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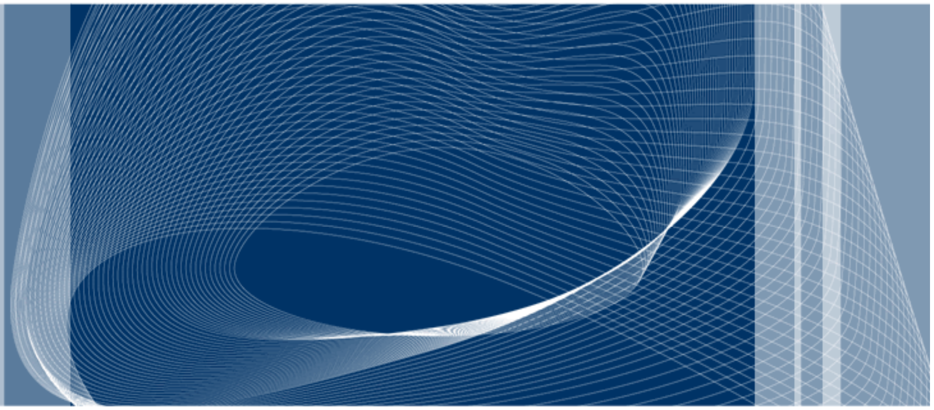

Simplified kinetic schemes for oxy-fuel combustion

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Outline

- CFD modeling of turbulent reacting flows

  Challenges for large-scale applications (industrial) – **oxy-fuel combustion**
- Role of detailed kinetics for pollutants prediction

  Coupling of detailed chemistry and fluid dynamics ⇒ Post Processing techniques

Cooperation with **More srl**

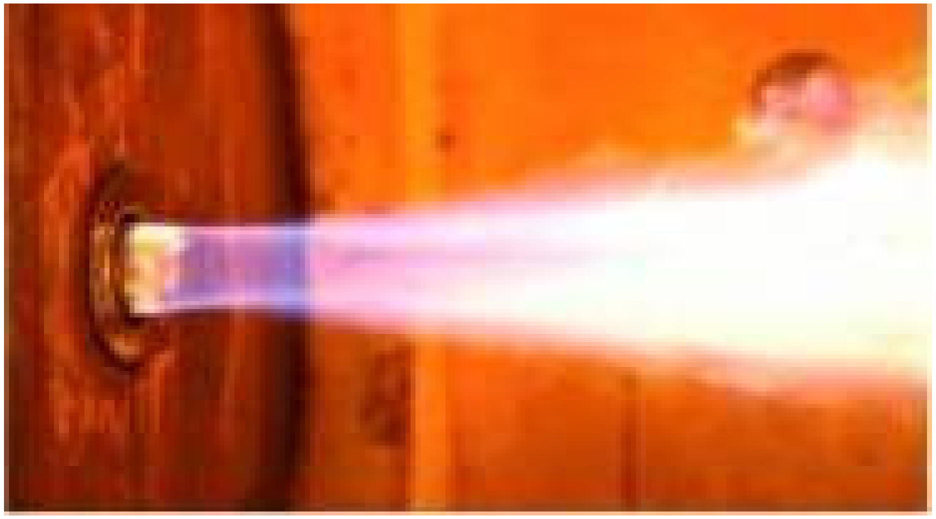
  - CFD modeling of heating systems (oxy-combustion)
  - **Need to predict temperature fields and emissions (NOx)**
- Assessment of Simplified (Global) kinetic mechanisms
  - Westbrook-Dryer and Jones-Lindstedt mechanisms
  - **Not applicable (directly) to oxy-fuel combustion**
- Methodology to calculate **optimized global schemes**
  - Minimizing the “distance” between Detailed Kinetic Mechanism and the optimal global mechanism
  - Role of dissociation reaction (radicals) peculiar of oxy-combustion
  - Effect on NOx prediction

Oxy-combustion

- CFD modeling of turbulent reacting flow

Oxidant:

pure oxygen or enriched air



High NOx emissions in case of presence of N_2 even in traces

Absence (or reduced) N_2

Very High Temperatures (T>2600-2800 [K])

High radiative heat transfer - Efficiency

Easier CO_2 capture. Reduced volume of the fue gases

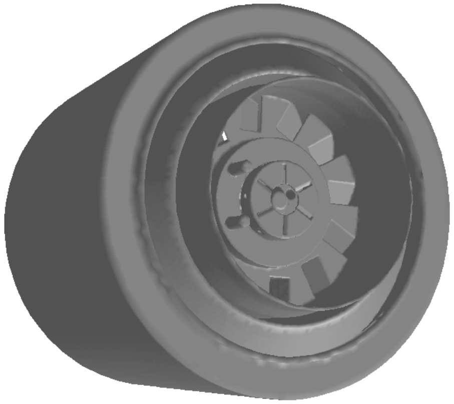
CFD modeling of flames, burners, furnaces

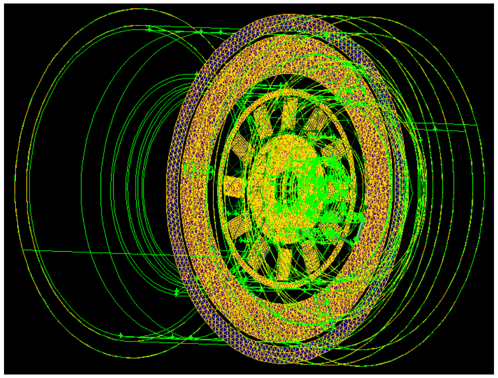
Computational Fluid Dynamics is a design tool for several engineering applications.

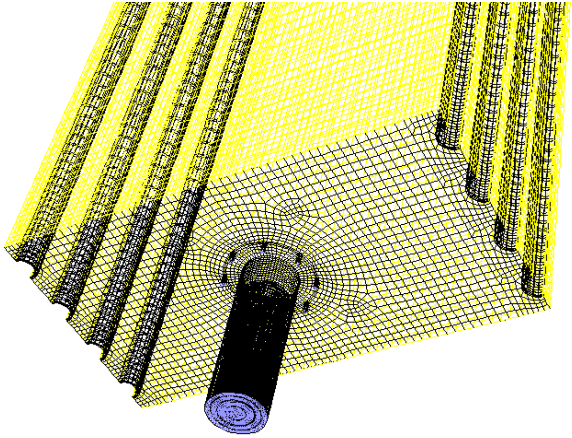
This presentation focuses on CFD modeling of **turbulent reacting flows (oxy-fuel combustion)**

The modeling of such systems requires the numerical solution of balance equations (mass, energy..) → 3D computational grids

Due to complex geometries, computational grids typically exceed 1-3 million elements

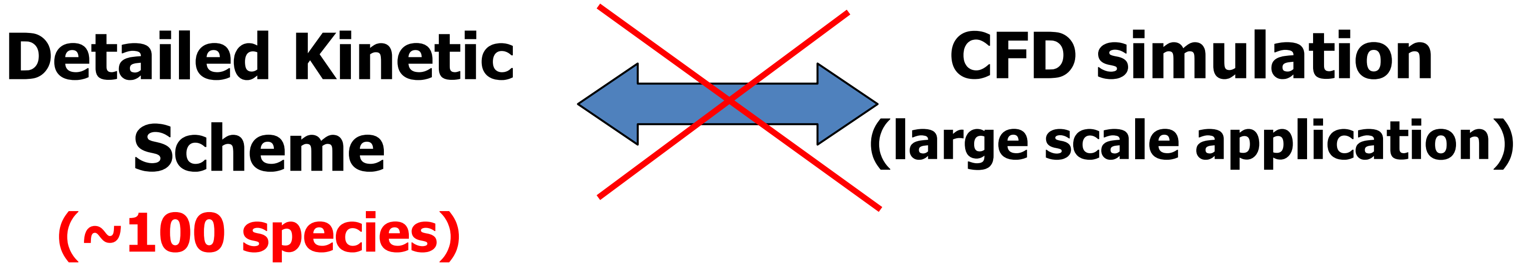






Kinetic mechanisms for CFD applications

Combustion is a complex process that involves **hundreds of species** and thousands of chemical reactions.



Detailed Kinetic Scheme

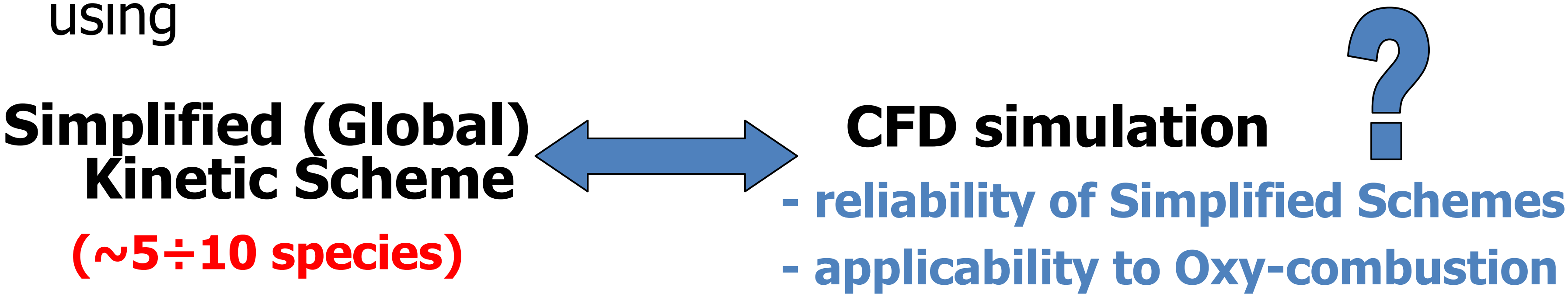
(~100 species)

CFD simulation

(large scale application)

Detailed kinetic mechanisms are available but cannot be handled by CFD codes…

…CFD simulations of complex geometries and large-scale application (practical industrial applications) are performed using



Simplified (Global) Kinetic Scheme

(~5÷10 species)

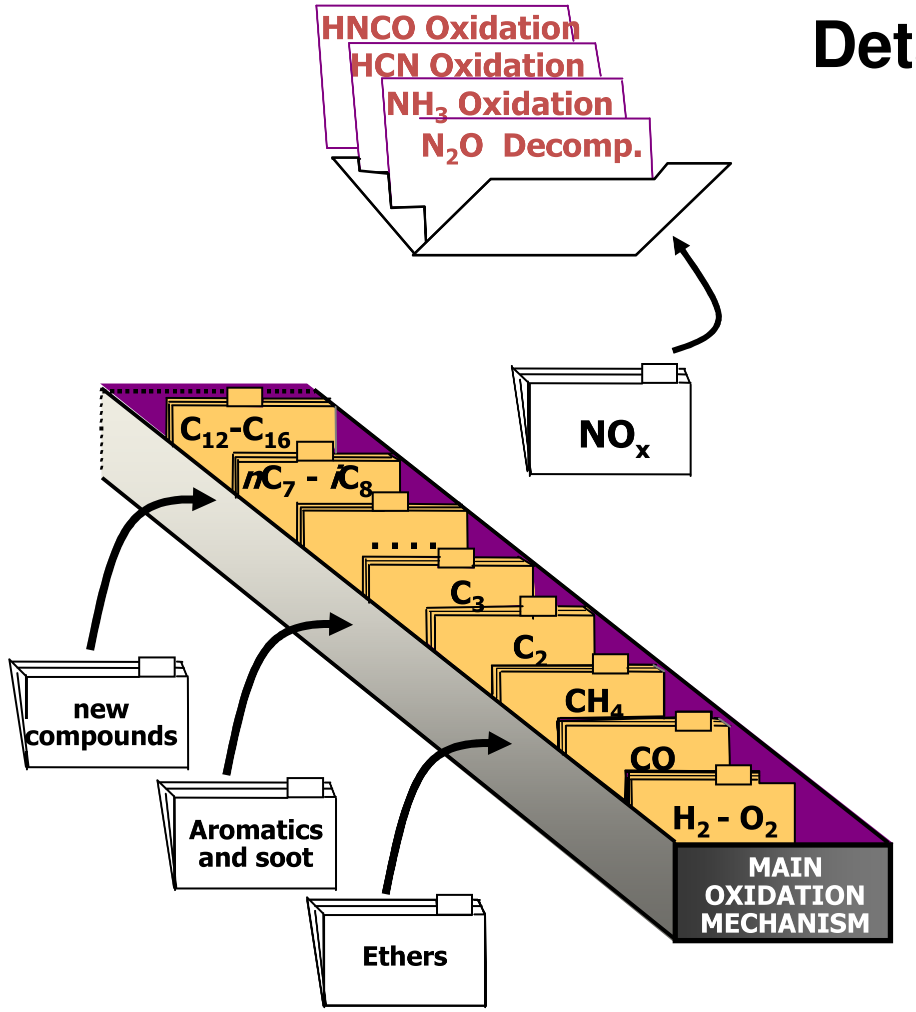
CFD simulation

- reliability of Simplified Schemes

- applicability to Oxy-combustion

Detailed Kinetic Mechanism (DKM)

(hundreds of species – thousands of reactions)



Starting Point:
Detailed Kinetic Mechanism

- Hierarchy and Modularity
- Analogies and similarities of reactions
- Simplifications and lumping

- Natural Gas
- Gasolines
- Kerosene & Jet Fuels

  (Surrogates)
- Biofuels

  Alcohols, biomasses,…
- Pollutants

  NOx, PAH, Soot,…

Ranzi et al.,
http://www.chem.polimi.it/CRECKModeling/

Global Mechanisms for CH_4: literature

Westbrook and Dryer

(1984): 2 steps and 6 species

$CH_4 + 3/2\ O_2 \rightarrow CO + 2\ H_2O$

$CO + 1/2\ O_2 \leftrightarrow CO_2$

Jones and Lindstedt

(1988): 4 steps and 7 species

$CH_4 + ½\ O_2 \rightarrow CO + 2\ H_2$

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

$CO + H_2O \leftrightarrow CO_2 + H_2$

$H_2 + ½\ O_2 \leftrightarrow H_2O$

$$aA + bB \rightleftharpoons cC + dD$$

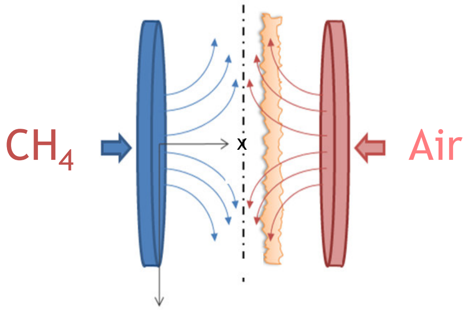
$$r_{rate} = A \cdot T^n \cdot e^{(-E/RT)} \prod_{i=1}^{NS} C_i^{\upsilon_{f,i}}$$

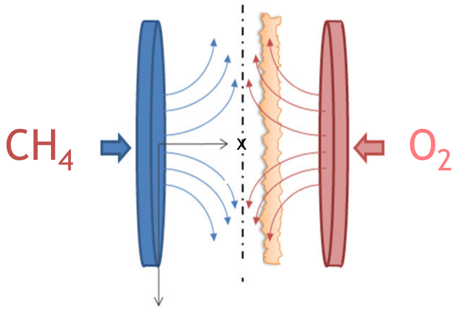
Reaction rate based on apparent global rate parameters empirically determined for **Air flames at 1 atm**.

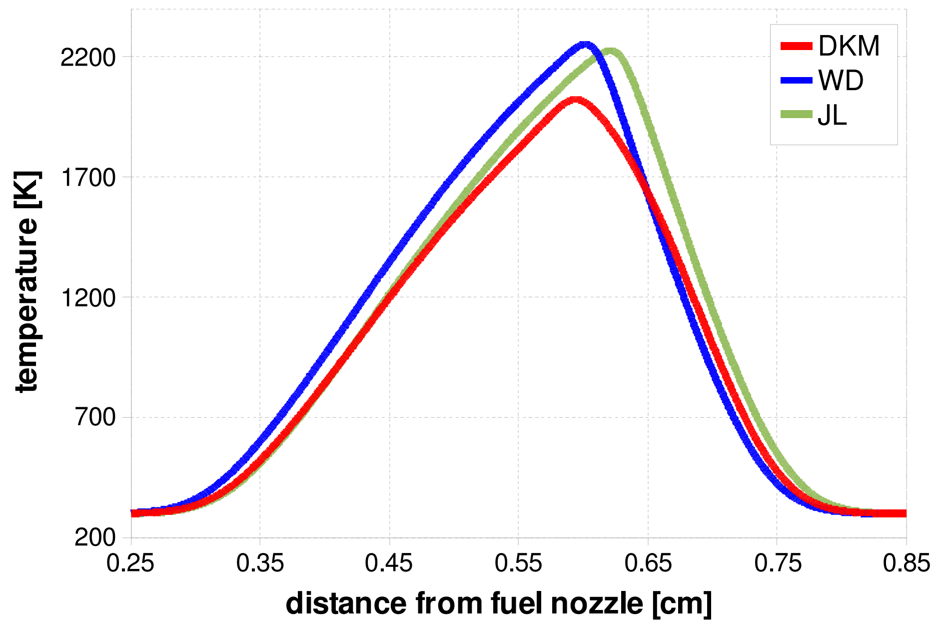
=>**How well do they perform in oxy-combustion**?

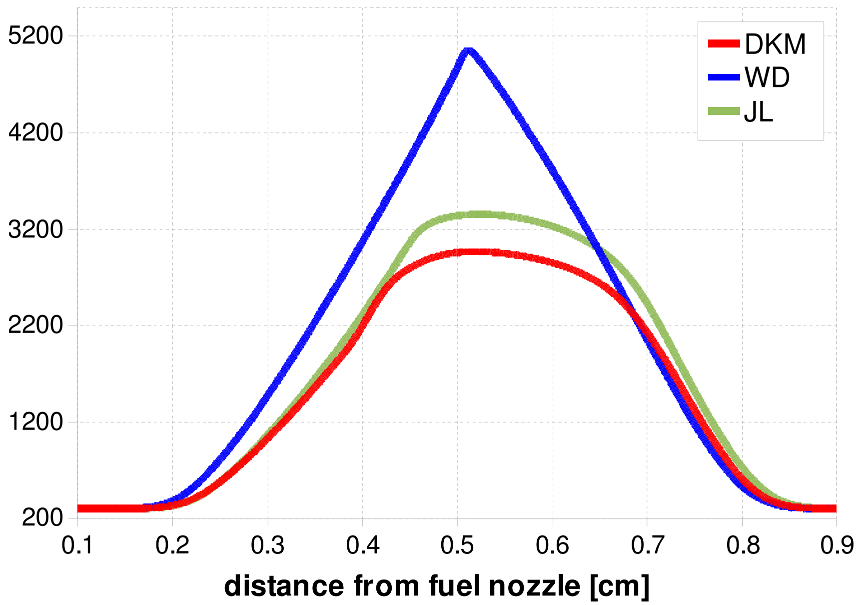
(=>**How well do they perform at high pressure**?)

Counterflow Flame Calculations (Flamelets)









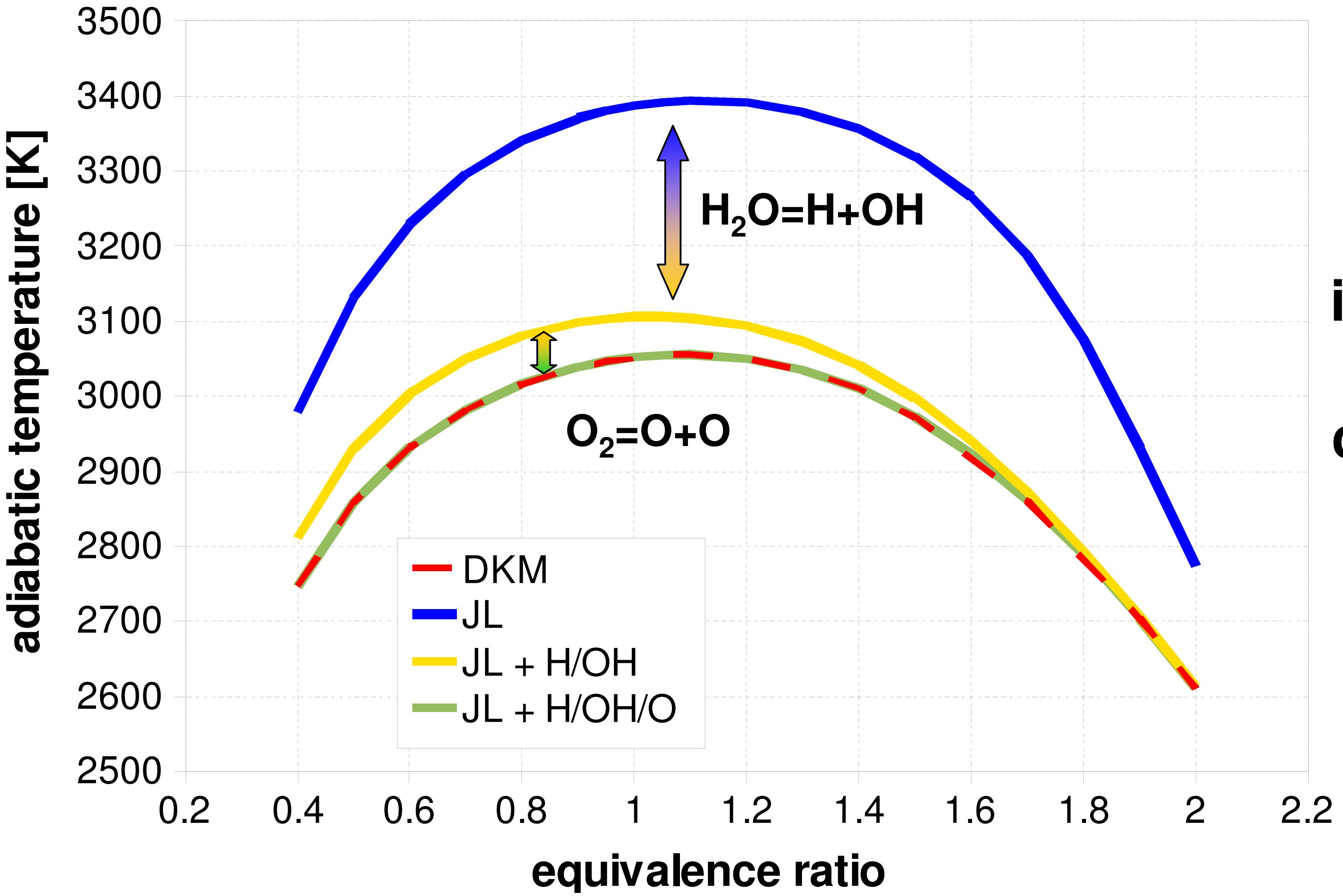
Global mechanisms contain only molecular species

=> **Bad performance in oxy-combustion**: role of dissociation reactions forming H_2, but also radicals H, OH, O

Simple equilibrium calculations

JL mechanism contains 6 species: CH_4, O_2, CO, CO_2, H_2O, H_2

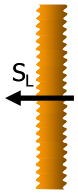
JL overestimates adiabatic T in oxy-combustion of ~350 K if compared to Detailed Kinetic Mechanism (DKM)



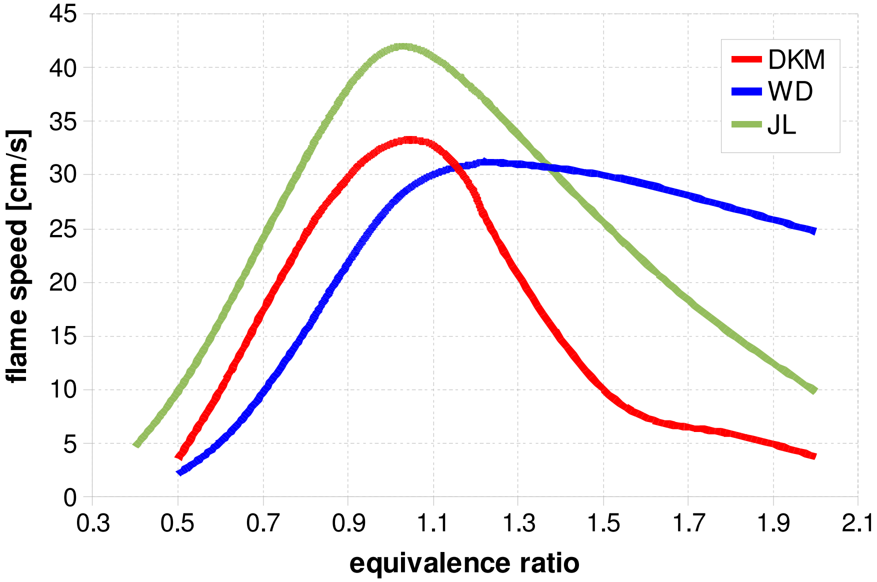
H, OH, O must be included for oxy combustion

6+3=9 Species

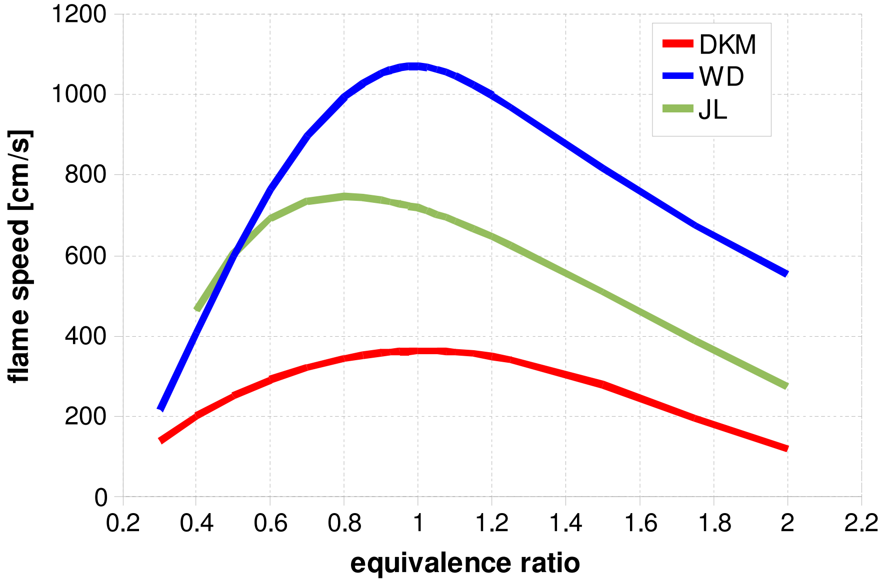
Flame Speed calculations



Air



Oxy-combustion



Also Flame Speed is overestimated

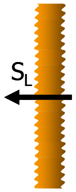
JL is better than WD especially in rich conditions (H_2)

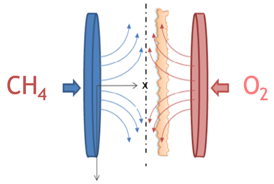
⇒ **Need to improve JL** (WD not interesting)

⇒ Use **optimization technique** (new reaction rate parameters)

Optimization Procedure

Variation of Rate Parameters (A,E,ν_i)





Simulation of a simple but meaningful reaction system

Comparison (deviation) SSErrors

min SSError function (T,Flame speed, etc)

min

JL scheme optimized

(Experimental Data)

Calculation with Detailed Kinetic Mechanism

New Mechanism: JL^{modified}, 6 steps

$CH_4 + ½\ O_2 \rightarrow CO + 2\ H_2$

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

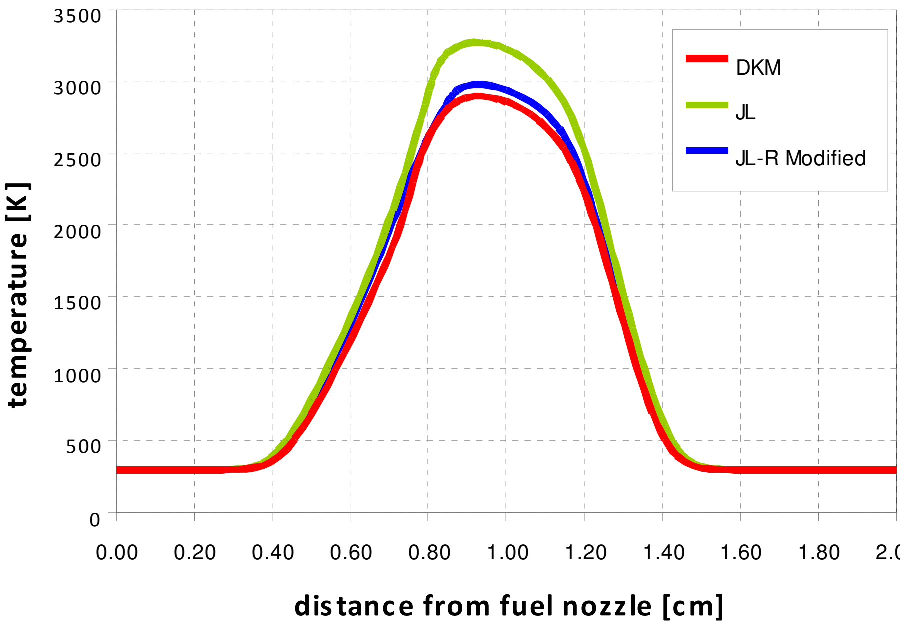
$CO + H_2O \leftrightarrow CO_2 + H_2$

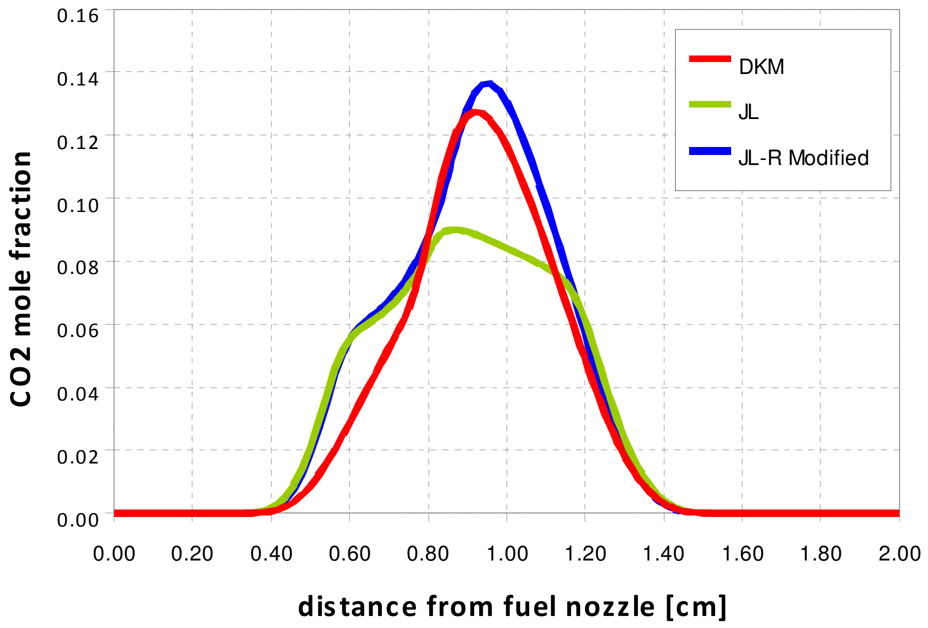
$H_2 + ½\ O_2 \leftrightarrow H_2O$

$H_2O \leftrightarrow H + OH$

$O_2 \leftrightarrow O + O$

Reaction	Parameter	Original Value	Optimized Value
1	A	$2.75 \cdot 10^{9}$	$2.63 \cdot 10^{10}$
1	E_a	20000	18500
2	A	$6.70 \cdot 10^{15}$	$6.80 \cdot 10^{14}$
2	E_a	40000	37700
3	A	$1.25 \cdot 10^{17}$	$1.07 \cdot 10^{18}$
3	E_a	98000	94000
2	υ_{f,H_2}	0.25	0.33
2	υ_{f,O_2}	1.50	1.40

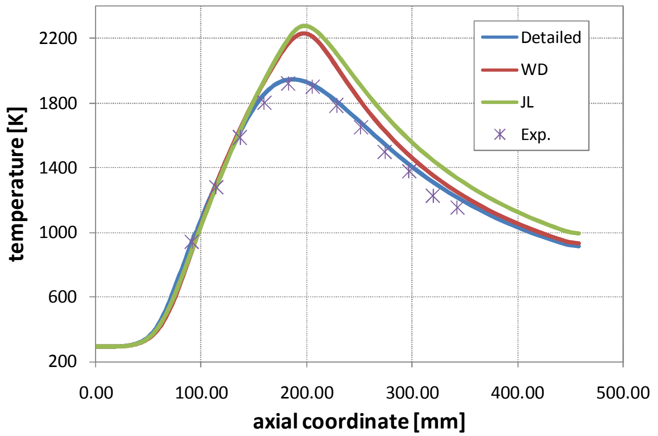


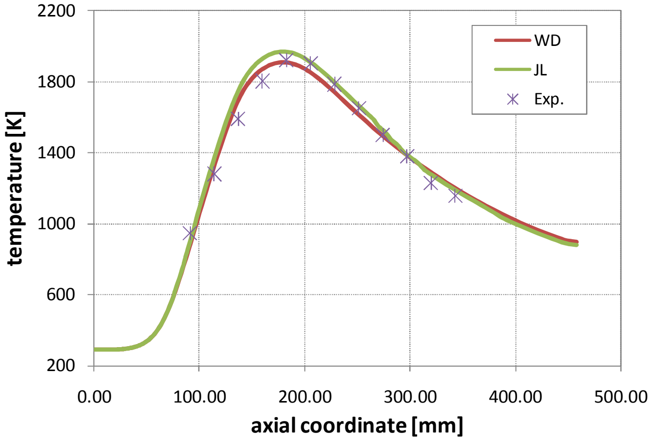


CFD simulations using optimized mechanisms

The improvement in CFD simulations is the same as the one obtained in counterflow flame calculations

Example: syngas/air turbulent flame (Cuoci et al, 2009)





Conclusion #1: Optimization procedure

-based on a series of **simple but physically meaningful** calculations (counterflow flame and flame speed)

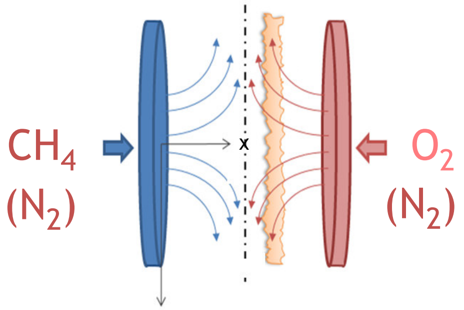
-allows to **automatically derive a global scheme** for the particular application (**oxy-combustion**, high pressures, new fuels, very lean conditions, H_2-enriched fuels)

-greatly improves the prediction of Temperature<=>NOx?

NOx emissions in oxy-flames

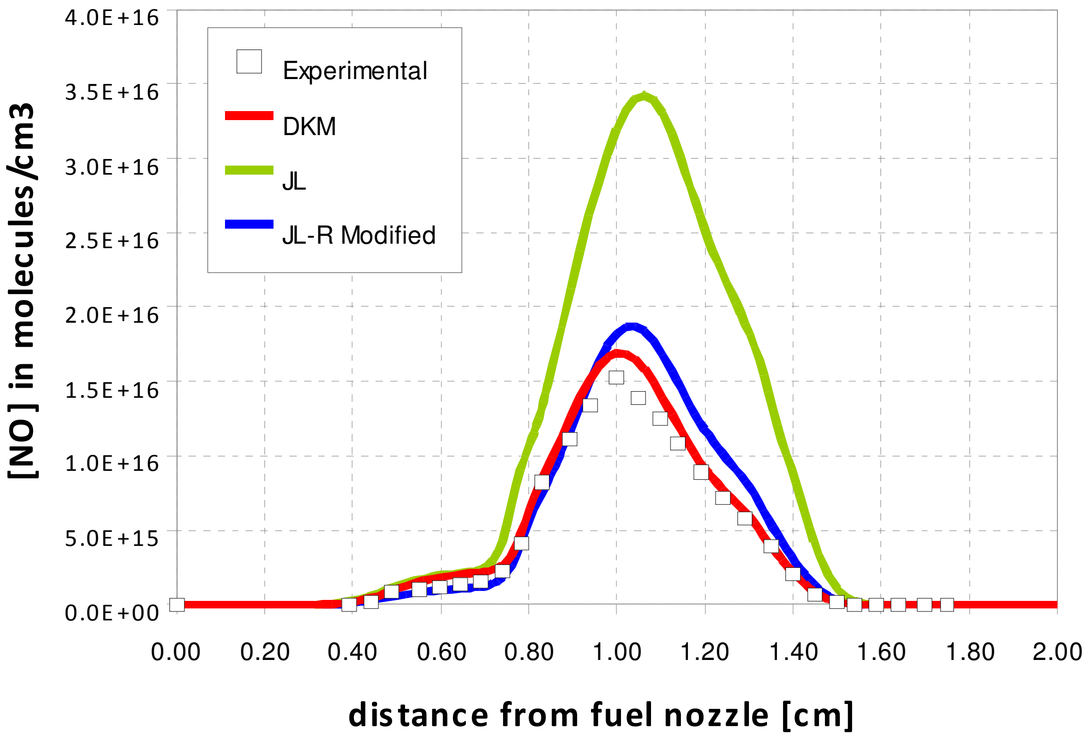
NOx emissions are typically calculated through **post- processing CFD calculation** => good prediction of temperature is needed

Study the effect of JL/JL^{modified} on NOx predicions in a counterflow diffusion flame. NOx calculated with DKM in a post-processing step.

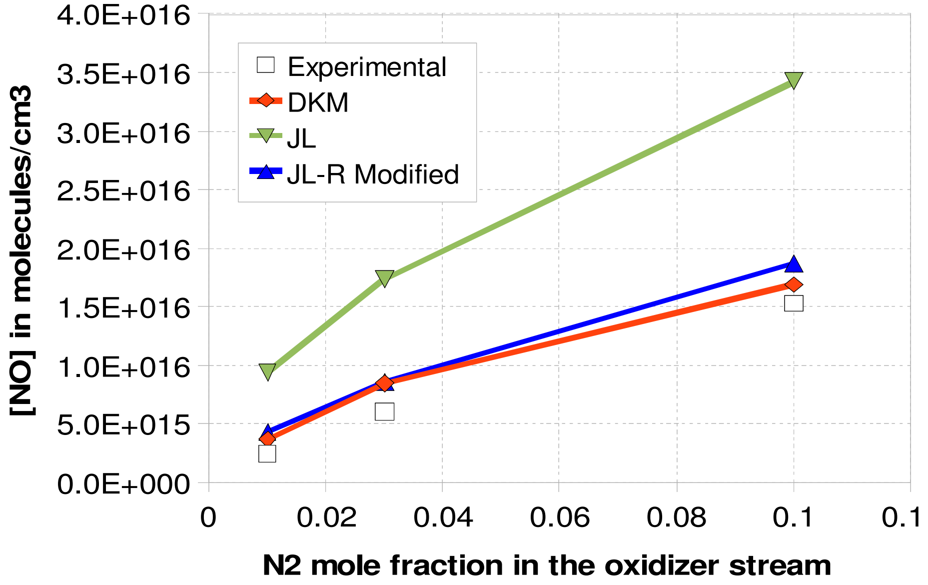


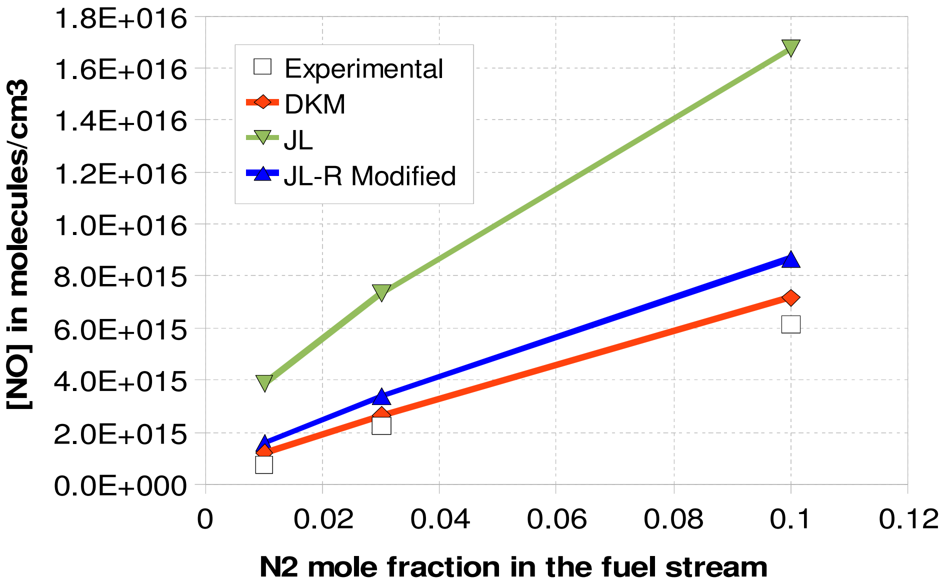
N_2 added in variable amounts to the fuel or to the oxidizer

Exp [Naik et al., C&F 2002, Purdue University]



NOx emissions in oxy-flames





- **Good agreement** between exp data and model prediction **(DKM)**
- Assuming the **original JL** temperature profile leads to **NOx overestimation** (double)=>not suitable for CFD simulations and post-processing
- The $\mathbf{JL}^{\mathbf{modified}}$ is able to predict correctly the **flame temperature** =>suitable for **CFD simulations**

(DKM is in better agreement because it includes soot (radiation))

Conclusions

- Need of simple but reliable global mechanism for CFD
- Problem: **Global mechanism are not general**

  => tailored for specific applications

  =>**lack of mechanisms for oxy-combustion**, high pressure and new fuels

- Procedure to **optimize existing mechanism**
  - Minimizing the distance form the detailed kinetic mechanism (general)
  - Distance: T, species profiles in Counterflow flames and flame speeds
  - Need to include dissociation reactions (H,OH,O)
- Comparison with experimental data
  - Optimized mechanism is very close to exp data in terms of temperature and NOx predictions

- Future work: use the $JL^{optimized}$ mechanism for CFD simulations of oxy-fuel turbulent flames
- Include simplified model for soot formation