Institute of Energy Process Engineering and Chemical Engineering

Towards a CFD Model for Industrial Scale Gasification Processes

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Content

Introduction and Problem Statement

- Partial oxidation/ gasification at high pressure up to 100 bar.
- Investigate of reactive flows with the following characteristics: turbulent mixing, combustion and downstream reactions.
- Large-scale reactors of several meters require steady-state solution techniques.

Goal

Stable steady-state solver capable of using detailed chemical reaction mechanisms.

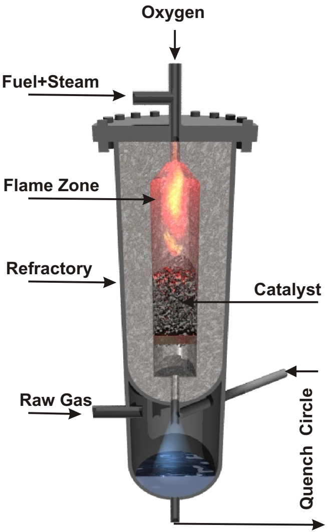
The HP POX Pilot Plant

HP-POX (High pressure patial oxidation) Pilot Plant, 5 MW thermal power, pressure up to 100 bar

Scheme of the HP-POX Pilot Plant (ATR Mode)

HP-POX

- Use of higher pressure levels to reduce size of plants and investment costs.
- Available modes: non-catalytic (POX), catalytic (ATR), liquid feedstock (MPG)
- Non-premixed educts ⇒ flame zone and reforming zone.



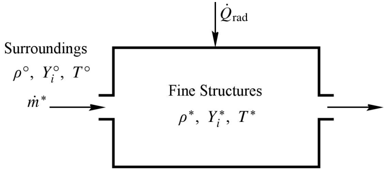
Development of a new OpenFOAM solver

- Unsatisfying results of commercial CFD-codes due to combustion models.
- Development of a steady-state OpenFoam solver for chemistry started: EDCSimpleFoam

Steps towards that solver

1. Steady-state solver for inert mixing using the SIMPLE algorithm for reactingFoam.
2. Integration of detailed chemistry mechanisms with the EDC model (Eddy dissipation concept) of Magnussen [MAGNUSSEN, 1989, Gran and Magnussen, 1996]
   - CVODE for stiff ODE
   - CANTERA for chemical source terms
3. Basis: EDMSimpleFoam of T. Lucchini

EDC Model Implementation



EDC reactor model from [Kleiveland, 2005]

- Consider a cell and assume that the reactions only take place where they are mixed at a molecular level: fine structure. The rest is inert: surrounding fluid.
- The zones exchange mixture with a rate $\frac{1}{\tau}$ (see eq. (2))

EDC Model Implementation II

Averaged chemical source terms RR_i for `YEqn.h` stem from a routine called `EDCSolve(`τ`, `γ`)` in class `chemistryModel` :

$$RR_i = \frac{\gamma^2 \rho}{\tau} \left(y_i^* - y_i^0 \right) \text{ in } \left[\frac{kg}{m^3 s} \right] \tag{1}$$

$$\gamma = C_\gamma \left(\frac{\nu \epsilon}{k^2} \right)^{0.25} \text{ and } \tau = C_\tau \left(\frac{\nu}{\epsilon} \right)^{0.5}$$

with ρ density, ν viscosity, y_i mass fractions of species i, k, ϵ turbulent kinetic energy and dissipation rate. Where '$*$' refers to fine structures and '0' to surrounding fluid.

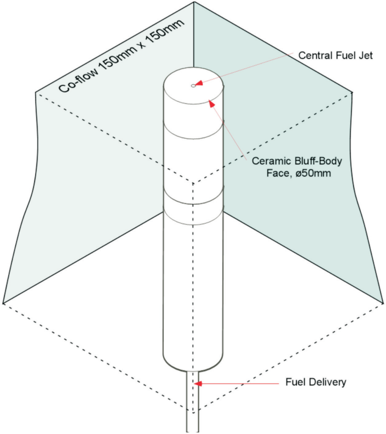
EDC Model Implementation III

Solve ODEs for an adiabatic ideal reactor (fine scales)

$$\frac{dy_i^*}{dt} = \frac{y_i^0 - y_i^*}{\tau} + \omega_i \tag{2}$$

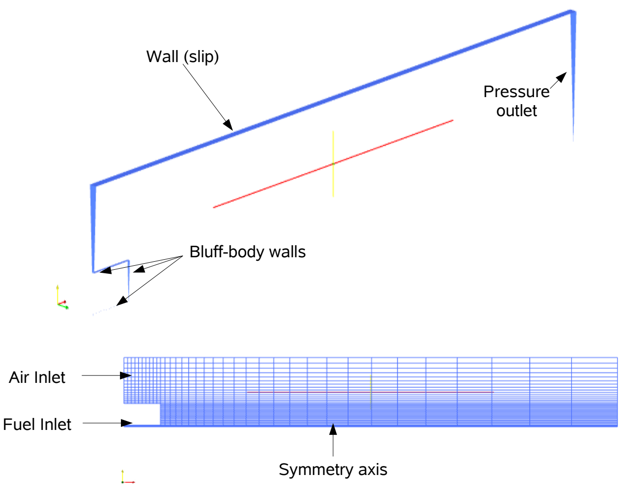
where $\bar{y}_i = \gamma^3 y_i^* + (1-\gamma^3) y_i^0$ and ω_i reaction rate

- Until steady-state of the system is reached (condition $\max(\Delta y, \Delta T/1000) < 10^{-5}$).
- This gives us y^*, y^0 for Eqn. (1).
- Integration with CVODE from SUNDIALS package.
- Reaction rates from CANTERA obtained with ATRMech [Zeißler, 2006] (28 Species, 112 Reactions, reduced version of GRIMECH 3.0 [et al,]).



Data from Sandia bluff-body flame HM1 and nonreacting jet NRBB conducted at Sydney university [Dally et al., 1998].

Boundary Conditions



Boundary Conditions II

Boundary conditions

- Diameters: $D_{jet} = 3.6$mm; $D_{channel} = 150$mm (300mm), $D_{bluffbody} = 50$mm
- Turbulence:8.5 % (2.5%) turbulence intensity , 0.135 mm (5.625 mm) mixing length for jet (co-flow)
- Mesh: from blockMesh with 1095 and 23640 cells

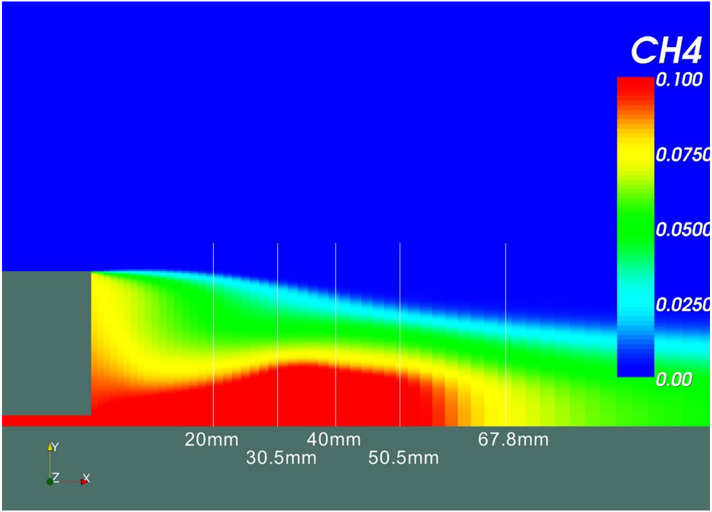
Three different inlet conditions:

- NRBB 1 (velocity): $U_{jet} = 61$m/s; $U_{coflow} = 20$ m/s
- NRBB 2 (inert mixing): $U_{jet} = 50$m/s; $U_{coflow} = 20$ m/s
- HM1 (reacting): $U_{jet} = 118$m/s $U_{coflow} = 40$m/s

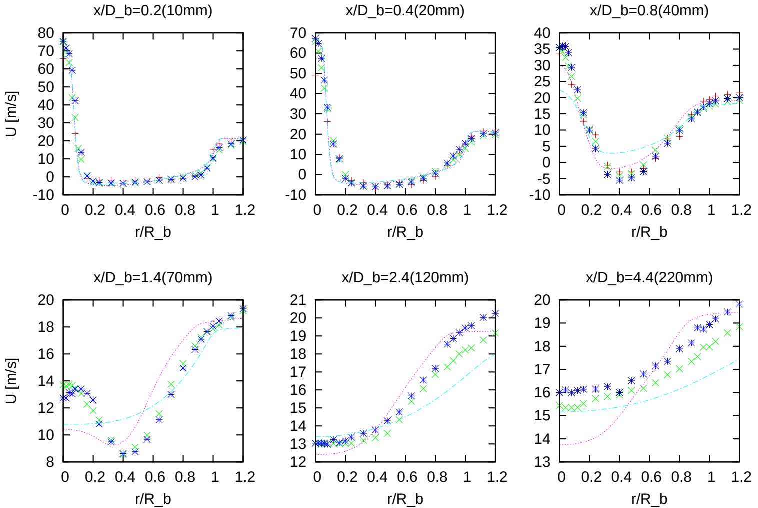
Other models:

- $k - \epsilon$/RKE turbulence model
- Non-reacting cases without energy equation

Points of measurement

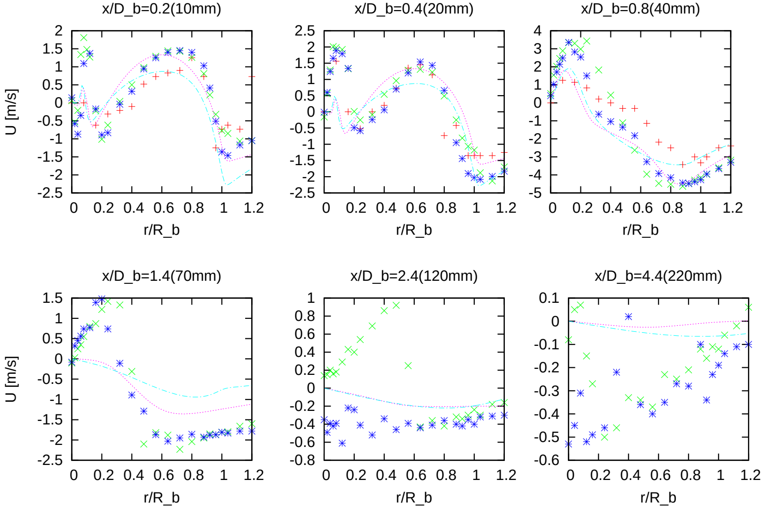


Results NRBB1 (Ux)



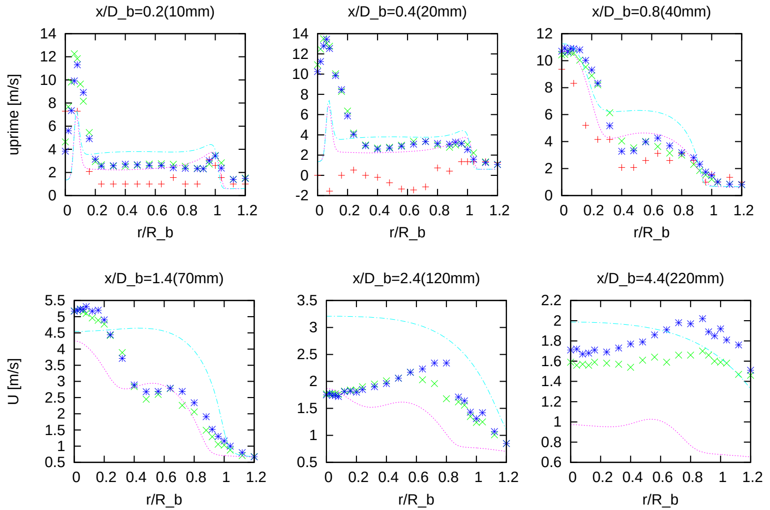
Axial velocity Ux, + HM1(exp.), lines EDCSimpleFoam, blue: geometry large; pink:geometry slim (as shown on page 11)

Results NRBB1 (Uy)



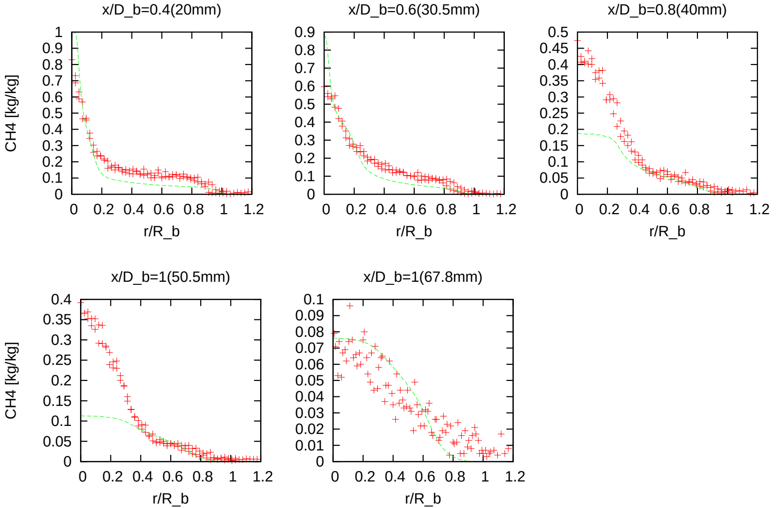
Radial velocity Uy, + HM1(exp.), lines EDCSimpleFoam, blue: geometry large; pink:geometry slim

Results NRBB1 (U′)



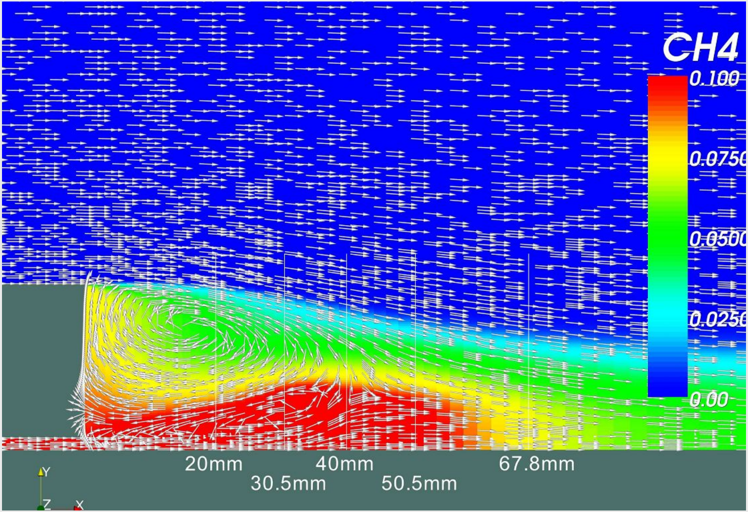
Fluctuation of velocity U', + HM1(exp.), lines EDCSimpleFoam, blue: geometry large; pink:geometry slim

Results NRBB2 (CH4)



Mass fraction CH4, + NRBB(exp.), lines EDCSimpleFoam

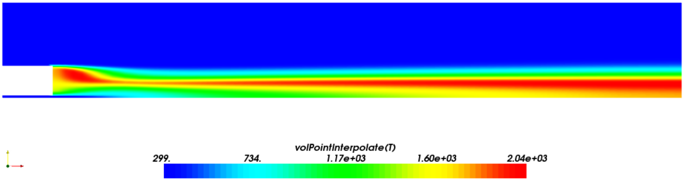
Recirculation at Bluff-body



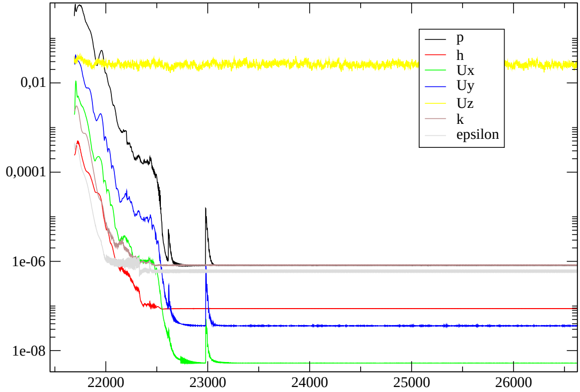
40mm, 50.5mm: CH4-under-predicted due to vortex

Flame Flame HM1

- Calculation of HM1 flame
- Up to now only solution for coarse mesh
- Difficult at start-up, under-relaxation important

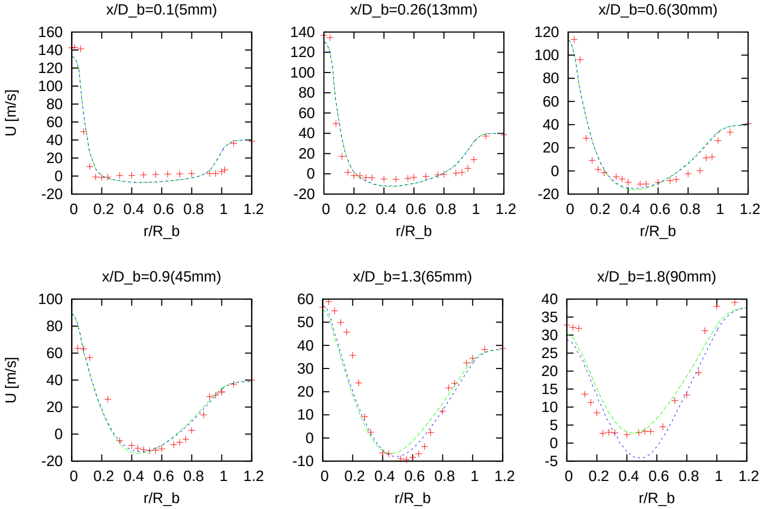


Results HM1 (Residuals)



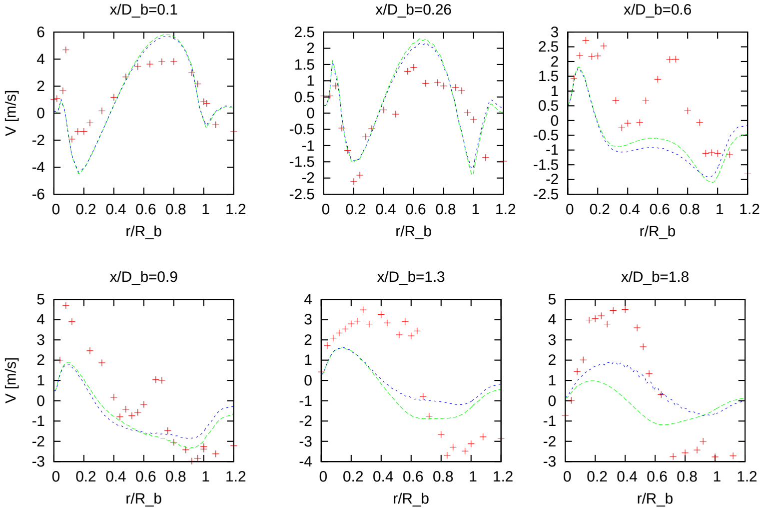
Residuals for calculation on coarse grid

Results HM1 (U)



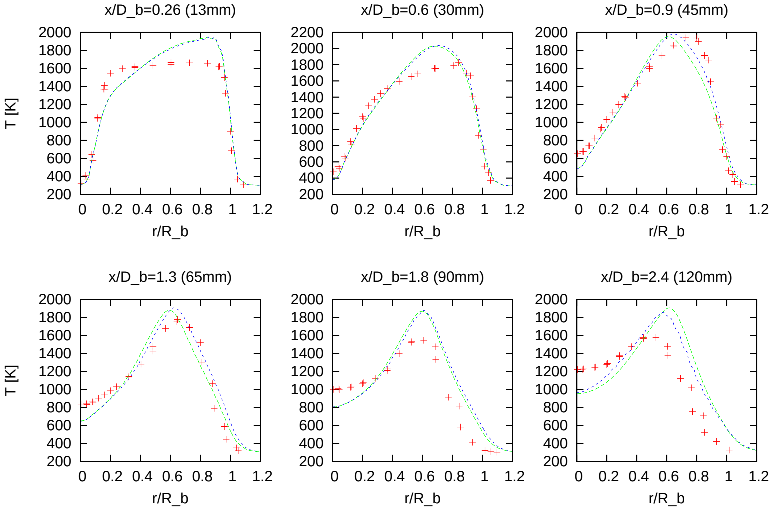
Axial velocity U, + HM1(exp.), lines EDCSimpleFoam

Results HM1 (V)



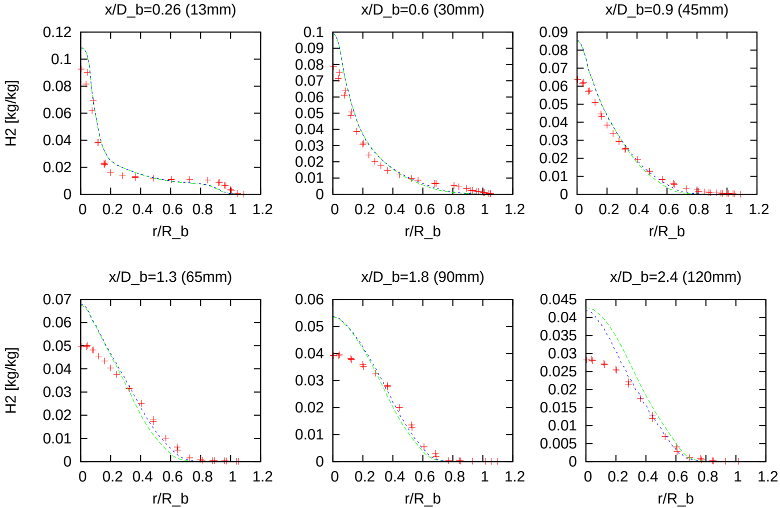
Radial Velocity V, + HM1(exp.), lines EDCSimpleFoam

Results HM1 (T) - Ensemble Mean Values



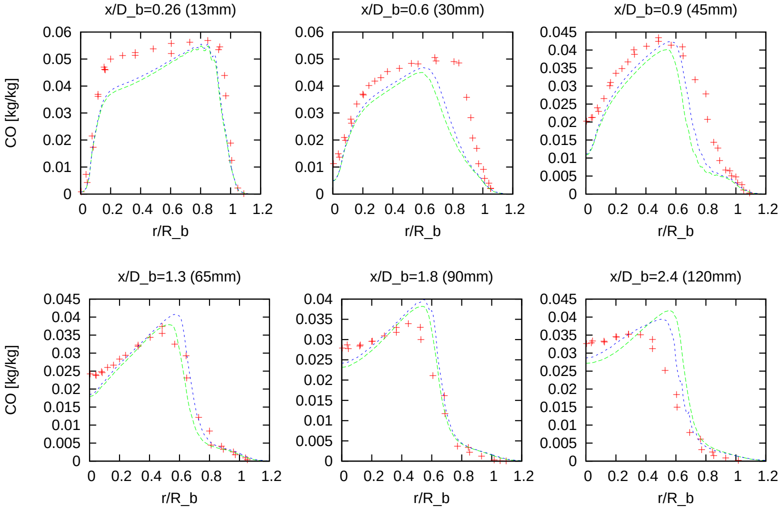
Temperature, + HM1(exp.), lines EDCSimpleFoam

Results HM1 (H2)



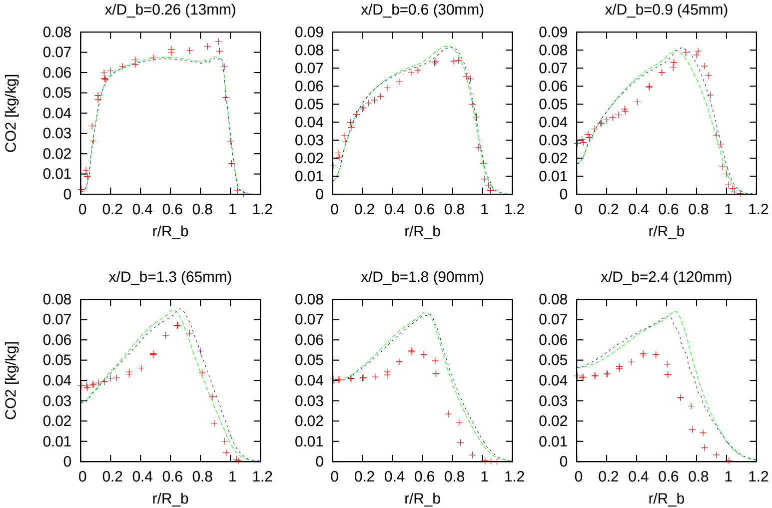
Hydrogen (H2), + HM1(exp.), lines EDCSimpleFoam

Results HM1 (CO)



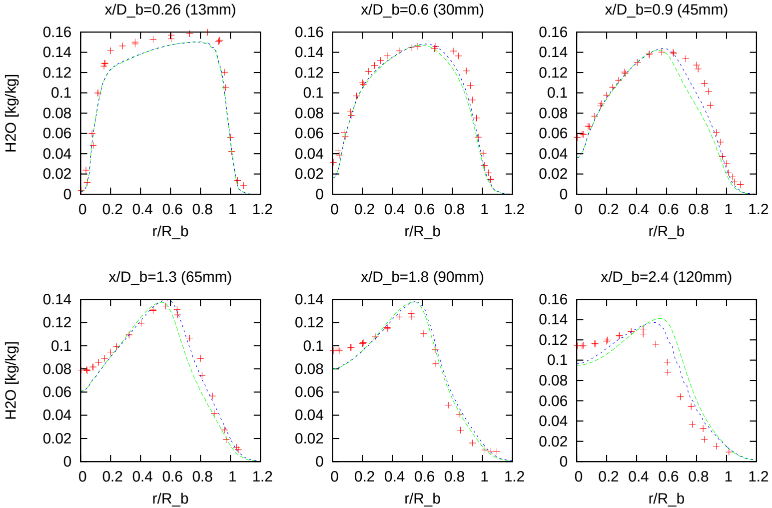
Carbon monoxide (CO), + HM1(exp.), lines EDCSimpleFoam

Results HM1 (CO_2)



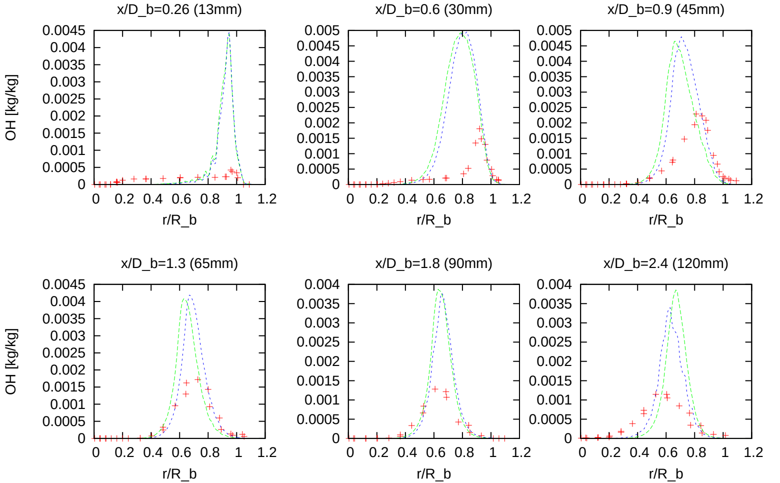
Carbon dioxide (CO_2), + HM1(exp.), lines EDCSimpleFoam

Results HM1 (H2O)



Hydrogen (H2O), + HM1(exp.), lines EDCSimpleFoam

Results HM1 (OH)



Hydrogen (OH), + HM1(exp.), lines EDCSimpleFoam

Problems

- Fluctuation and residual of Uz
- Temperature at mixing point where shear-stresses are highest (jet inlet)
- EDCFoam for unsteady calculation doesn't give same results yet

Future plans

- Further study of the flame and checking of the results
- Stable solution for fine mesh
- Checking of unsteady solver EDCFoam
- Reduction of chemistry (ISAT and/or ILDM)
- Application to the whole HP-POX reactor
- Optimization and readability of code
- New class `canteraThermo` for chemistry, viscosity, diffusivity, ...
- Virtuhcon launch in 2009 will contribute to the development of high temperature conversion processes, too (see flyers).

Acknowledgements

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Literature I

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