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MODELLING METHANE COMBUSTION UNDER MAST CONDITIONS

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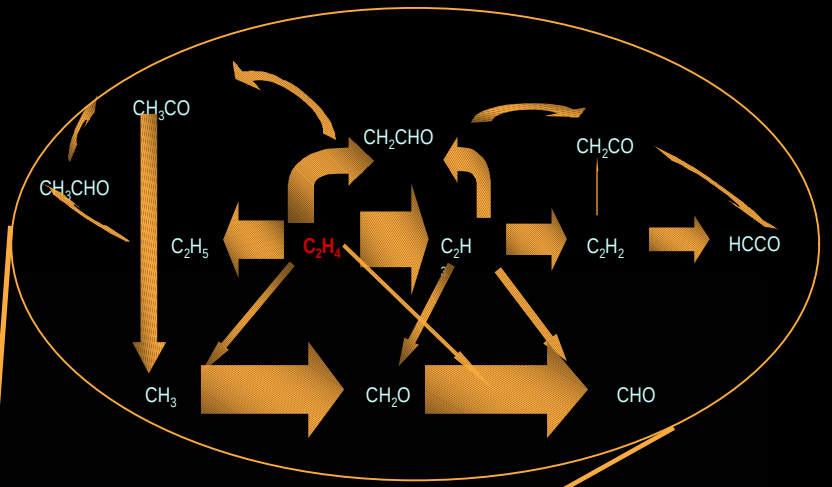
The Practical Problem

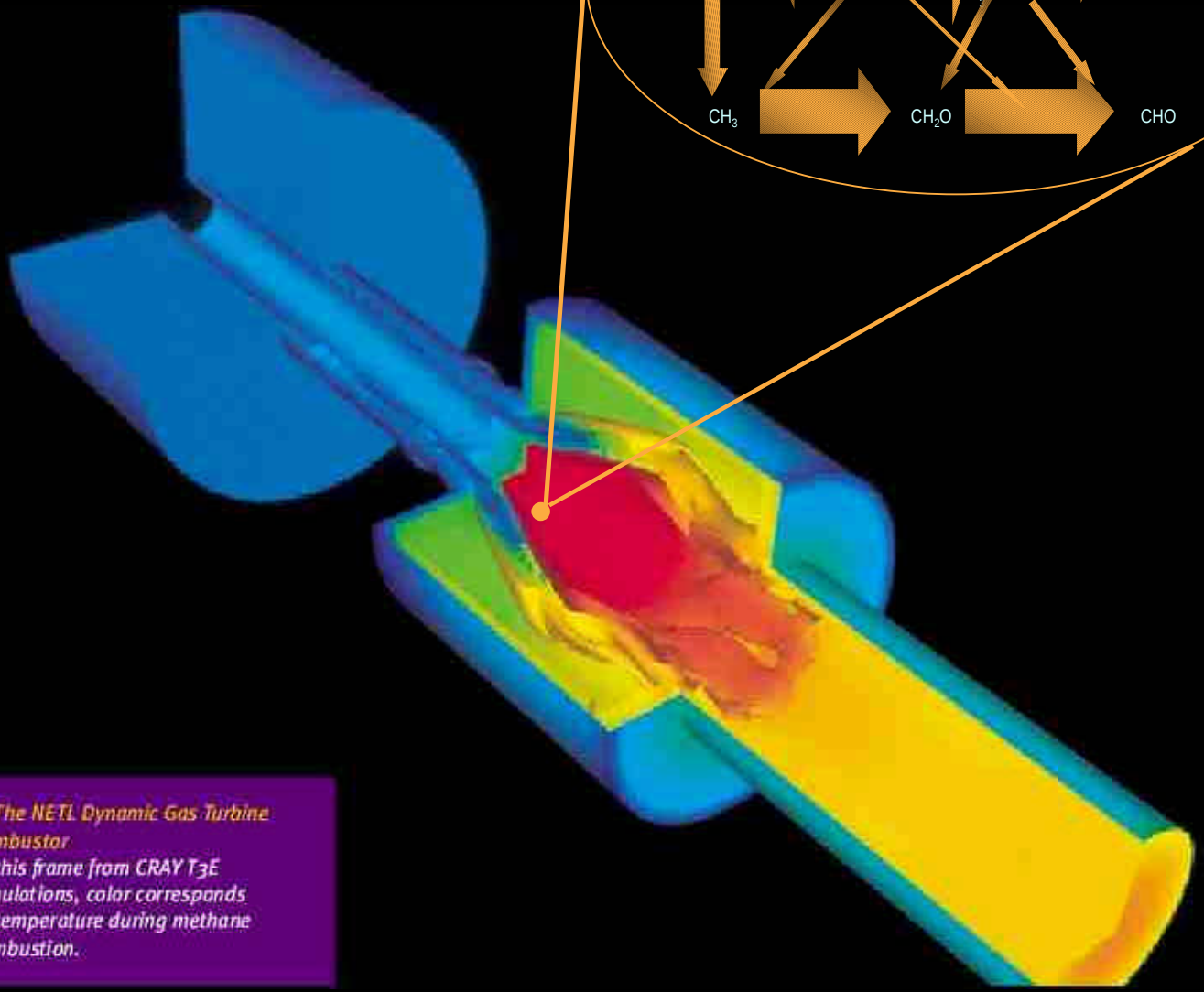
- Lower emissions while retaining efficiency and power output from power generating gas turbines
- Water or steam addition to gas turbine combustor increases turbine mass flow and output power (e.g., Horlock, 1998)
- Reduction of nitrogen oxide emissions in premixed and non-premixed modes of operation (e.g., Bhargava *et al*., 2000)

Objectives

- Combustion chemistry and flow-chemistry interactions under high-pressure and high-humidity conditions
- Simulations of turbulent flow field with realistic chemistry
- Development of systematically reduced kinetic mechanisms

Reduced Mechanisms





▲ *The NETL Dynamic Gas Turbine Combustor*
In this frame from CRAY T3E simulations, color corresponds to temperature during methane combustion.

Reduced Mechanisms
CSP Formulation

The CSP algorithm constructs a reduced mechanism given a detailed kinetic mechanism (K reactions, N species, E elements), a numerical solution to the physical problem and the desired number of global steps (N-M-E)

$$\frac{\partial \mathbf{y}}{\partial t} = \mathbf{L}(\mathbf{y}) + \mathbf{g}(\mathbf{y})$$

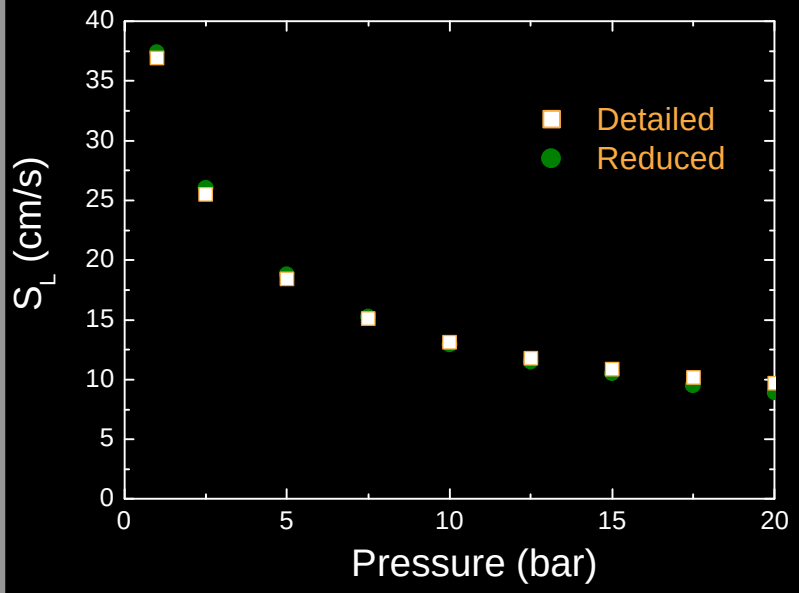
Mechanism reduction through use of steady-state approximations

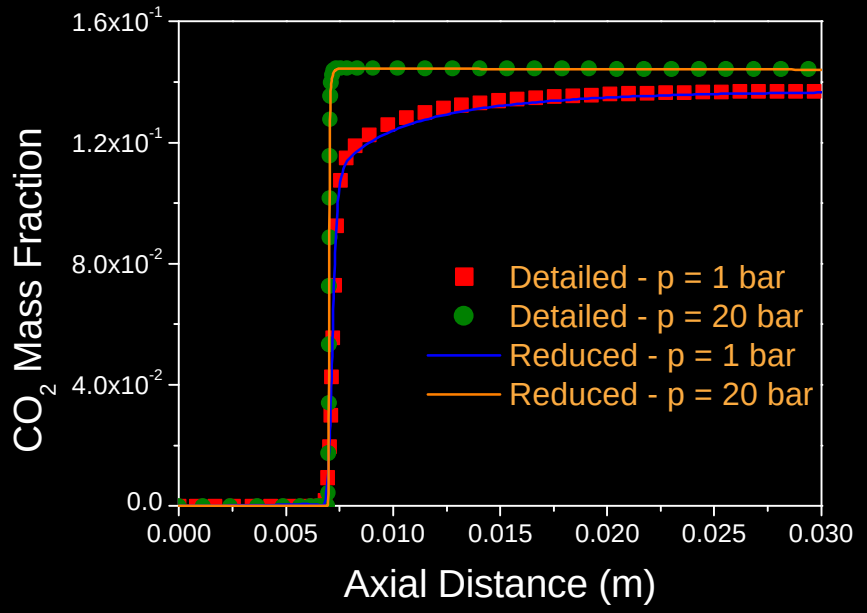
Detailed chemistry of GRI-3.0 mechanism (53 species and 325 elementary reversible reactions)

Reduced Mechanisms
Validation

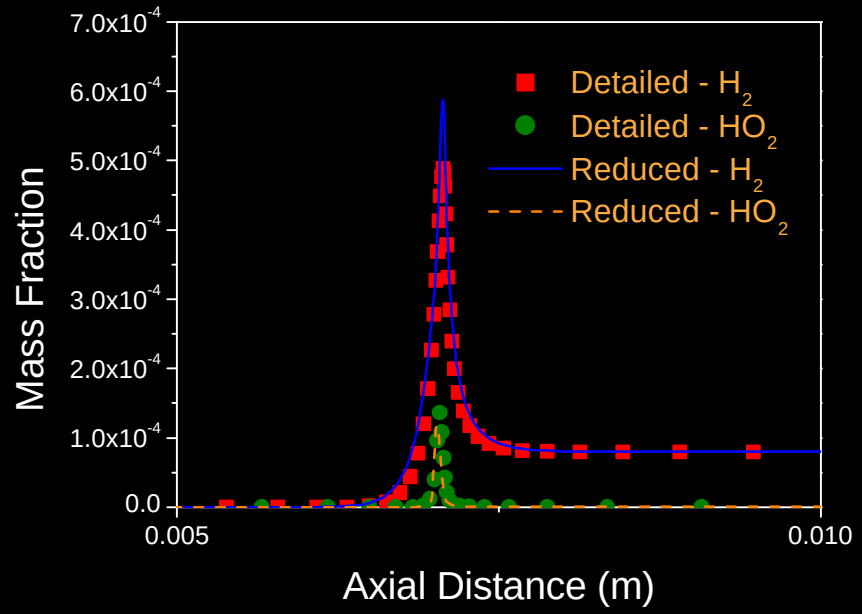
I	CH_4	+	OH	=	CO	+ $2.5H_2$
II	$2CO$	+	O_2	=	$2CO_2$	
III	$2H_2$	+	O_2	=	$2H_2O$	
IV	H_2	+	O_2	=	$2OH$	
V	H_2			=	$2H$	
VI	N_2	+	$0.5O_2$	=	N_2O	
VII	$0.5N_2$	+	$0.5O_2$	=	NO	

Methane-Air flame,
p = 1 bar, ƒ = 1.00
GRI-3.0 mechanism





Reduced Mechanisms
MAST Chemistry



Methane-Air flame, p = 20 bar, ƒ = 1.0,
T_{in} = 500 K, w =20%
GRI-3.0 mechanism

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T_{in} = 500 K
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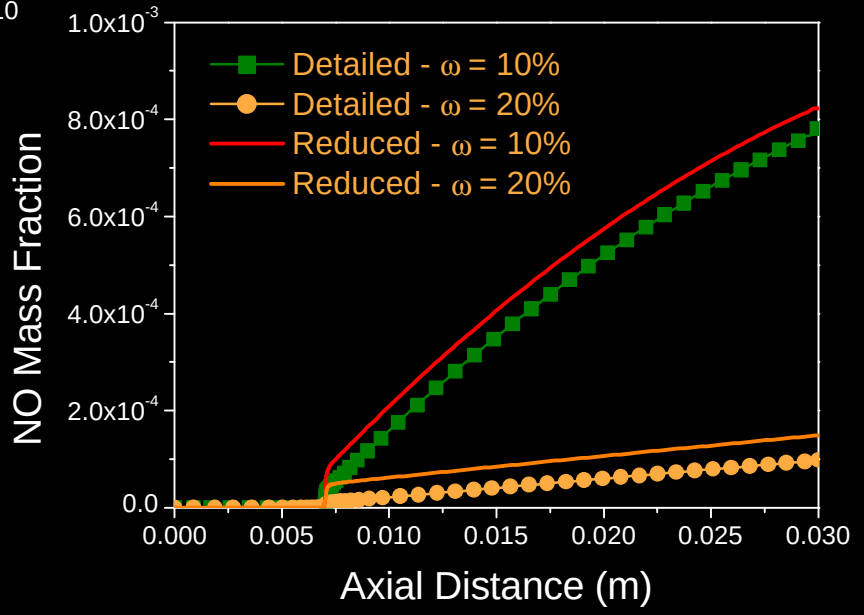


Humidity and Combustion Chemistry

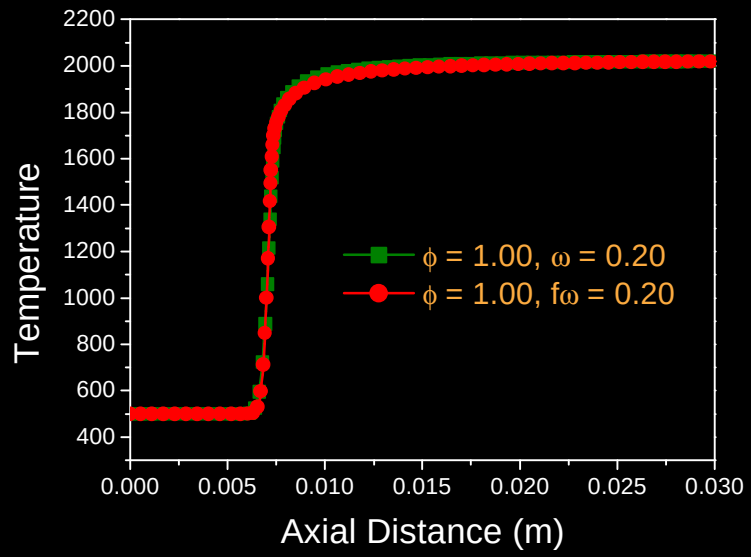
Combustion chemistry dynamics at high humidity ratios.

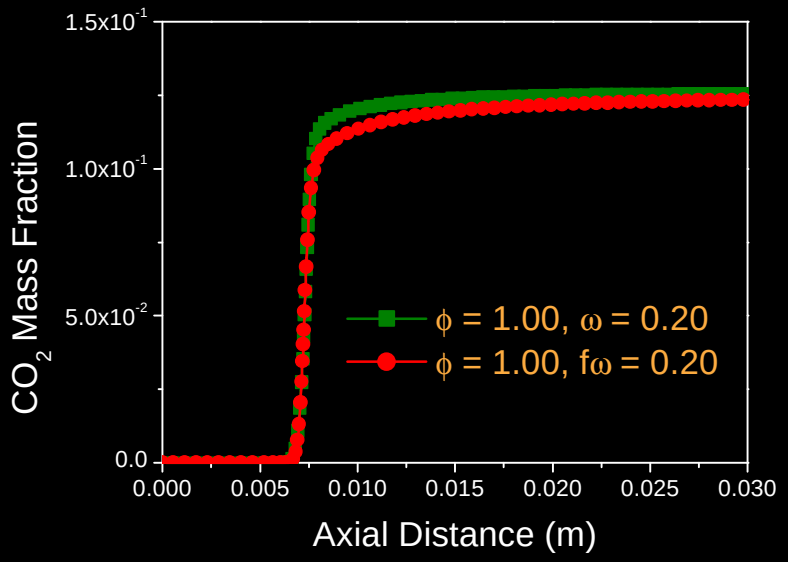
- Temperature effects (e.g. Dlugogorski *et al.*, 1998)
- Chemical effects (e.g. Zhao *et al.*, 2002)
- Dilution effects

- Replace ***normal*** water with ***fictitious*** water (same thermochemical and transport properties but no participation in chemical reactions – e.g. Liu *et al.*, 2001)
- Global flame structure and reaction path analysis
- CSP analysis for pollutants and crucial intermediates

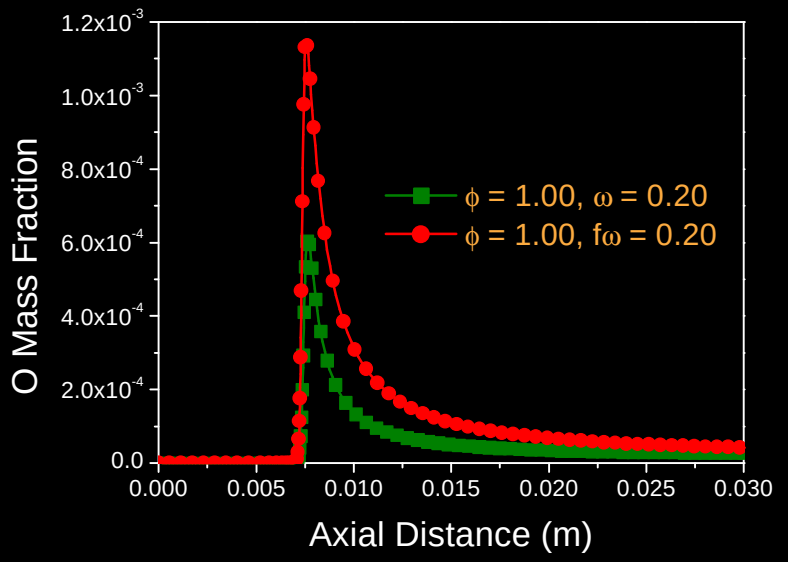
Humidity and Combustion Chemistry

Flame Structure



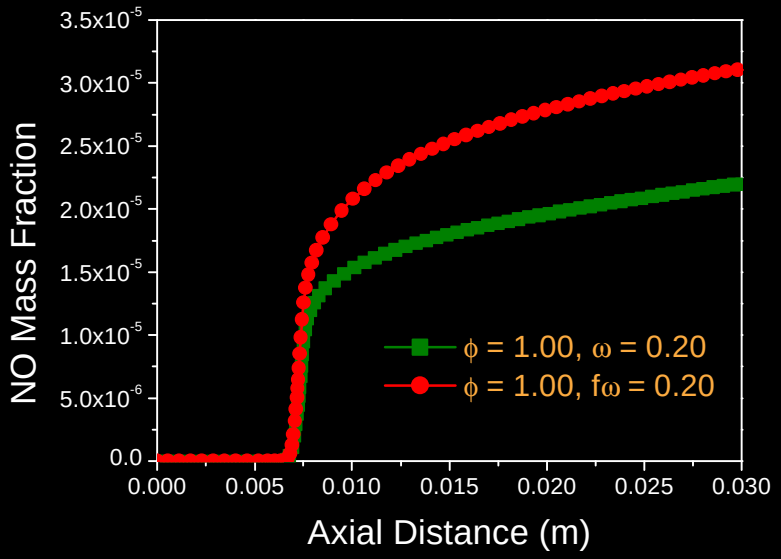


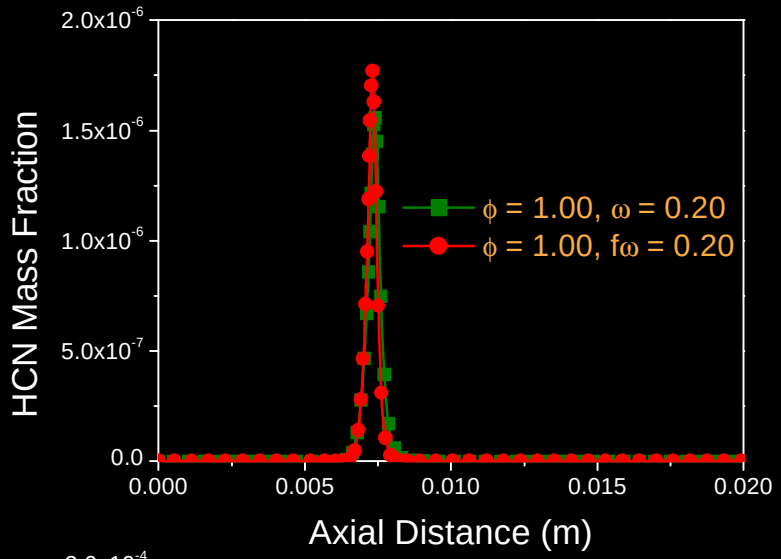
Methane-Air flame, p = 1 bar, f = 1.0,
T_{in} = 500 K, w =20%
GRI-3.0 mechanism



Humidity and Combustion Chemistry

Pollutants





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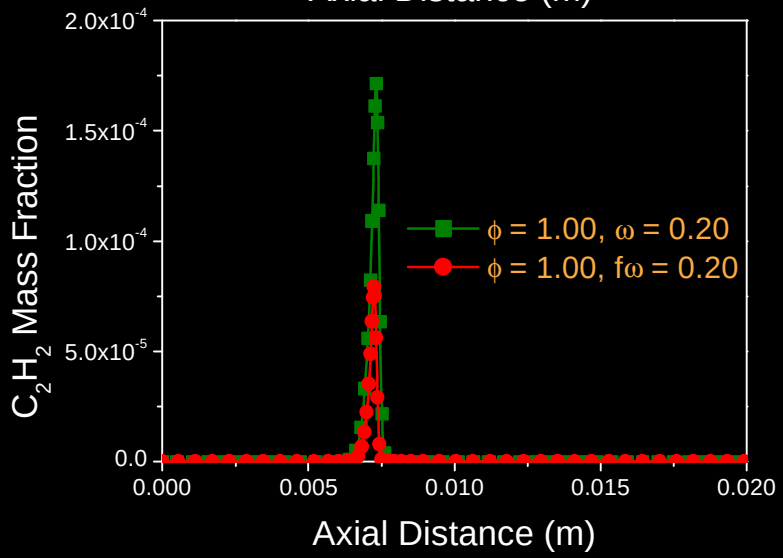


Humidity and Combustion Chemistry
Reaction Path Analysis

- Oxygen atom suppression through reaction

$$O + H_2O = OH + OH$$

- Reduction in thermal NO concentration

$$O + N_2 = NO + N$$

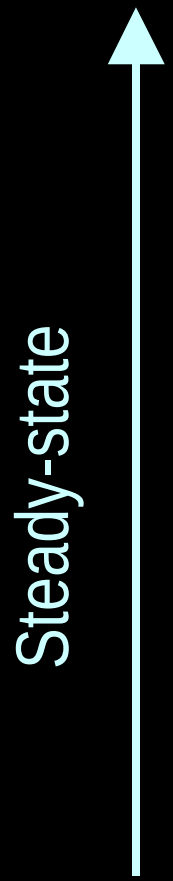
- Increase in acetylene levels due to slower consumption reactions

$$C_2H_2 + O = {}^3CH_2 + CO$$

$$C_2H_2 + O = HCCO + H$$

Humidity and Combustion Chemistry

Integrated CSP Pointers



Integrated CSP Pointers		
	Normal Water	Fictitious Water
20	NO	C_2H_4
19	C_2H_6	C_2H_6
18	O	C_2H_2
17	HCN	HCN
16	CH_3	CH_3
15	H	O
14	OH	H
13	C_2H_2	OH
12	CH_2CO	CH_2CO
11	C_2H_4	NO
10	CH_4	HCNO
9	HCNO	CH_4
8	N_2O	N_2O
7	H_2	H_2
6	O_2	O_2
5	CO	CO
4	H_2O	H_2O
3	CO_2	CO_2
2	N_2	N_2
1	Ar	Ar

Humidity and Combustion Chemistry
Conclusions

- Humidity *does not* appear to significantly alter overall flame structure
- Significant O atom suppression through elementary reaction $O + H_2O = OH + OH$
- *Thermal* NO chemistry influenced by humidity
- Substantial increase in acetylene levels!

Does humidity enhance soot formation? **Possibly**

Do we need further investigations? **Definitely**

The FIRST Model
Formulation

- Reaction progress is modelled through Reaction Progress Variables (RPV's).

-RPV's are linear relations amongst species mass fractions

-RPV's are governed by transport equations which replace the species equations.

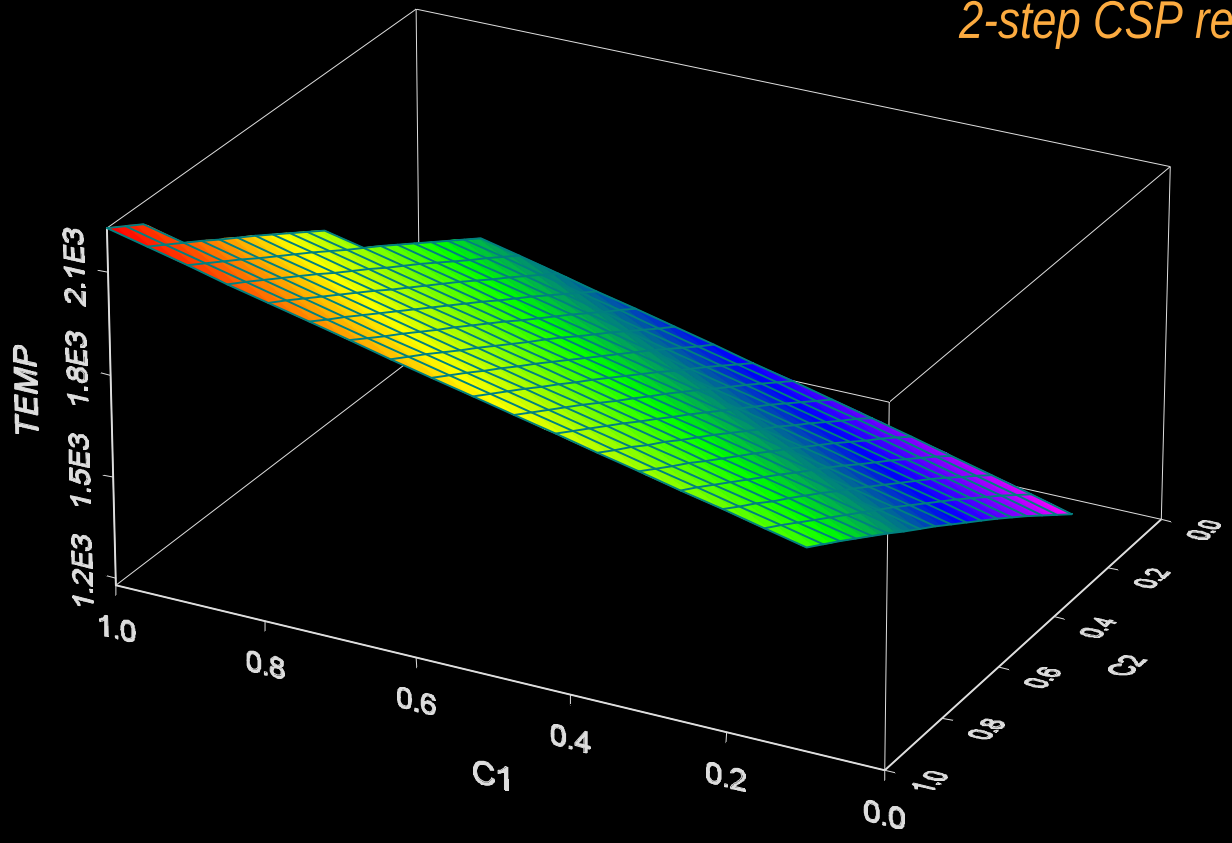
-RPV's constructed by CSP guarantee that the simplified problem is the most accurate and the least stiff, accelerating considerably the computational speed.

-In a pre-processing step data files are constructed for RPV source terms as a function of the RPV's, which are later used in the CFD computations.

The FIRST Model

Results

Methane-Air flame,
p = 1 bar, f = 1.00
2-step CSP reduced mechanism

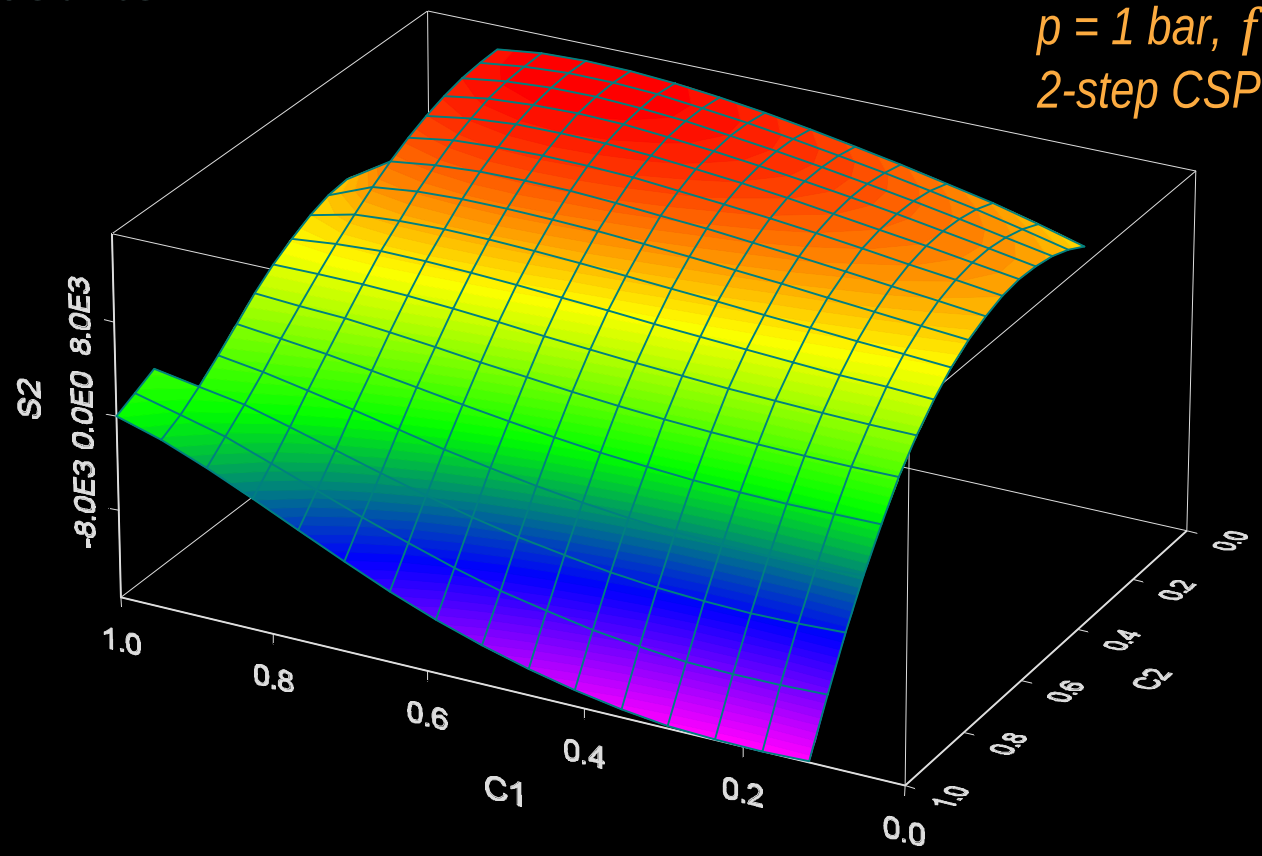


- *Temperature as a function of the 2 RPV's: linear behaviour*

The FIRST Model

Results

Methane-Air flame,
p = 1 bar, f = 1.00
2-step CSP reduced mechanism



- *Source term of RPV 2 as a function of the 2 RPV's:*
  - *-Smooth surface*
  - *-Both positive and negative source term values*
  - *-Zero source term value at equilibrium*

Conclusions

- Accurate reduced mechanism for methane combustion under MAST conditions developed using CSP
- A 2-step reduced mechanism constructed for turbulent calculations
- Generated smooth, "low-dimensional" thermochemical databases very suitable for use in turbulent combustion simulations
- Modelling work in progress, implemented in a turbulent CFD code (CFX-5.5)

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