3rd Oxyfuel Combustion Conference, Ponferrada, Spain, 2013

Evaluation of Global Reaction Mechanisms for CFD Modelling of Oxy-Fuel Combustion

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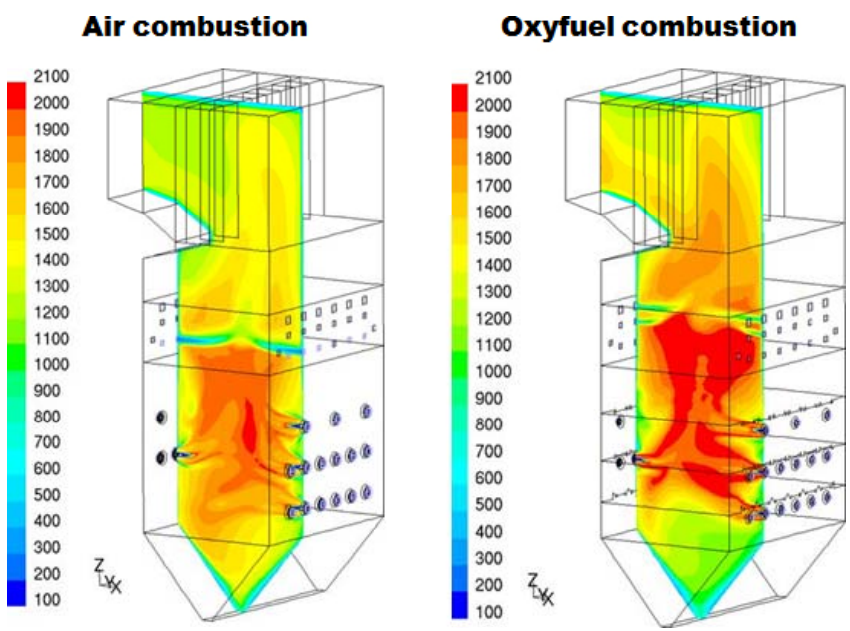
Background

Purpose	To obtain information for development of commercial oxy-fuel boilers
Progress of work	Chalmers 100 kW oxy-fuel unit Oxy-CFB combustion Series of experimental and modelling studies
Content of work	Combustion issues Emissions (NO_x and SO_x) Heat transfer
Present presentation	Evaluation of reduced reaction mechanisms for CH oxidation in CFD simulations

Computational Fluid Dynamics



Source: www.hightech.fi

Complex Geometries
Complex Turbulent Flames

↓

Simplified reaction mechanisms

↓

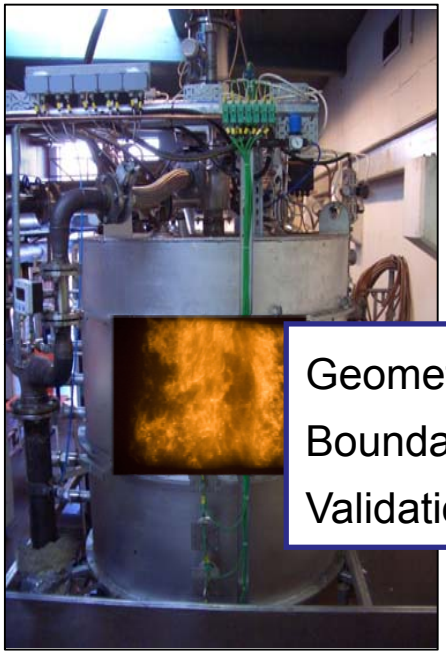
Limited generalizability

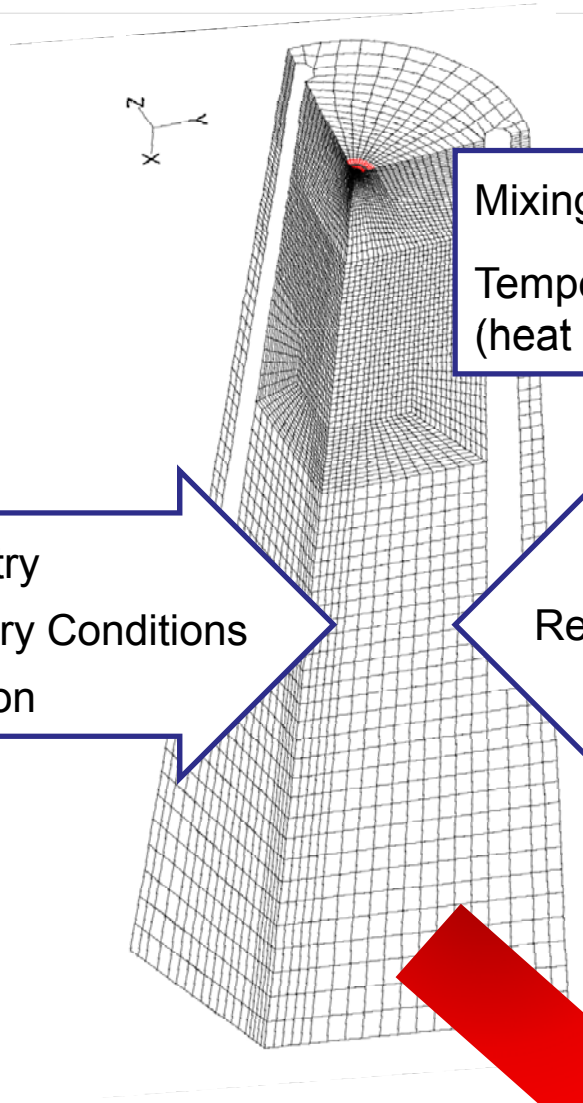
↓

Applicability to oxy-fuel combustion with high CO_2 concentration?

Global Reaction Mechanisms

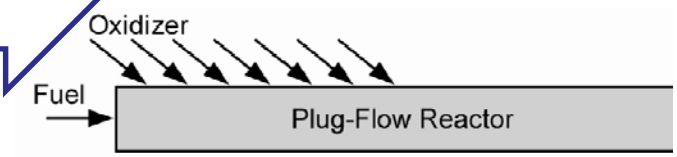
		Air	Oxy-fuel		
		JL	3-step	4-step	6-step
Fuel Oxidation	$C_3H_8 + 1.5\,O_2 \rightarrow 3\,CO + 4\,H_2$	x	x	x	x
	$C_3H_8 + 3\,H_2O \rightarrow 3\,CO + 7\,H_2$	x		x	x
Intermediates Oxidation	$H_2 + 0.5\,O_2 \leftrightarrow H_2O$	x	x	x	x
	$CO + H_2O \leftrightarrow CO_2 + H_2$	x		x	x
	$CO + 0.5\,O_2 \leftrightarrow CO_2$		x		
Radical Formation	$O_2 \leftrightarrow 2O$				x
	$H_2O \leftrightarrow H + OH$				x
		Jones & Lindstedt, 1988	Leiser et al 2007	Glarborg et al, 2009	Frassoldati et al 2009





Mixing (turbulence)

Temperature
(heat transfer)



Geometry

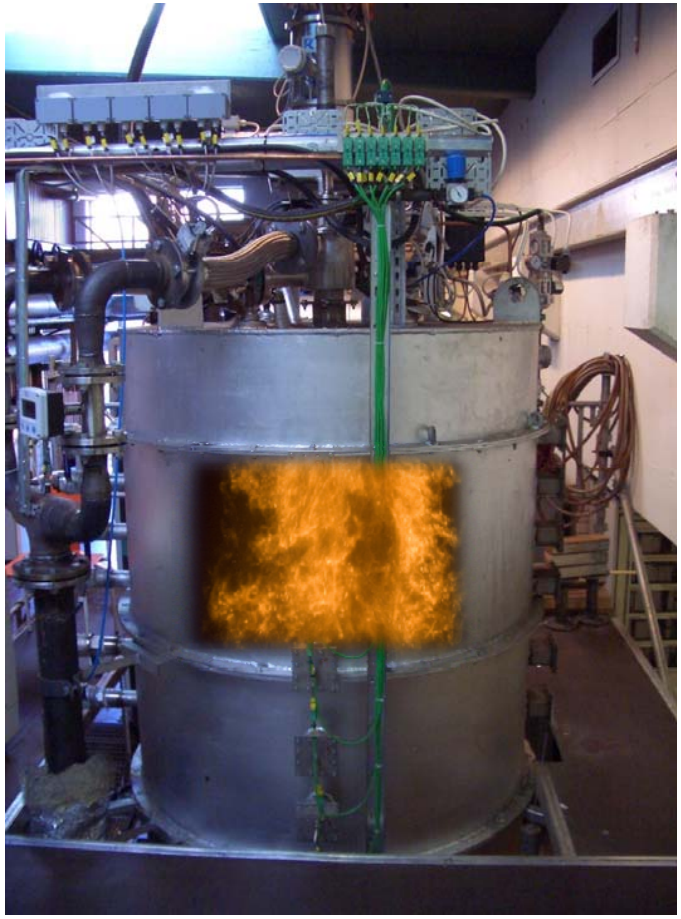
Boundary Conditions

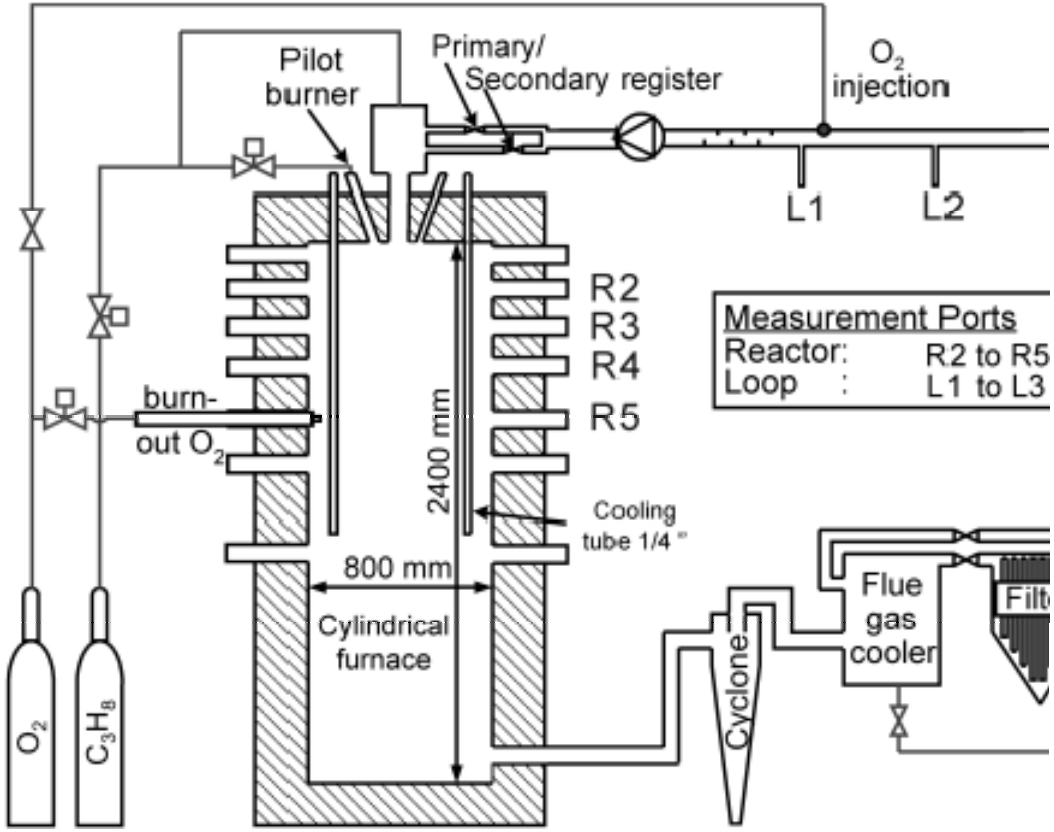
Validation

Reaction Mechanism

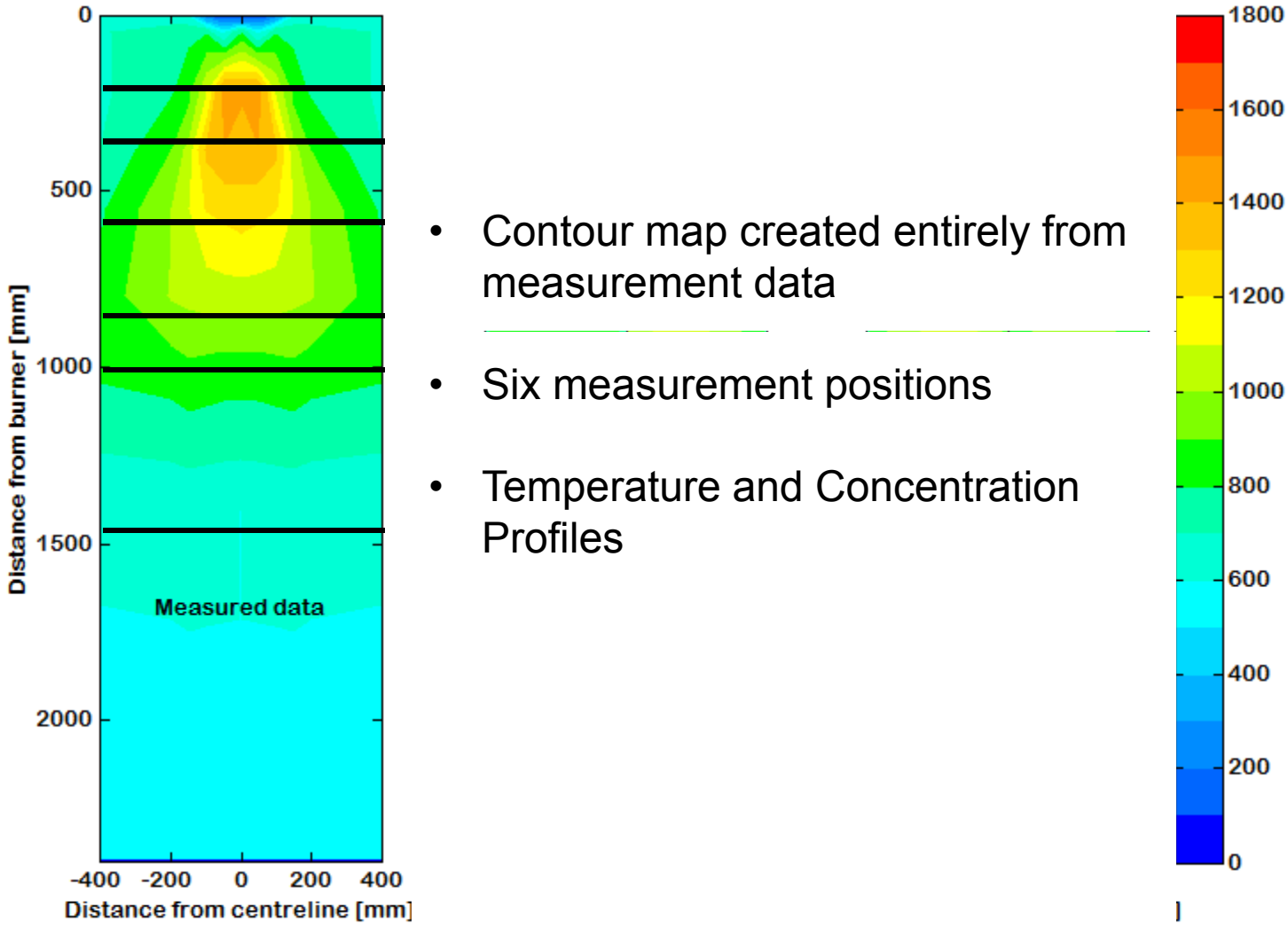
Burner and Boiler Optimization

Mapping of 100 kW Oxy-Propane Flame





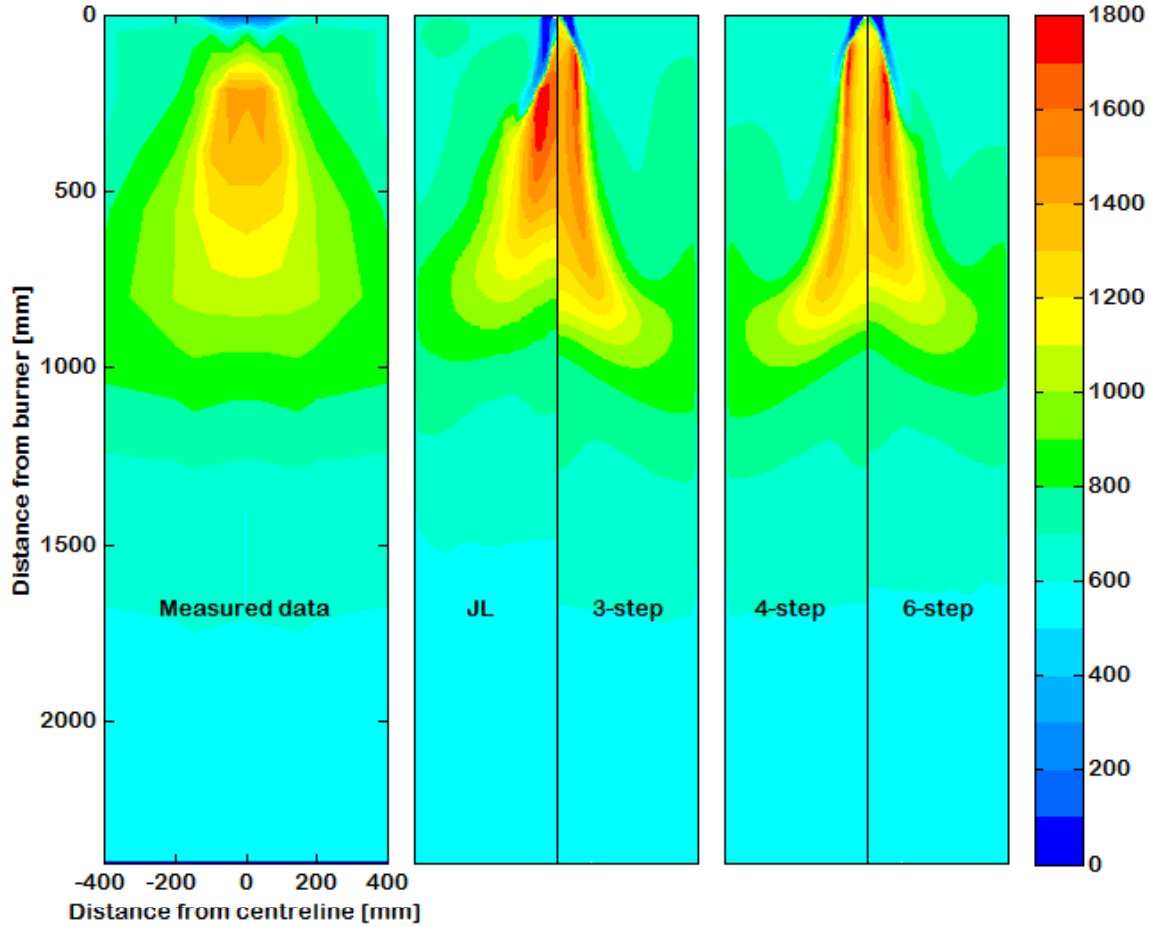
Temperature Measurements



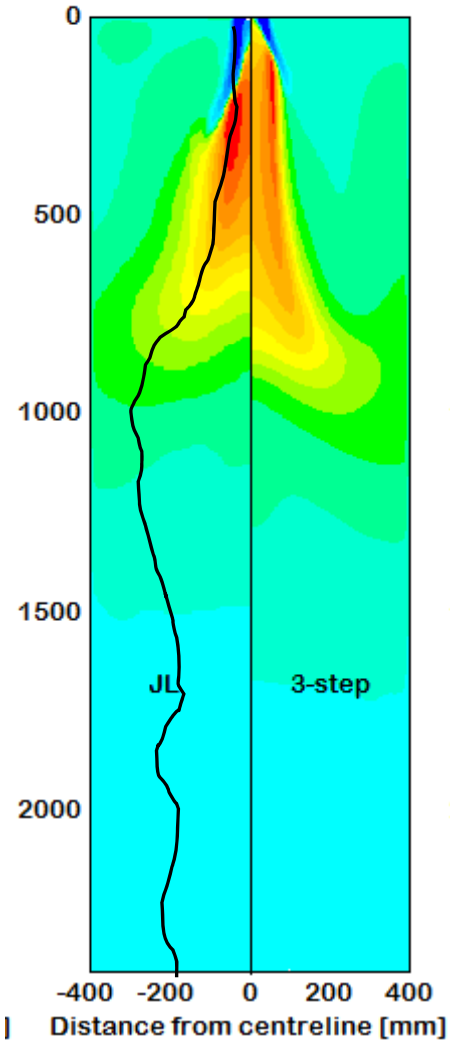
- Contour map created entirely from measurement data
- Six measurement positions
- Temperature and Concentration Profiles

3D CFD Model

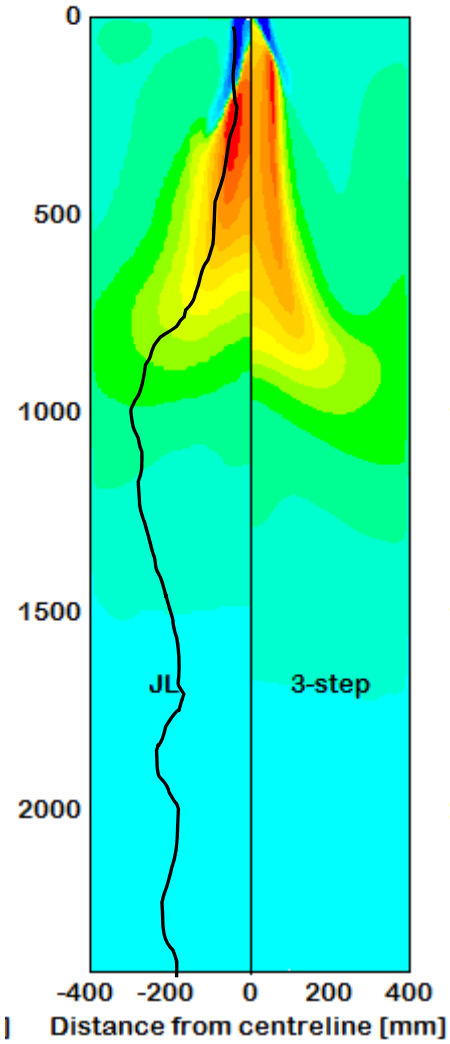
- Sub-models:
  - k-ε Realizable turbulence model
  - Eddy Dissipation Concept
  - Discrete Ordinates model with a WSGG model for oxy-fuel conditions (grey)
- Flame shape
  - JL predicts a wider and shorter flame than the oxy-fuel derived mechanisms
- Concentration of CO
  - JL and 3-step yield the predictions which are most in line with measured data

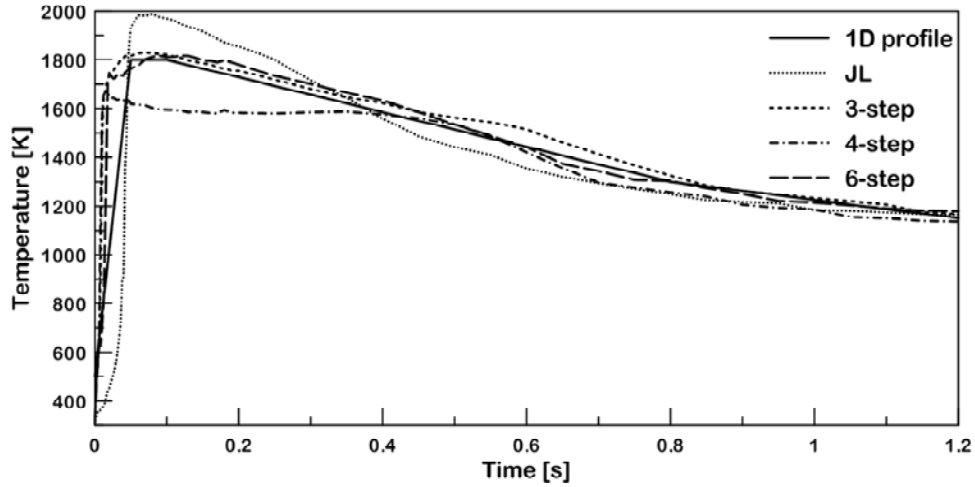


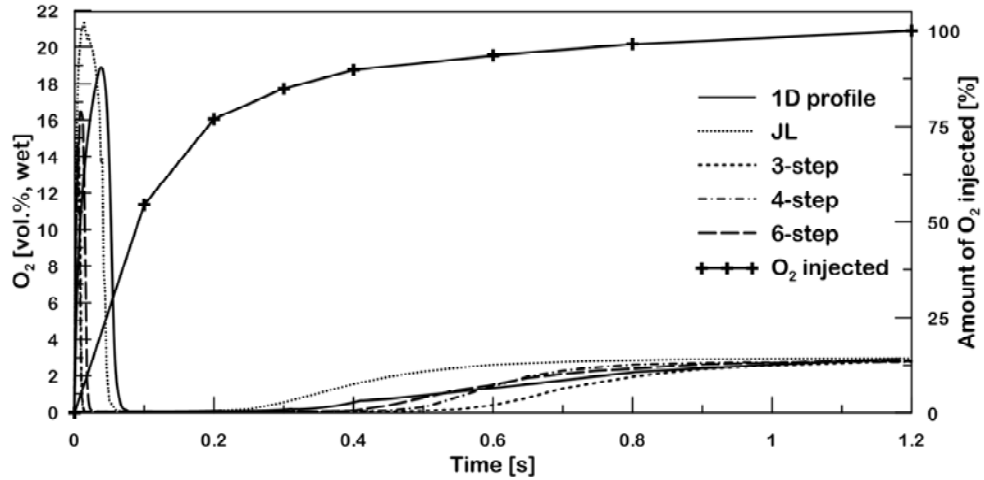
Generation of 1D-Model

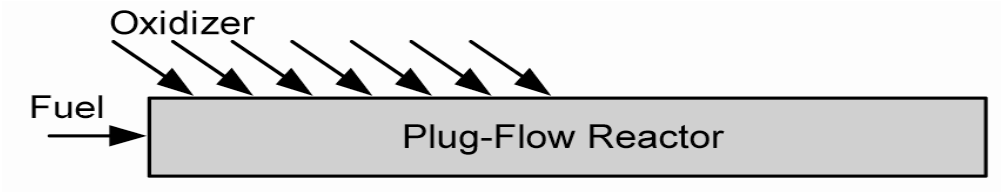


- Traced a “particle” from the fuel inlet throughout the furnace
- Recorded O_2 concentration and temperature


0
500
1000
1500
2000
JL
3-step
-400
-200
0
200
400
Distance from centreline [mm]

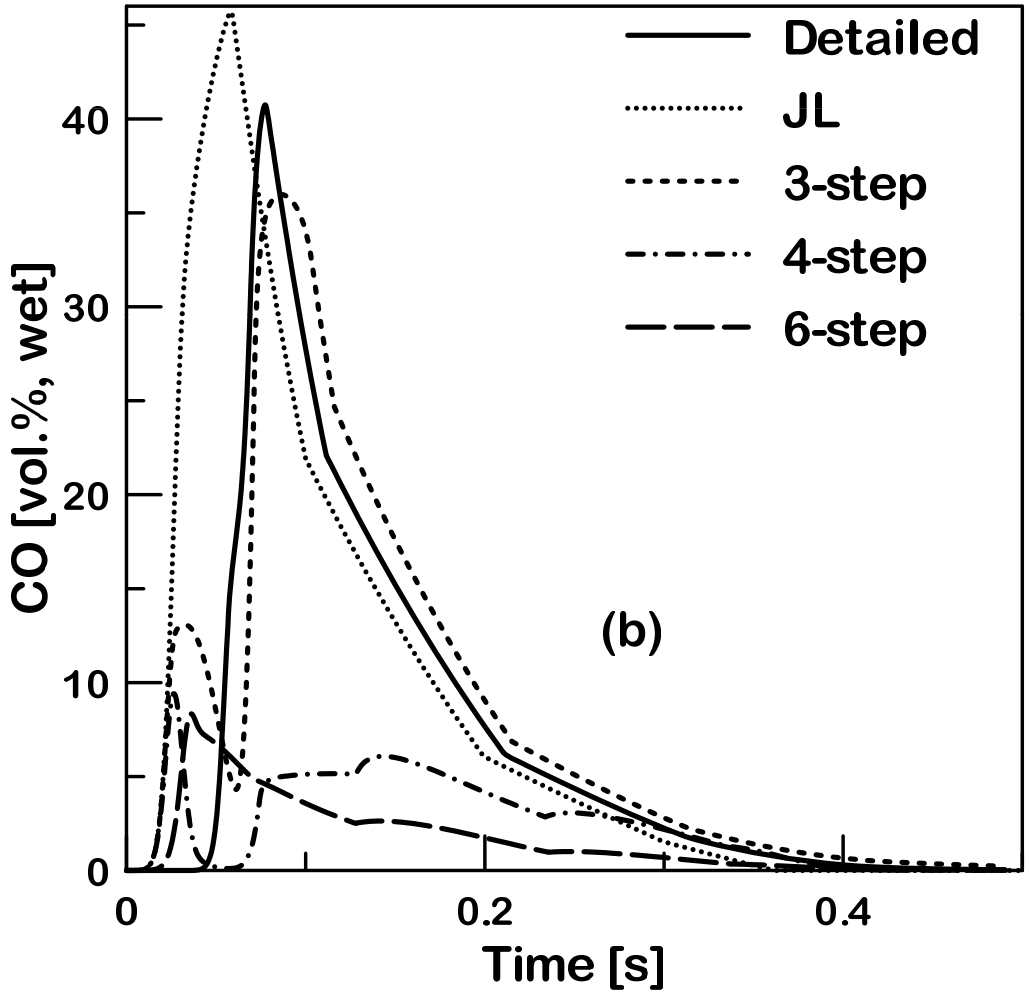

Temperature [K]
Time [s]
1D profile
JL
3-step
4-step
6-step


O2 [vol.%, wet]
Amount of O2 injected [%]
Time [s]
1D profile
JL
3-step
4-step
6-step
O2 injected


Oxidizer
Fuel
Plug-Flow Reactor

Comparison – CO concentration

- The propane-fired Chalmers 100 kW OF27 flame
- Includes comparison with a detailed scheme
- Path-line data from CFD calculations is used in the PFR model
  - Temperature
  - O_2 concentration
- Large discrepancies between the global models.



Comparison - Reaction Dynamics

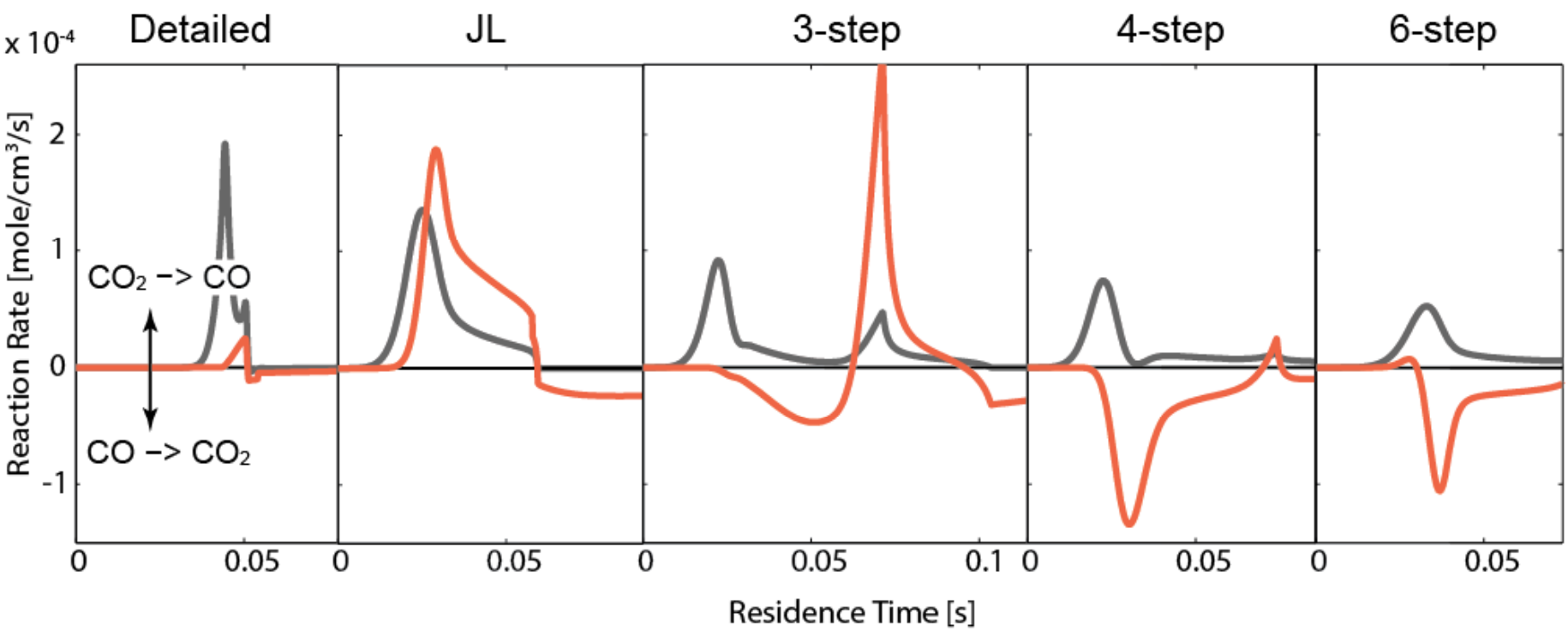
Fuel Oxidation

$$C_3H_8 + 1.5\ O_2 \rightarrow 3\ CO + 4\ H_2$$

CO Oxidation

$$CO + 0.5\ O_2 \leftrightarrow CO_2$$

$$CO + H_2O \leftrightarrow CO_2 + H_2$$



Conclusion

- There is a significant improvement potential for global oxy-fuel reaction mechanisms and, thus, a need to develop a refined global reaction mechanism.
- Simply adjusting the reaction parameters to compensate for quantitative errors (such as over-predicted CO concentration or combustion temperature) may lead to errors in the reaction dynamics
- A qualitatively incorrect behavior reduces the generic nature and applicability of the mechanism.

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http://www.chalmers.se/en/projects/Pages/forbrannings--och-koldioxidinfangningstekniker.aspx