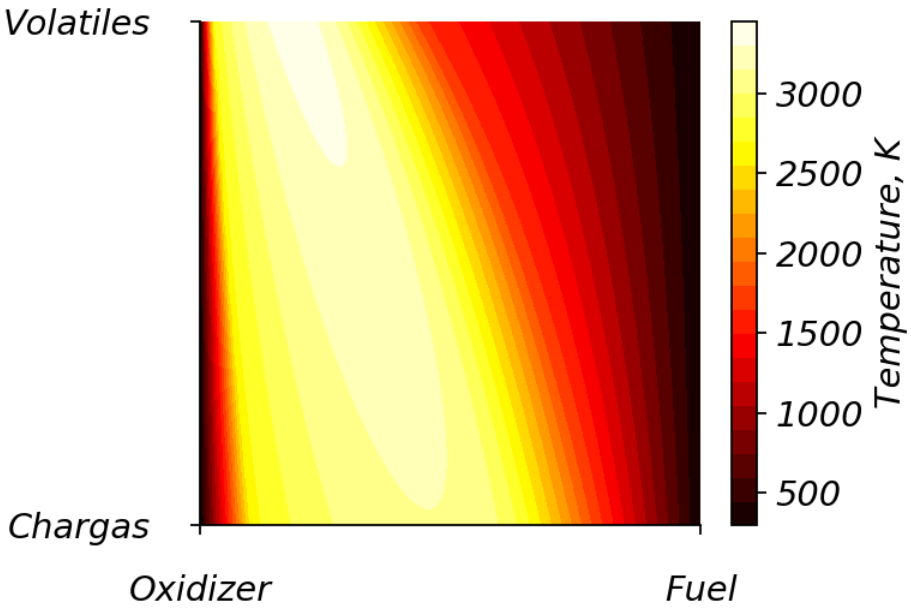
- PDF-equilibrium stores gas equilibrium as a function of the mixture fraction
- New PDF-equilibrium solver implemented in Ansys-Fluent as proof of concept
- Efficient and flexible table generation using **ULF** and **pyFLUT** (in-house NTFD codes)
- Coupled to the Memory Abstraction Layer (**MAL**) flamelet table reader for an optimal management of the memory[1]
- The new solver will be the starting point for more advanced tabulation strategies, such as **FPV**.

1. Weise et al. (2013). An abstraction layer for efficient memory management of tabulated chemistry and flamelet solutions. *Combustion Theory and Modelling*, *17*(3), 411–430.

Mixture fractions in coal gasification



- Different fuel streams in coal thermo-conversion
  - Pyrolysis
  - Char burn gases
- These streams are represented by different mixture fractions

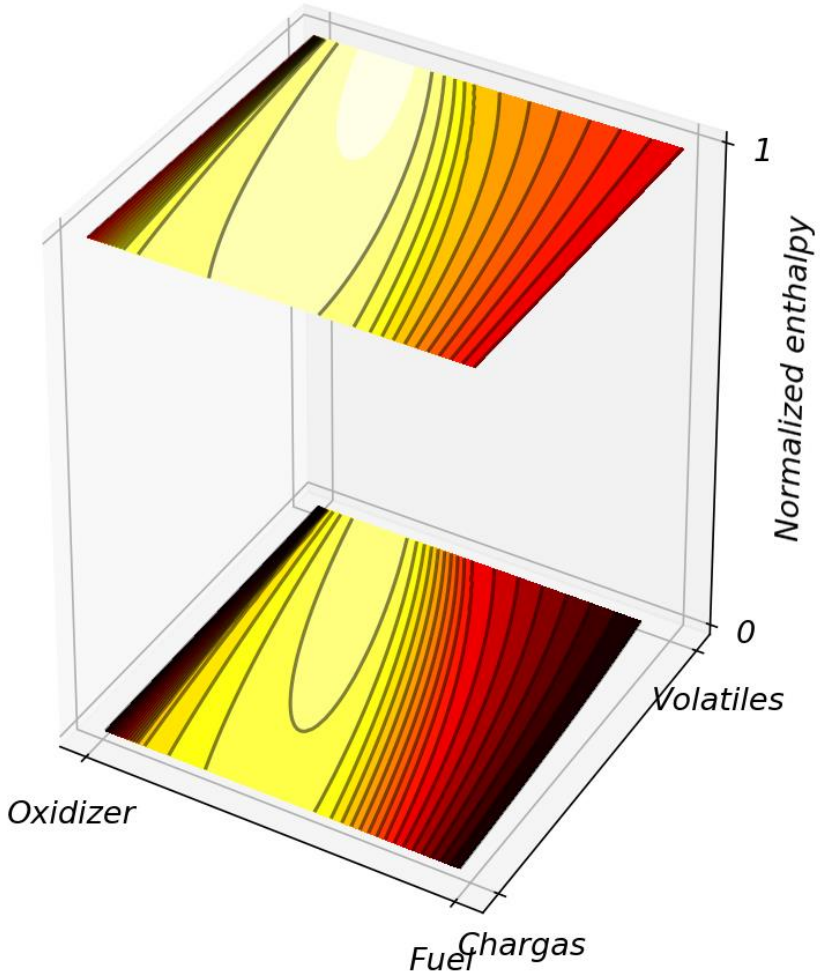


Enthalpy defect in the look-up table

- Gas phase exchanges heat with
  - Coal particles
  - External environment (wall)

- **Normalized enthalpy** is added as additional input parameters in the look-up table

- Different enthalpy levels are generated considering unburned fuel and oxidizer at different temperatures



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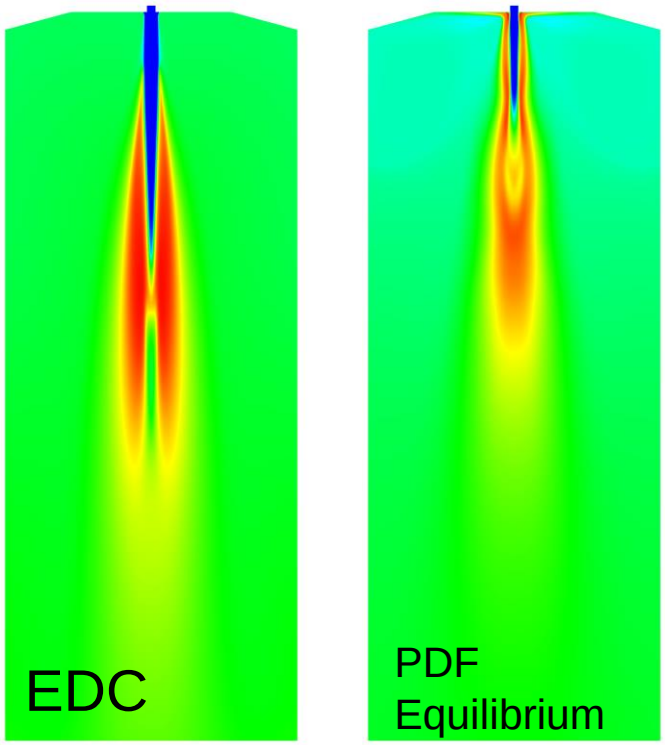
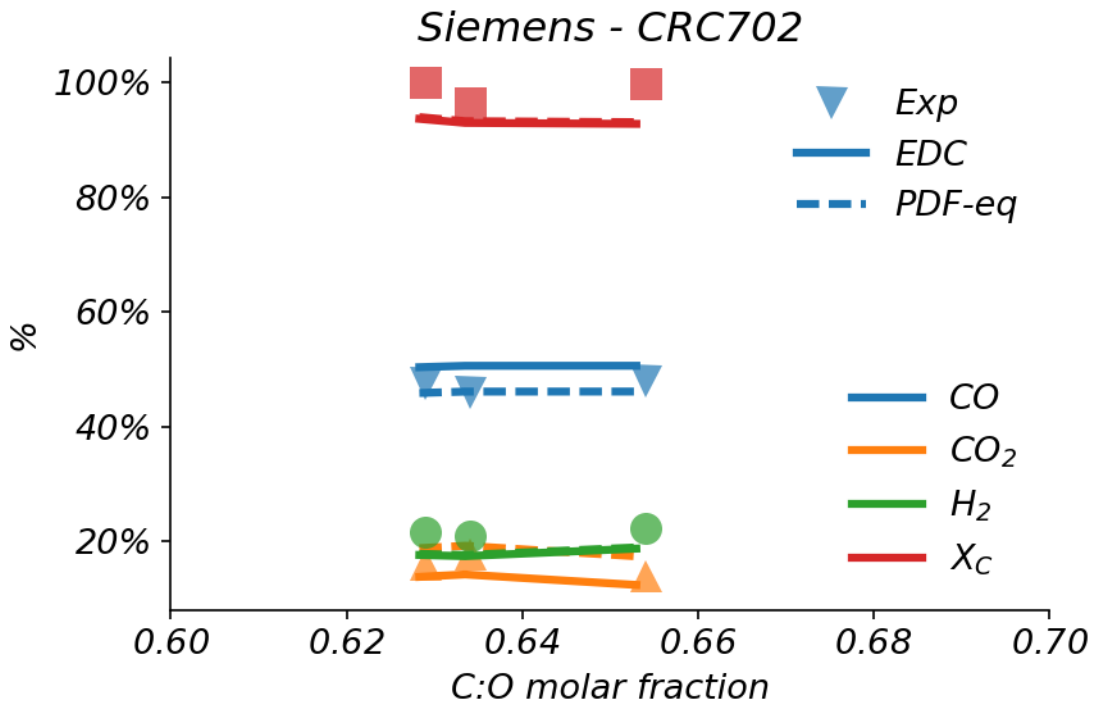
Results

- PDF-equilibrium tested on 5MW pilot-scale Siemens gasifier
- PDF-equilibrium shows satisfactory results compared to EDC
  - Differences are related to the equilibrium assumption
- Sensible speed-up on the solution of the gas phase ***~20x***
  - EDC 0.470 sec/iteration – PDF-eq: 0.022 sec/iteration on 16 cores with 21k cells





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Conclusions and next steps

- Performances of entrained-flow coal gasification can be accurately modeled using CFD
  - Detailed kinetics of coal conversion and homogeneous reactions
  - Accurate modeling of turbulent flows in the reactors => residence time
- Accurate estimation of the turbulent flows can be obtained with LES
  - Computationally expensive
  - Efficient modeling approaches
- Tabulation strategies allow efficient computation of homogeneous reactions
- A PDF-equilibrium solver implemented in Anysis-Fluent as proof of concept
- Considerable speed-up in gas phase computation ~20x
- Extend PDF-equilibrium solver including the progress variable (FPV) => accounts for finite rate chemistry

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Thank you for your attention!

Questions?

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