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Effects of Reduced Kinetic Models on the Simulation of sCO_2 Oxy-Combustion

Zefang Liu*, Xiang Gao, Miad Karimi, Bradley Ochs, Vishal Acharya, Wenting Sun*
Georgia Institute of Technology

Jacob Delimont, Nathan Andrews
Southwest Research Institute

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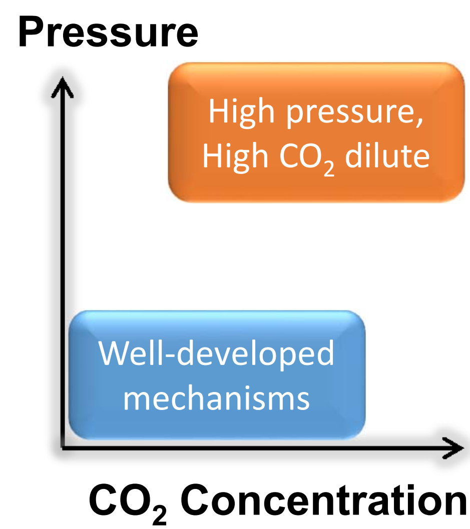
Contents

Introduction

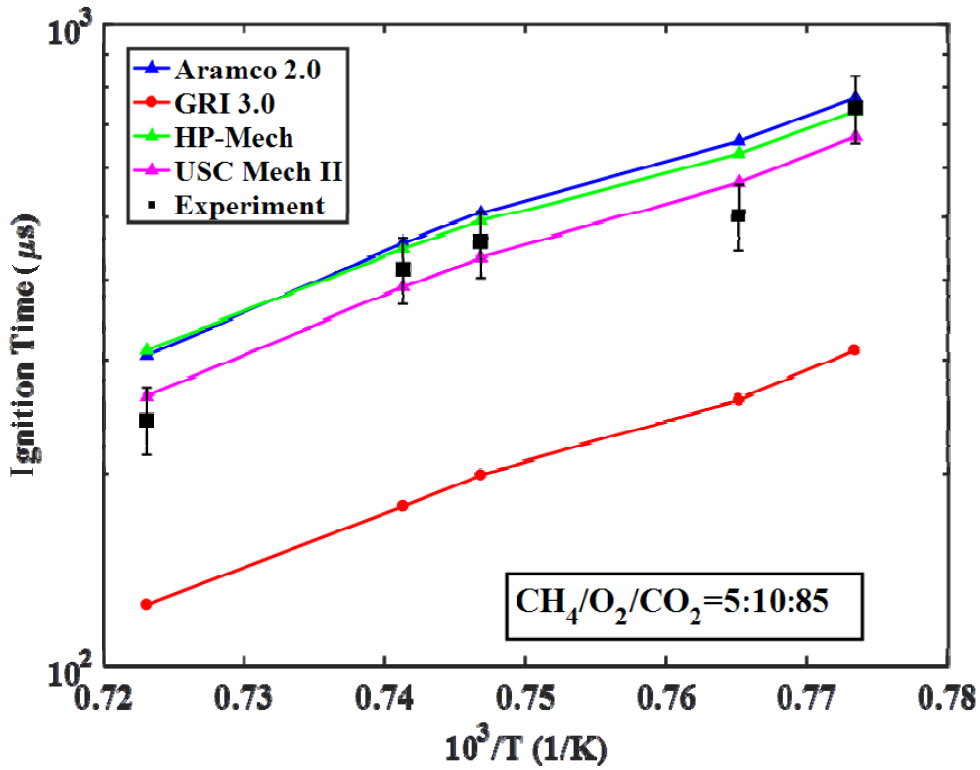
- Advantages of directly fired supercritical carbon dioxide (SCO_2) oxy-combustion power cycle:
  - Increase the efficiency
  - Capture up to 99% of carbon
- A validated kinetic model is missing but needed:
  - Lack relevant experimental data for kinetic model validation
- Our goals:
  - Demonstrate the effect of kinetic model selection on combustor design
  - Reduce computational resource from using detailed kinetic models



Kinetic model reduction and optimization

- Kinetic model selection
- Kinetic model reduction and optimization

Kinetic model reduction and optimization: Model selection



Measured autoignition delays of $CH_4/O_2/CO_2$ mixture (5:10:85) and simulation using kinetic models at 105 atm
(preliminary data of the shock tube from Dr. Sun's group)

- To: select a proper kinetic model for sCO_2 condition
- The experimental results deviate approximately 40% for **USC Mech II** and 100% for GRI 3.0
- Also, *Coogan et al.* (2016) also shows "**USC Mech II** has the best overall performance" (over 70% CO_2 dilute and 10-85 atm)
- Reduction & optimization: USC Mech II → **13 species model**
- Comparison: GRI 3.0 → **24 species model** by Global Pathway Selection (GPS[1]) algorithm (reduction only)

1. Gao, X., Yang, S., and Sun, W., "A global pathway selection algorithm for the reduction of detailed chemical kinetic mechanisms," Combustion and Flame, Vol. 167, 2016, pp. 238-247. doi: 10.1016/j.combustflame.2016.02.007.

Kinetic model reduction and optimization: Model reduction & optimization

- To: get an optimized 13 species kinetic model
- **Reduction**:
  - based on the **USC Mech II (111 species and 784 reactions)**
  - **13** species selected with **GPS**
- **Optimization**:
  - a genetic algorithm
  - objective function: autoignition delay
  - “genes”: pre-exponential factors
- Covering conditions:
  - Pressure:150 - 300 bar
  - Temperature: 900 - 1800 K
  - Equivalence ratio: 0.7 - 1.3
  - CO_2 dilute: around 90%
- Less than 13% error relative to that of USC Mech II → accuracy & efficiency

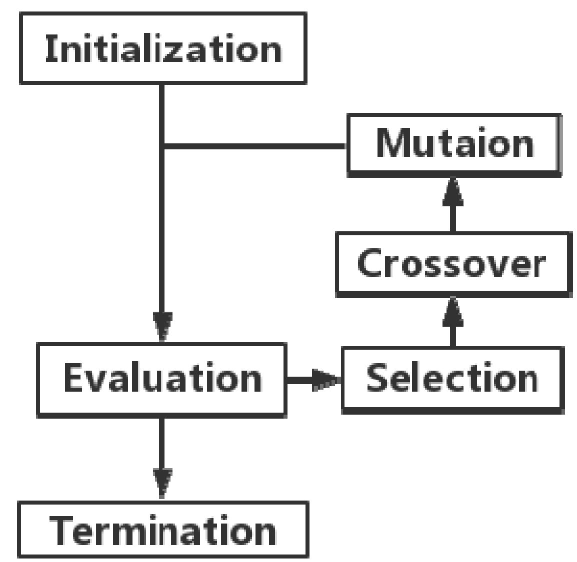
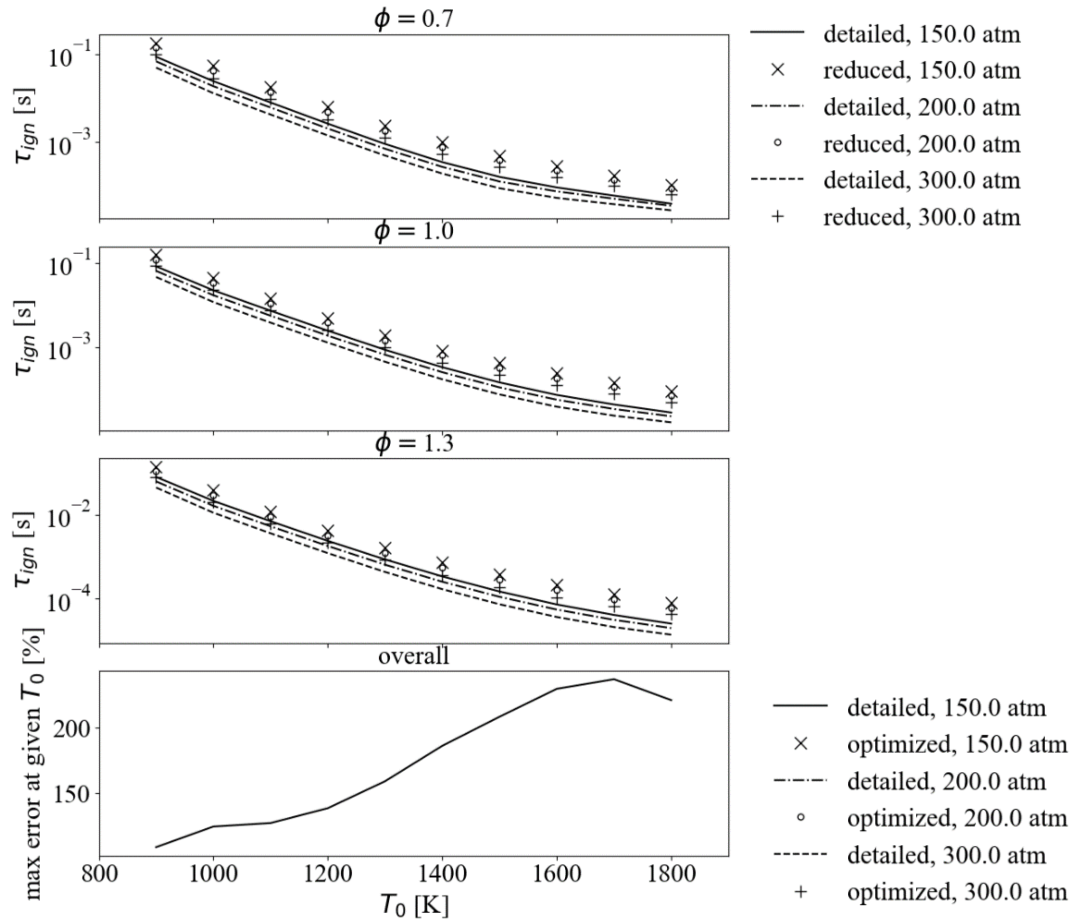


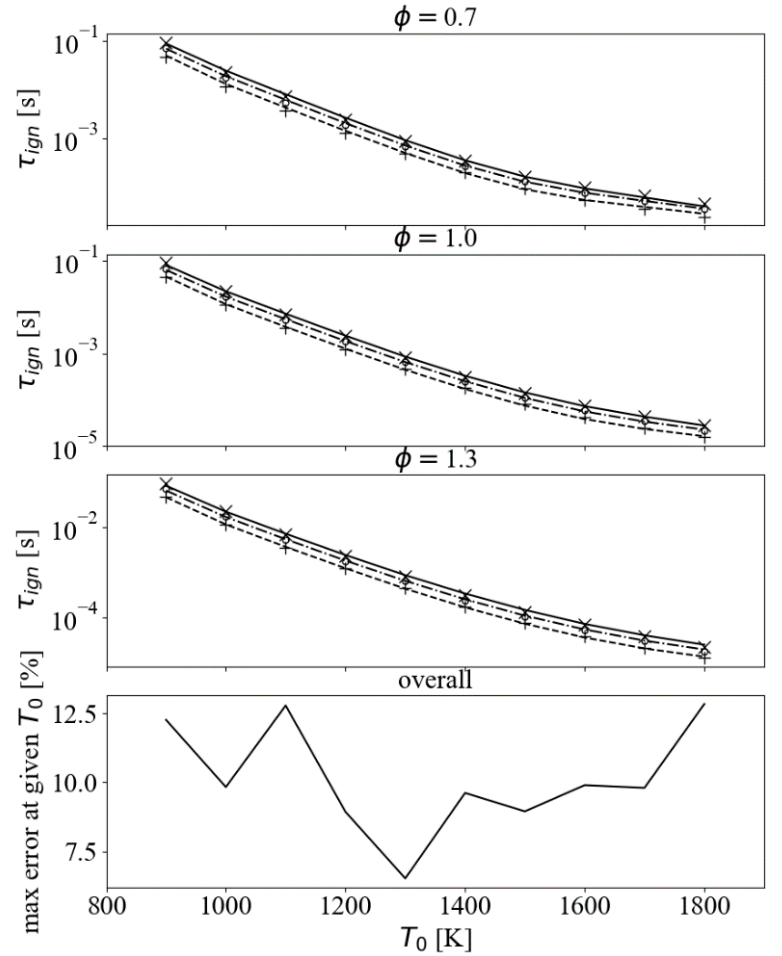
Fig. Flowchart of genetic algorithm

Kinetic model reduction and optimization: Model optimization

Before optimization



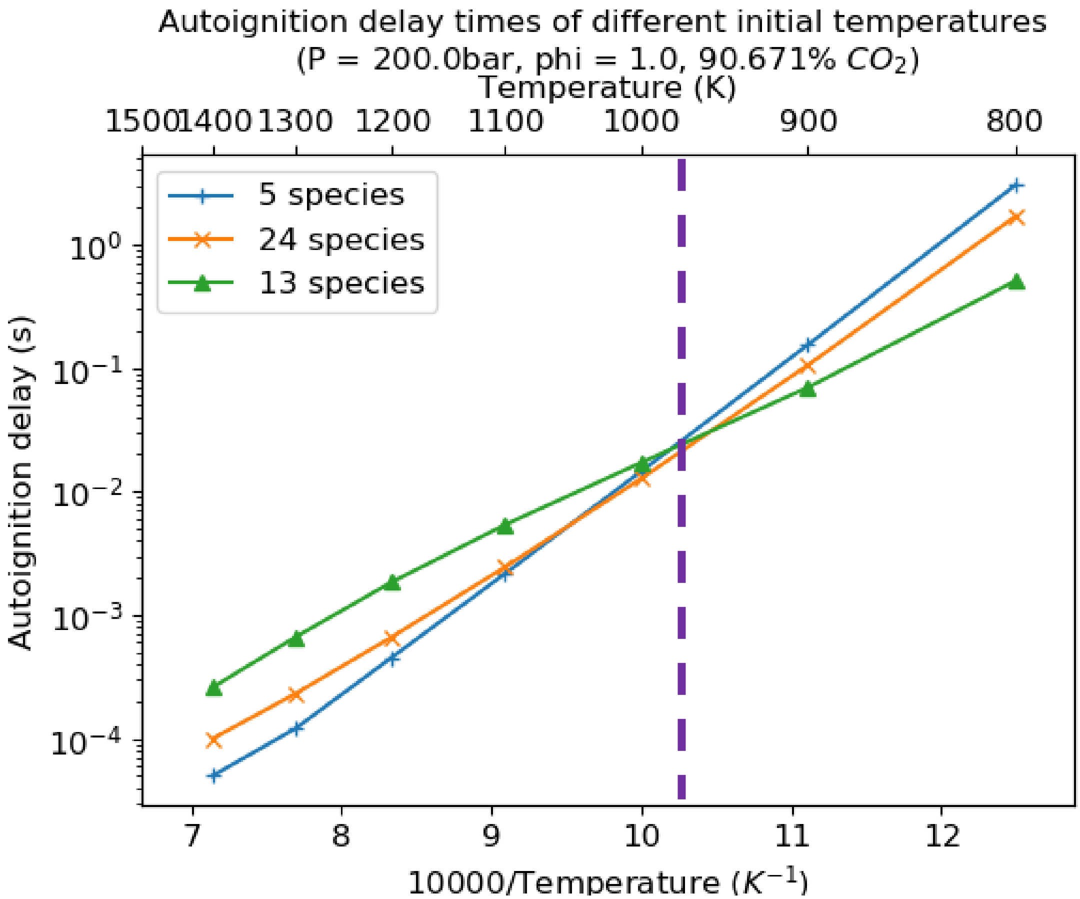
After optimization



Numerical simulations using 3 different kinetic models

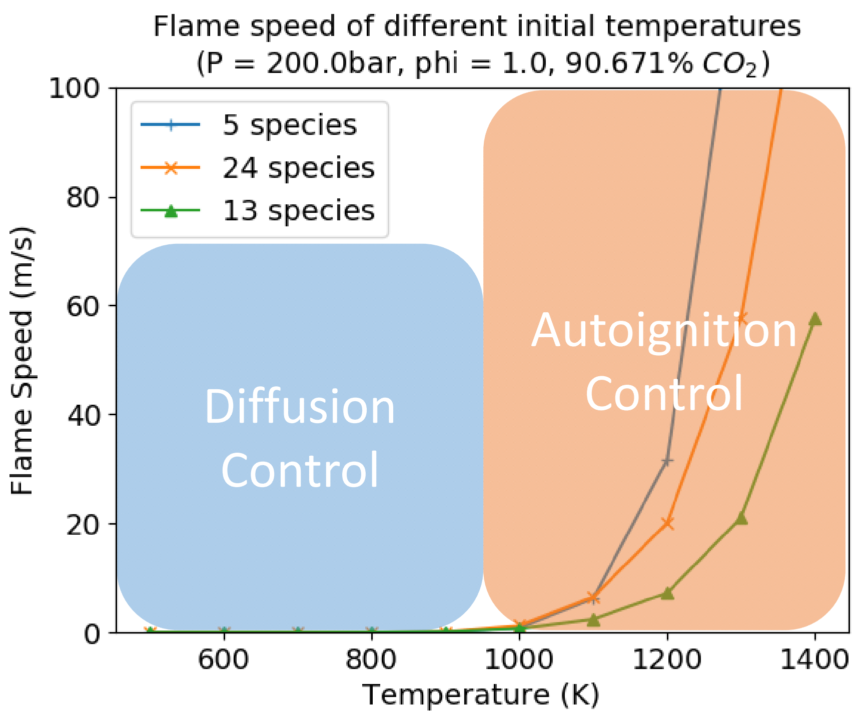
- **5 species** model built in ANSYS Fluent
- **24 species** model reduced from GRI Mech 3.0
- **13 species** model reduced and optimized from USC Mech II

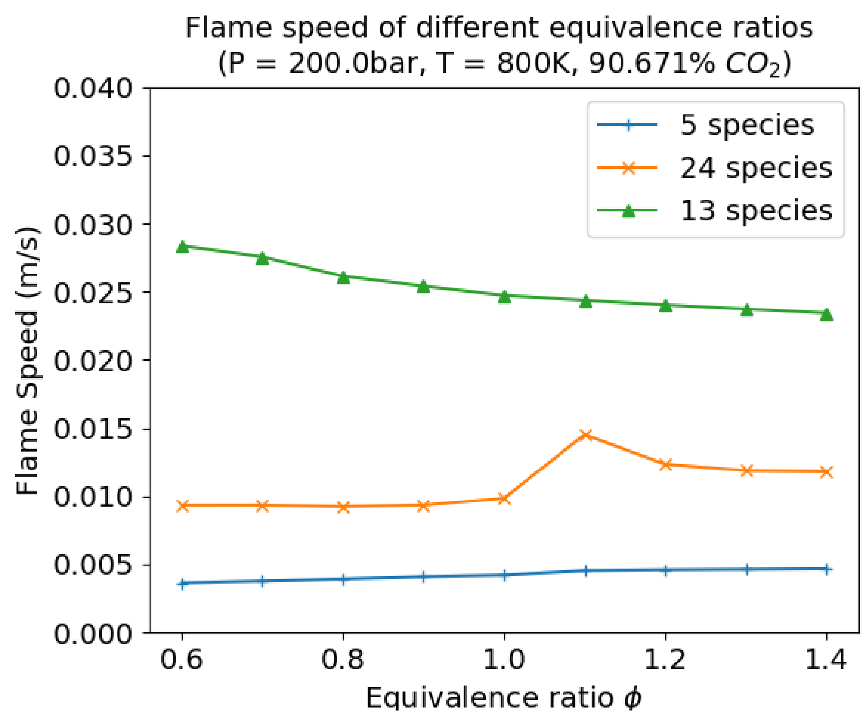
Numerical simulations using 3 different kinetic models: 0D, autoignition delay



- Model: Cantera – ideal gas constant pressure reactor
- Autoignition delay time:
  - Lower T_0: 5 species > 24 species > 13 species
  - Higher T_0: 13 species > 24 species > 5 species

Numerical simulations using 3 different kinetic models: 1D, laminar flame speed

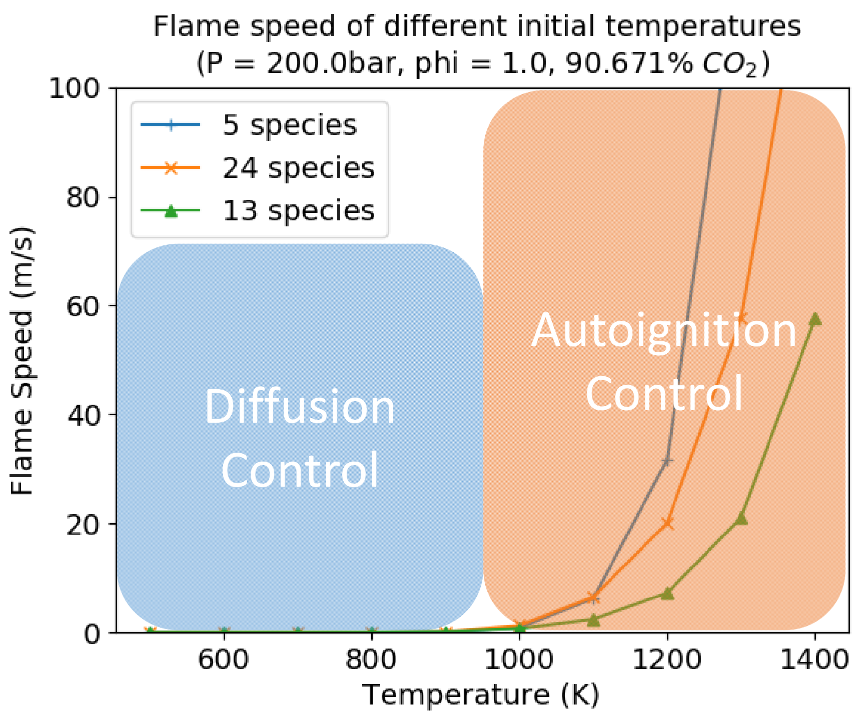


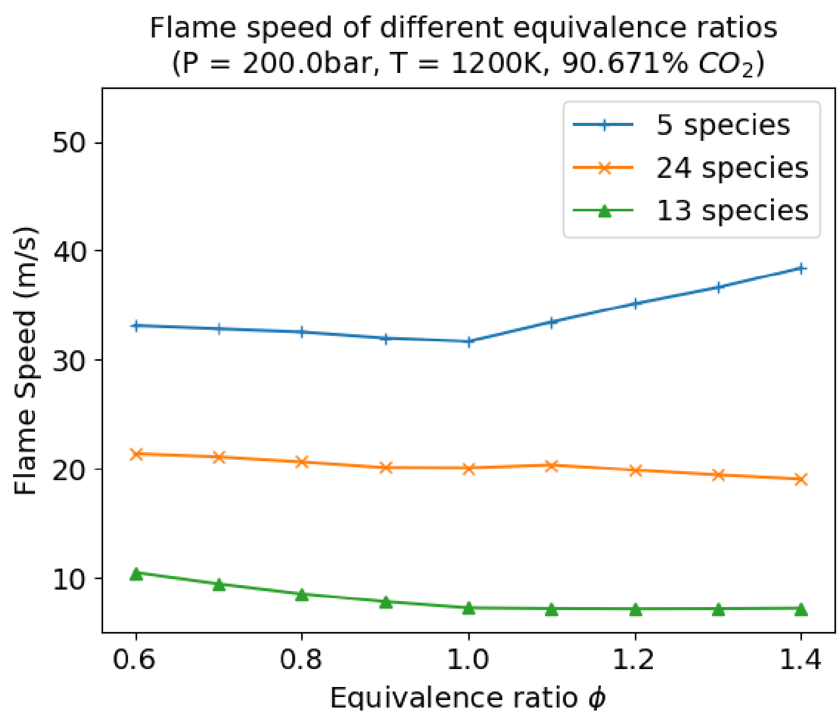


- Model: Cantera – free flame
- Flame speed: diffusion control vs. autoignition control

- T_0=800K: 13-species > 24-species > 5-species, little change with ϕ

Numerical simulations using 3 different kinetic models: 1D, laminar flame speed

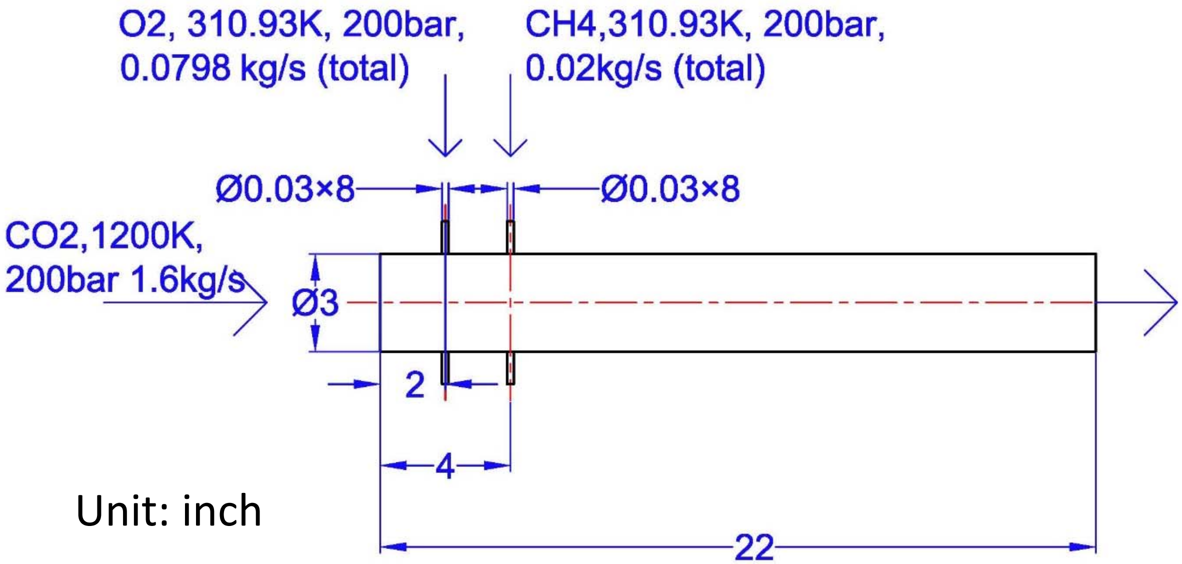


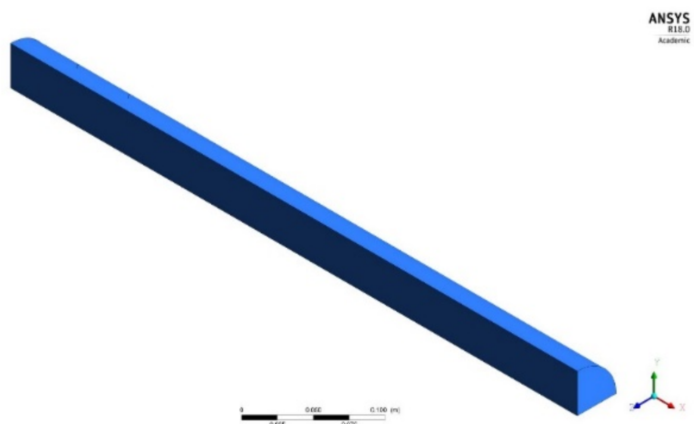


- Model: Cantera – free flame
- Flame speed: diffusion control vs. autoignition control

- T_0=1200K: 5-species > 24-species > 13-species, little change with ϕ

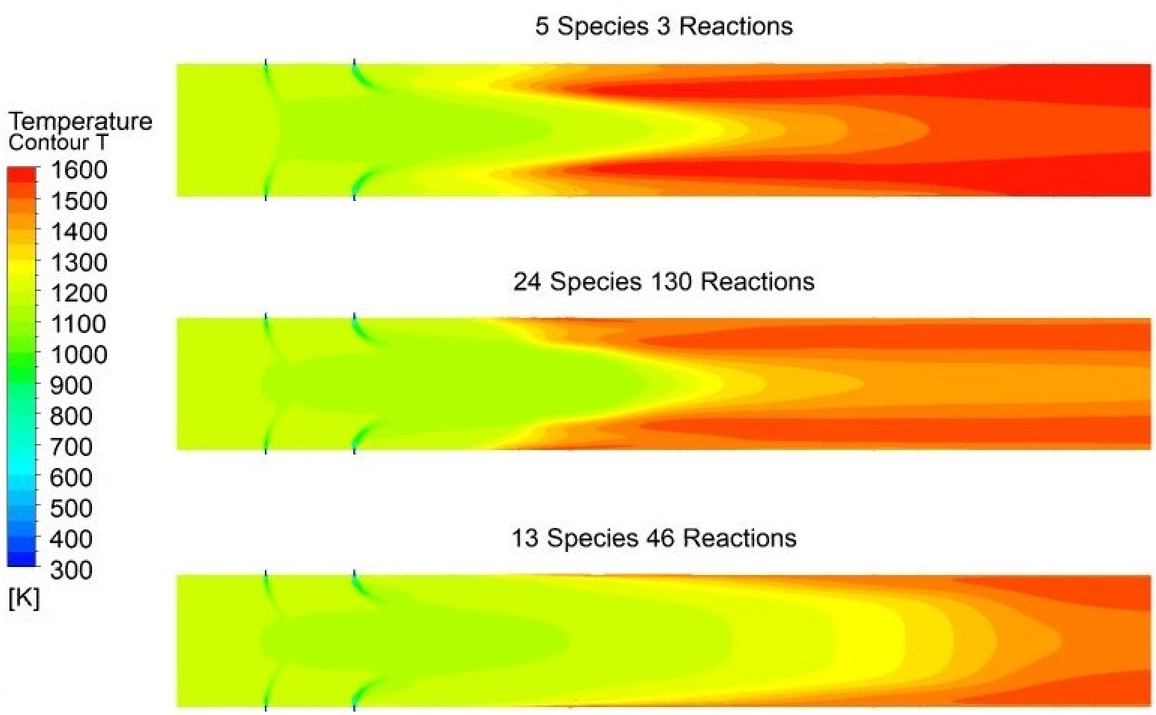
Numerical simulations using 3 different kinetic models: 3D, crossflow combustor





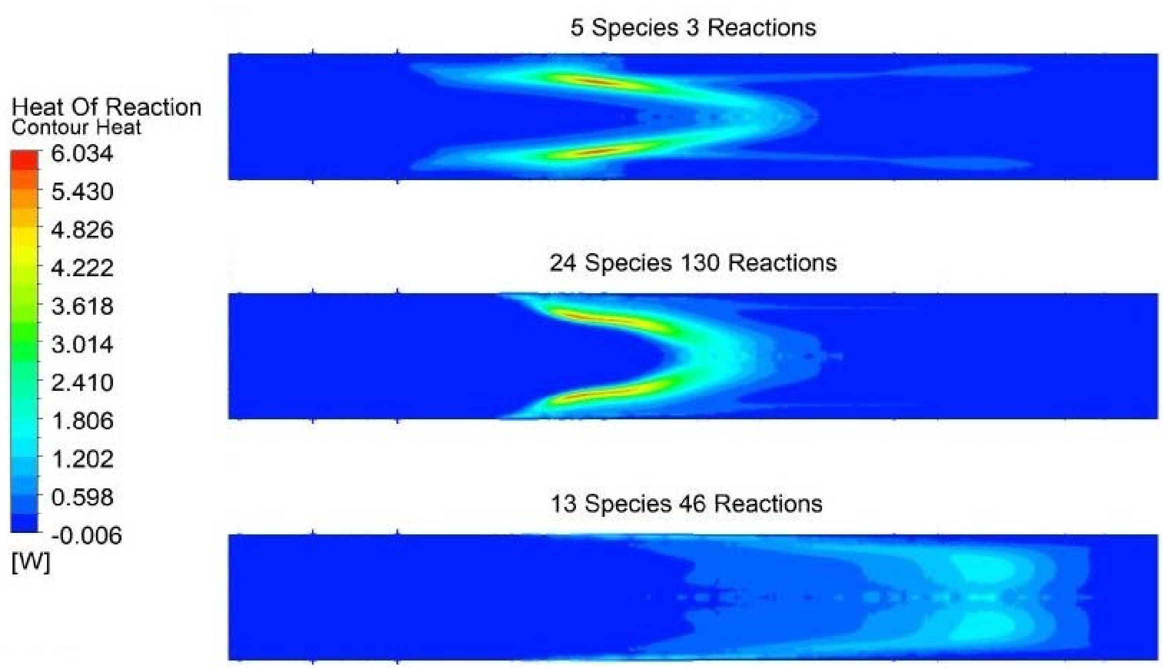
Software	ANSYS Fluent
Mesh	783,936 elements (quarter model)
Turbulent model	k-epsilon
Turbulence -chemistry interaction	Eddy-Dissipation Concept (EDC)
Equation of state	ideal-gas (for simplicity)
Results	Steady

Numerical simulations using 3 different kinetic models: 3D, temperature



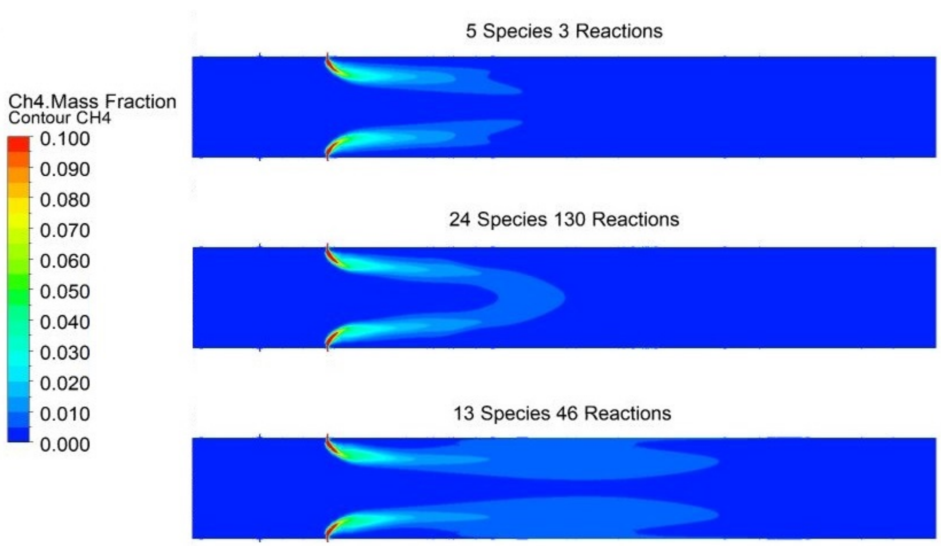
- **5 species**: 2 steps chemistry, fastest temperature raising
- **24 species**: faster chemistry
- **13 species**: slower temperature raising, a longer autoignition delay
- Similar results with the autoignition delay (0D model) of 91% CO_2 dilute and 1200 K

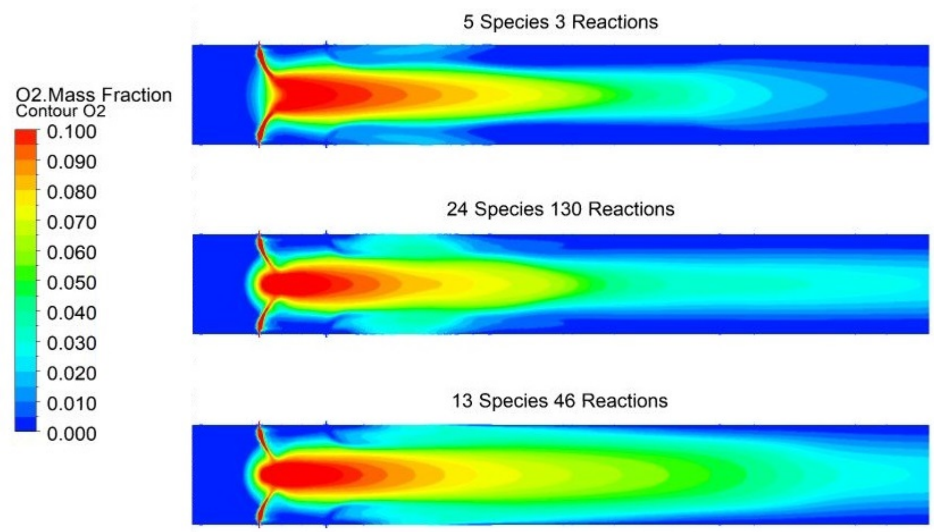
Numerical simulations using 3 different kinetic models: 3D, heat of reactions



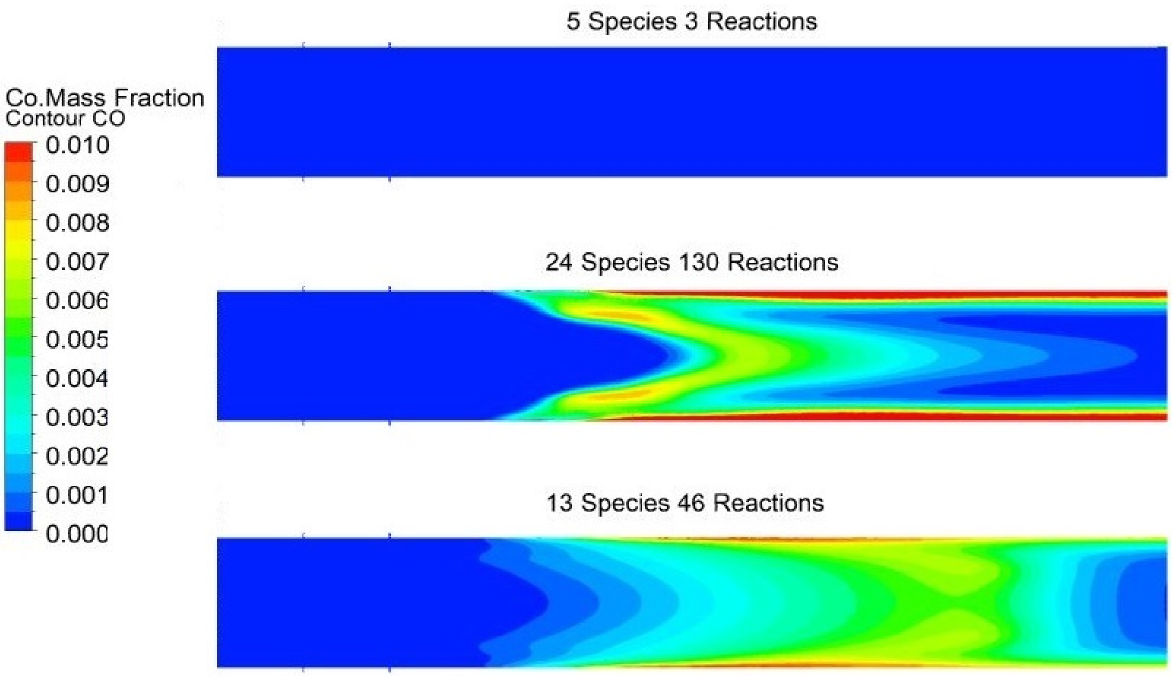
- **Reaction speed**: 5 species > 24 species > 13 species
- Similar results with the autoignition delay (0D model) of 91% CO_2 dilute and 1200 K

Numerical simulations using 3 different kinetic models: 3D, CH_4 & O_2 mass fraction





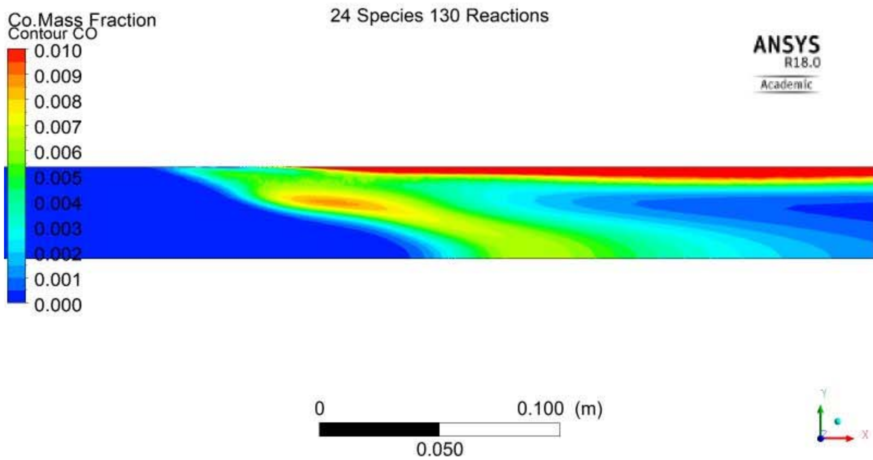
Numerical simulations using 3 different kinetic models: 3D, CO mass fraction

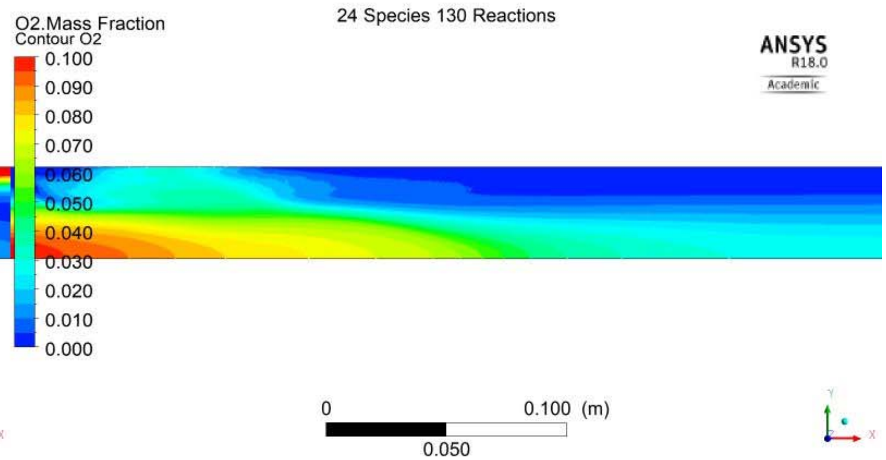


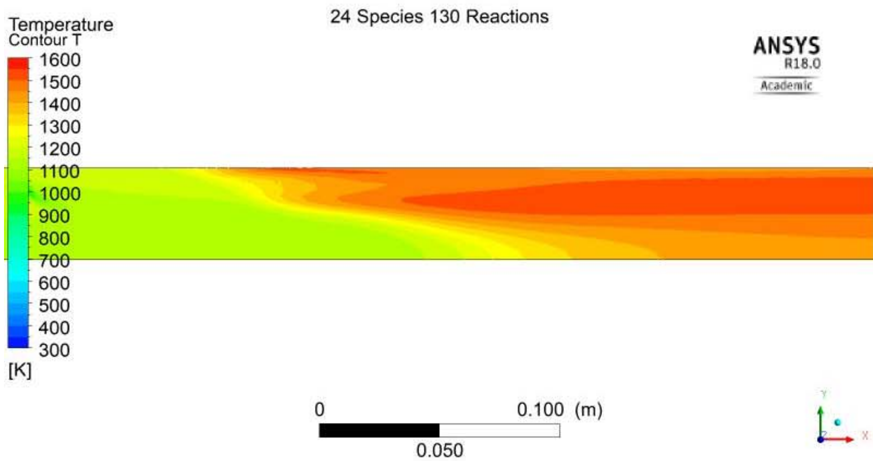
- **5 spceies model**:
  - Y(CO) < 0.05%
  - 2-step chemistry
- **24 spceies model**:
  - High CO mass fraction near the wall
  - Diffusion from flame and production from HCCO and CH_3 (lack of O_2)
- **13 species model**:
  - larger reaction zone

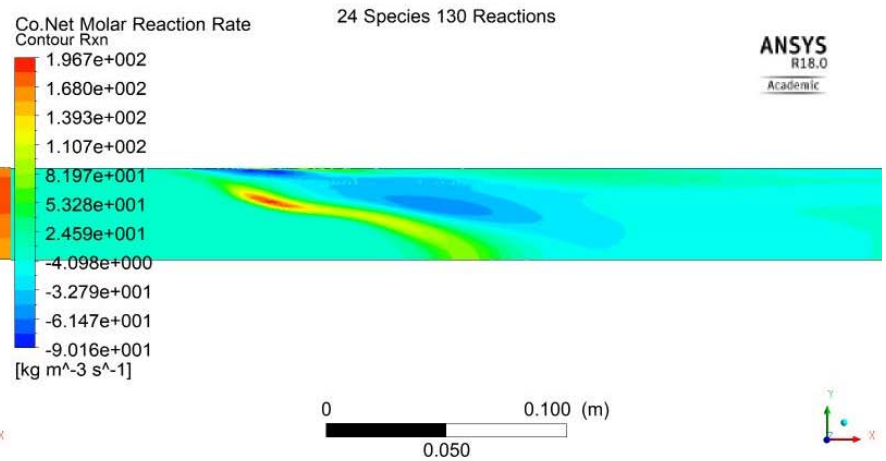
Kinetic model	Area-weighted average mass fraction of CO at outlet
5 species	4.876e-5
24 species	4.476e-3
13 species	3.065e-3

Wall Effect – 24 Species

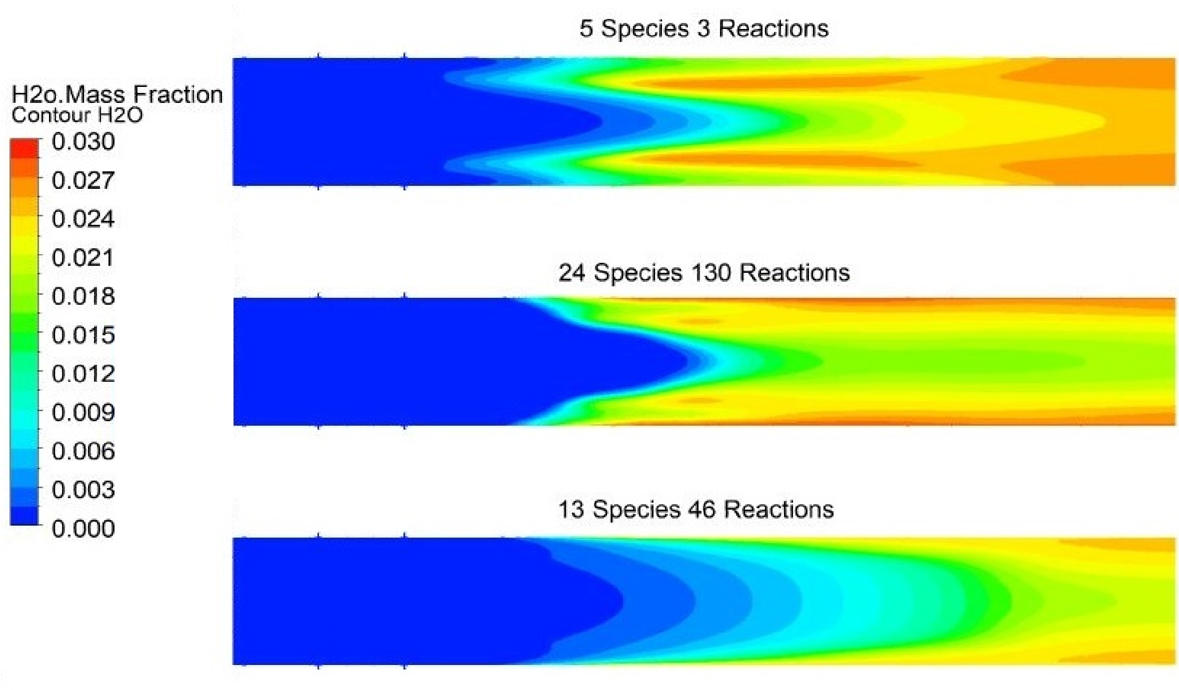






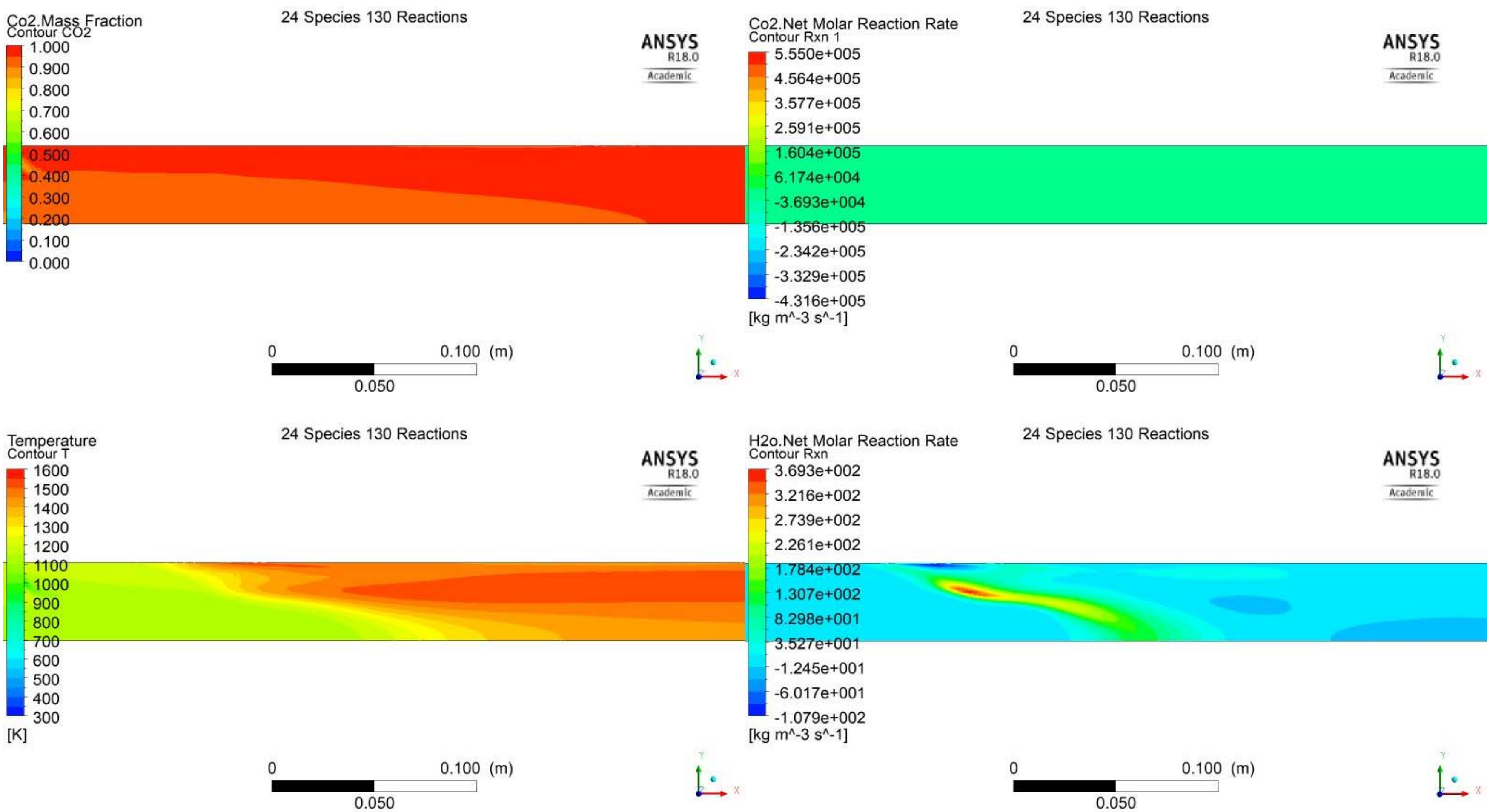


Numerical simulations using 3 different kinetic models: 3D, H_2O mass fraction



- Similar to temperature result
- Most heat: H_2O

Wall Effect – 24 Species



Conclusions

- Kinetic model reduction and optimization:
  - Section: USC Mech II
  - Reduction: 13 species kinetic model by Global Pathway Selection
  - Optimization: optimized 13 species kinetic model by genetic algorithm (13% error)
- Numerical comparison between 3 different kinetic models:
  - autoignition delay (200bar, 91% CO_2 dilute):
    - T_0<1000K: 5 species > 24 species > 13 species
    - T_0>1000K: 13 species > 24 species > 5 species
- The simulation is sensitive to kinetic models
  - 200bar, 1200K and 91% CO_2:
    - 5 species: faster chemistry
    - 24 species kinetic model: wall effect
    - Optimized 13 species kinetic model: longer autoignition delay → incomplete combustion

Questions?

Kinetic models

- **Optimized 13 species kinetic model**
- **13** species: CH_4, CH_3, CH_2O, HCO, CO, H, O, O_2, OH, H_2O, H_2O_2, HO_2, and CO_2
- Download: http://sun.gatech.edu/download.htm

Kinetic models

24 species kinetic model

- From GRI 3.0
- 24 species: $CH_2(S)$, CH_2O, O_2, CH_2CHO, CH_3O, H_2O_2, CH_2, CH_3, CH_4, HO_2, HCCO, CO, H, O, C_2H_6, C_2H_5, C_2H_4, C_2H_3, HCO, OH, H_2, H_2O, CH_2CO, and CO_2
- 130 reactions

5 species kinetic model

- From ANSYS Fluent
- 5 Species:
  - CH_4, O_2, CO, CO_2, and CH_4
- 3 reactions:
  - $CH_4 + 1.5O_2 \rightarrow CO + 2H_2O$
  - $CO + 0.5O_2 \leftrightarrow CO_2$

Numerical simulations using 3 different kinetic models: 3D, CO_2 mass fraction