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A skeletal mechanism for n-heptane MILD combustion

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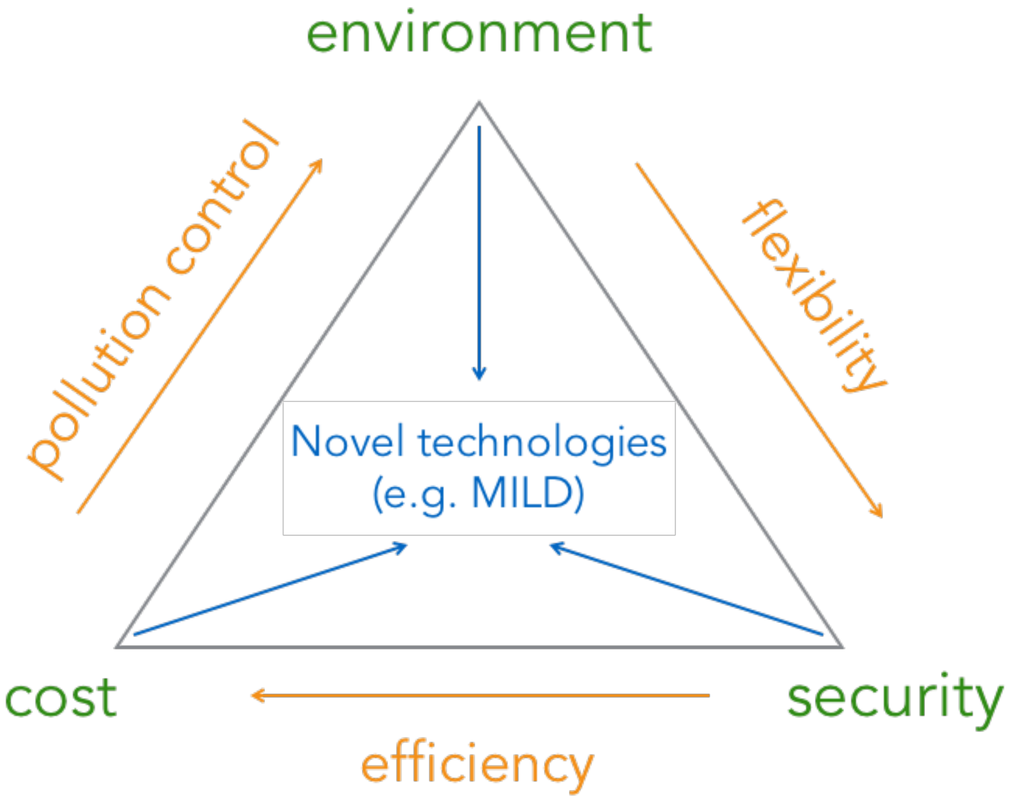
Motivation: challenges



adapted from de Joannon, 2015

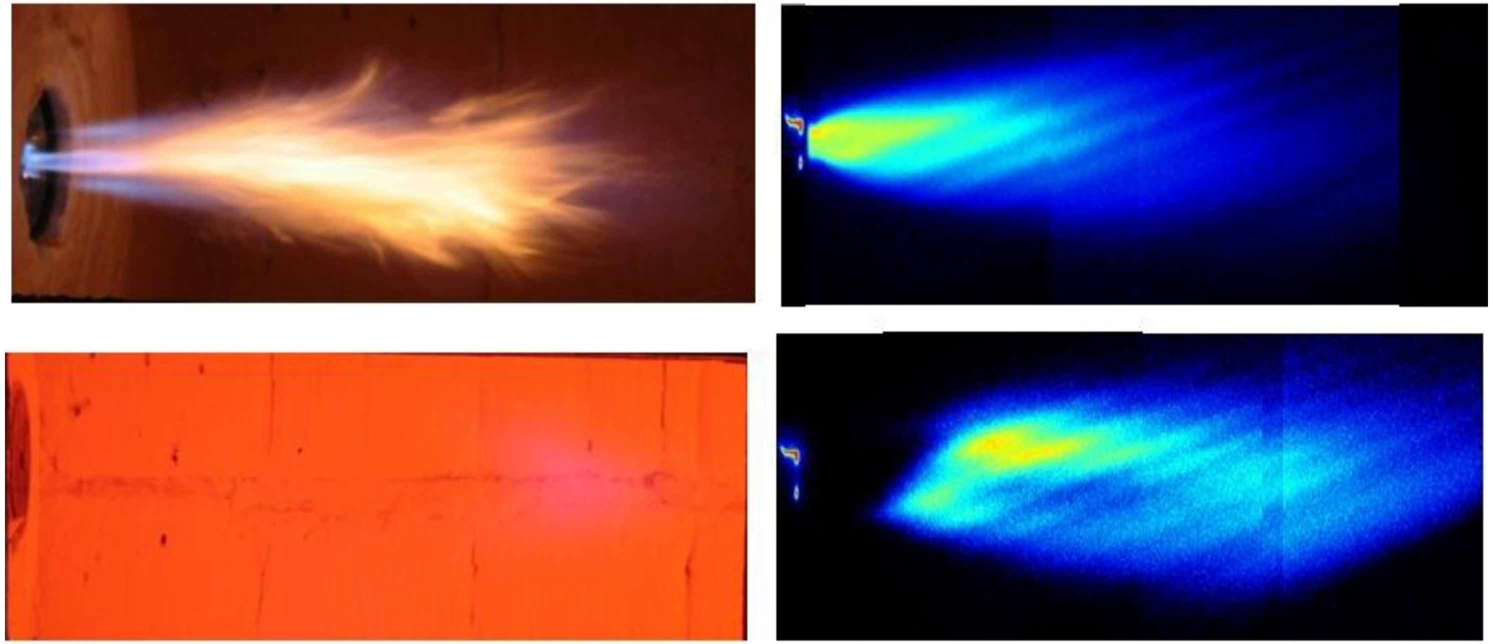
MILD: Moderate or Intense **Low oxygen Dilution** combustion

Motivation: MILD combustion

OH* chemiluminescence image

Conventional:

MILD:



Jörg Leicher et al, 2013

Motivation: advantages of MILD combustion

Features of MILD combustion:

- Distributed reaction zone
- More uniform temperature field
- Ideally no visible flame

Advantages of MILD combustion:

- High efficiency
- Low emissions (especially thermal NOx)
- Large fuel flexibility
- Low noise level

J. A. Wünning and J. G. Wünning, Progress in Energy Combustion and Science, 1997.

A Cavaliere and M de Joannon, MILD Combustion. Prog. Energy Combust. Sci., 2004.

Minamoto el al., Combust. Sci. Technol., 2014

Motivation: why is such mechanism needed?

- Simple gaseous fuels (methane, hydrogen, ethylene) have common characteristics.
- Oxygenated fuels and long-chain alkanes show distinct features:
  - increased pollutants emission
  - appearance of visible flames

- LES and DNS are needed to study these distinct features: no. of species below 40
- Current skeletal mechanisms for n-heptane available are mainly used for engine conditions, not for MILD conditions.

Model: Computer Assisted Reduction Method (CARM)

- **DRGEP** method is used as first reduction step with target species of fuel, major products and H, allowing a cut-off threshold value of 0.01.
- A starting skeletal mechanism with high accuracy of laminar flame speed is generated.
- The **trial-and-error brute force method TSA** is applied on the starting skeletal mechanism for further reduction. Species with removal error larger than 10% will be kept or otherwise removed. The **flame speed set is kept** when using TSA.

- Low temperature range (< 950 K) is not considered in the reduction process.

- More details of the method can be found here:

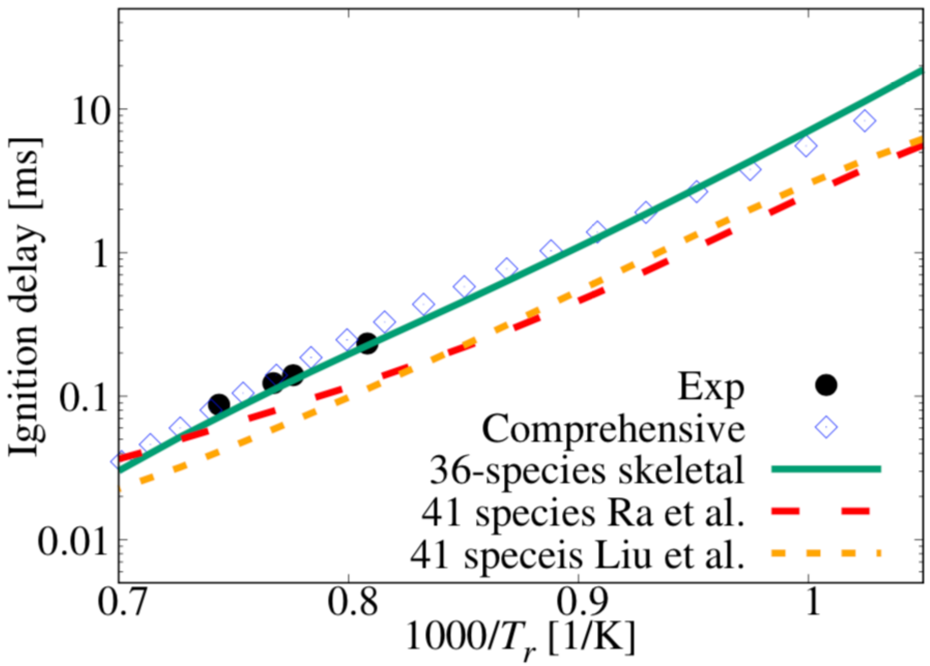
J.-Y. Chen, A general procedure for constructing reduced reaction mechanisms with given independent relations, Combustion Science and Technology 57 (1-3) (1988) 89–94.

J.-Y. Chen, Automatic generation of reduced mechanisms and their applications to combustion modeling, Zhongguo Hangkong Taikong Xuehui Huikan/Transactions of the Aeronautical and Astronautical Society of the Republic of China 33 (2) (2001) 59–67.

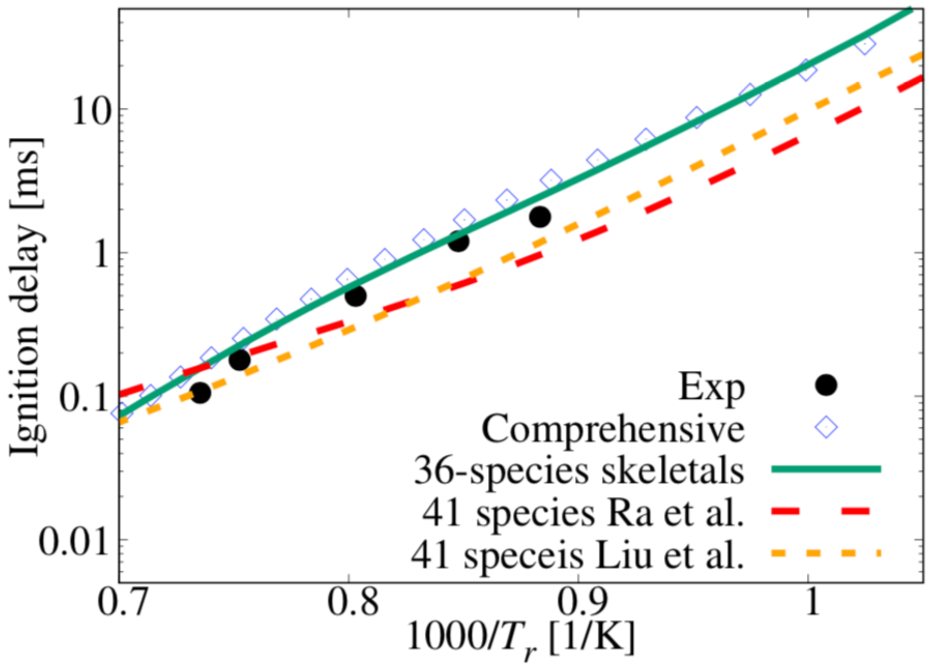
Validation: mechanisms

- Comprehensive mechanism (Zhang et al, 2016): 1268 species, 5336 reactions.
- Skeletal mechanism in the present work: 36 species, 205 reactions. For pure n-heptane, low temperature range excluded.
- Skeletal mechanism from Ra et al, 2008: 41 species, 130 reactions. For primary reference fuel, engine condition.
- Skeletal mechanism from Liu et al, 2012: 41 species, 124 reactions. For primary reference fuel, engine condition.
- Skeletal mechanism from Ranzi et al, 2014: 106 species, 1738 reactions. For pure n-heptane with low temperature.

Validation: ignition delay time



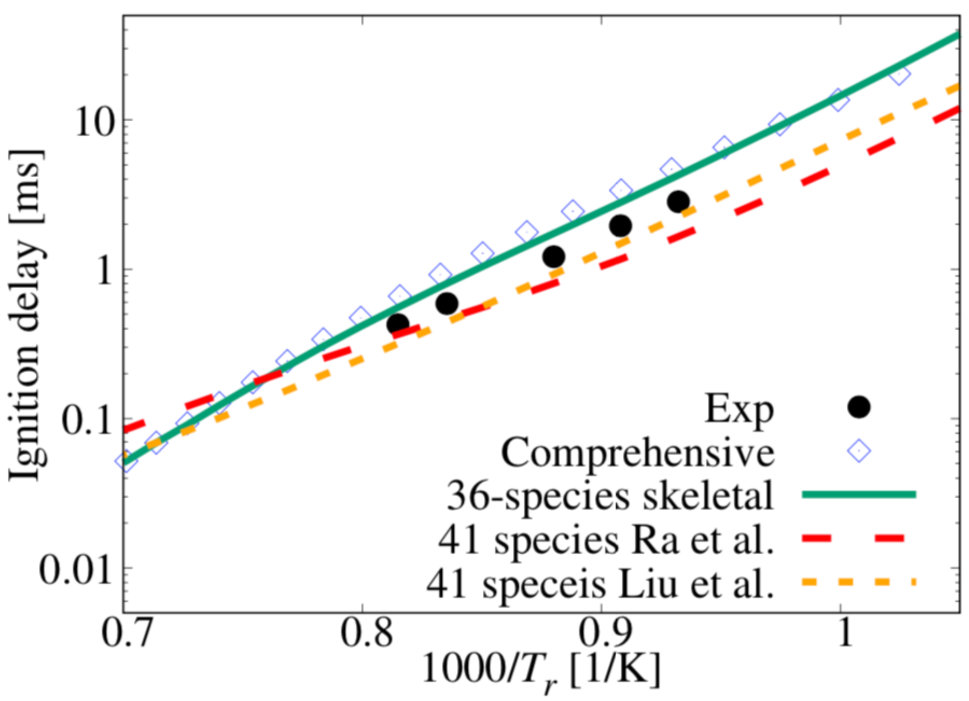
(a) 10 atm, $\phi = 1.0, \alpha = 0$



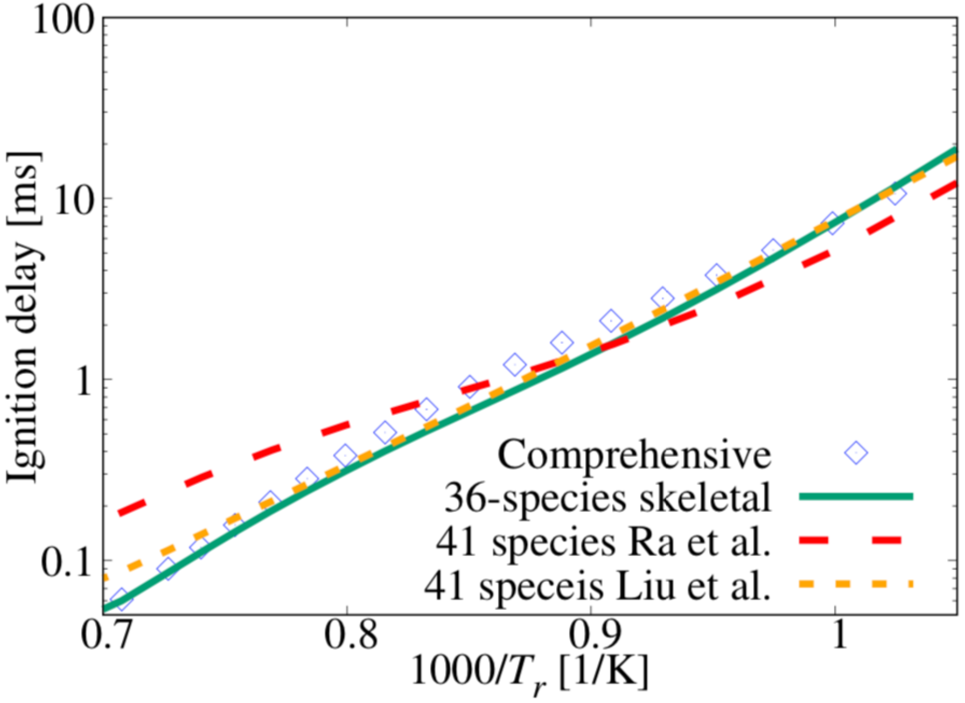
(b) 3.2 bar, $\phi = 1.0, \alpha = 0$

ϕ: *equivalence ratio* α: *dilution level*

Validation: ignition delay time



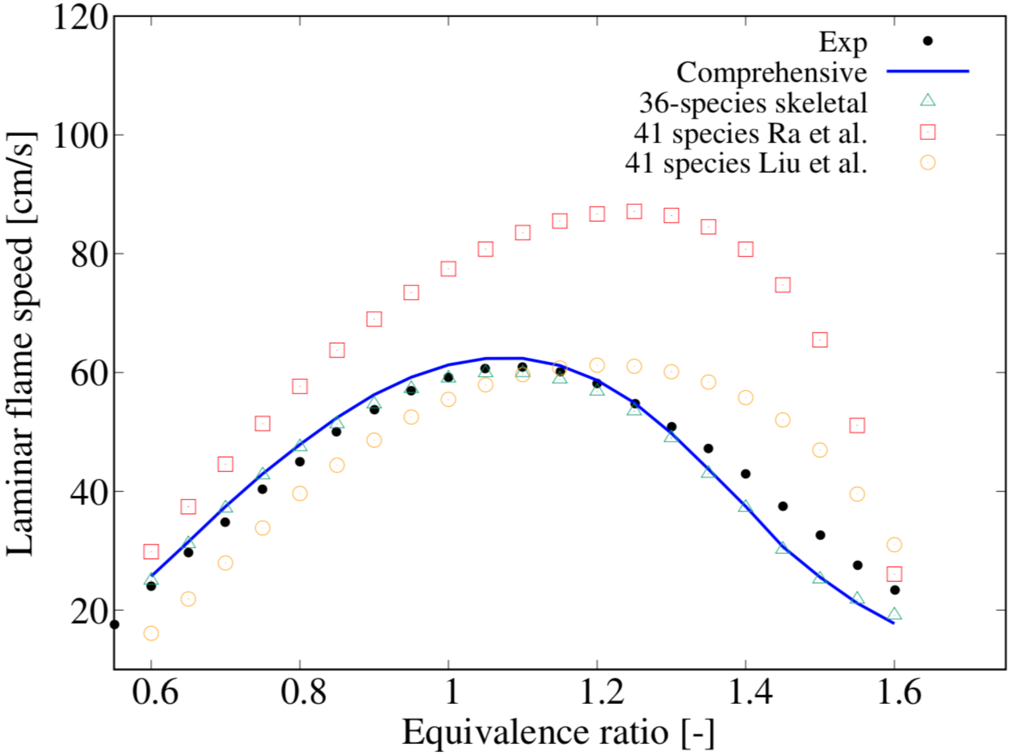
(a) 6.5 atm, $\phi = 0.75$, 15%O_2/5%CO_2/Ar



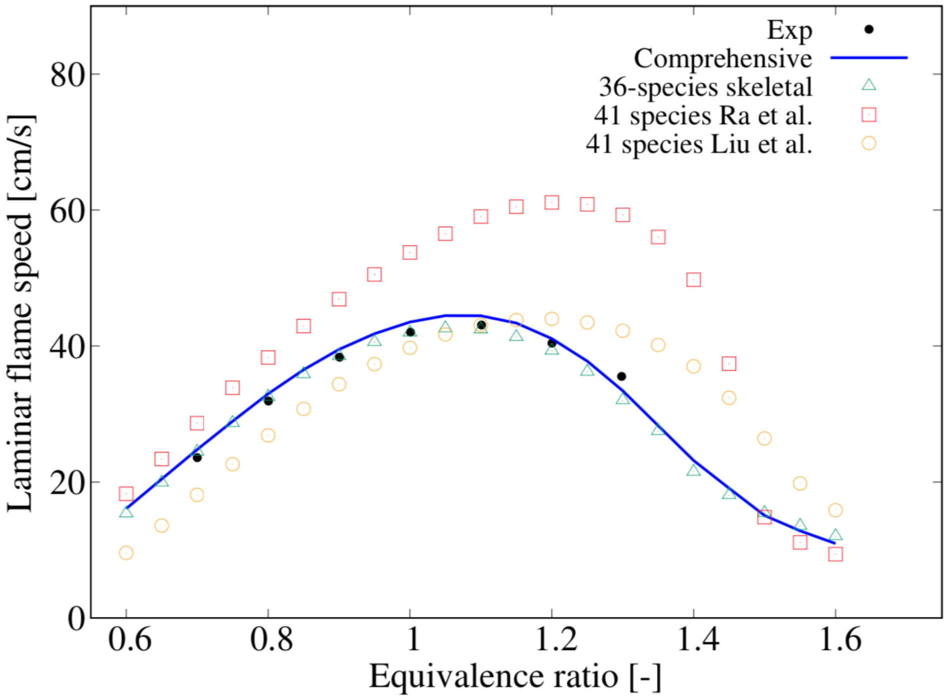
(b) 5 atm, $\phi = 1.0, \alpha = 40\%$

ϕ: *equivalence ratio* α: *dilution level*

Validation: laminar flame speed



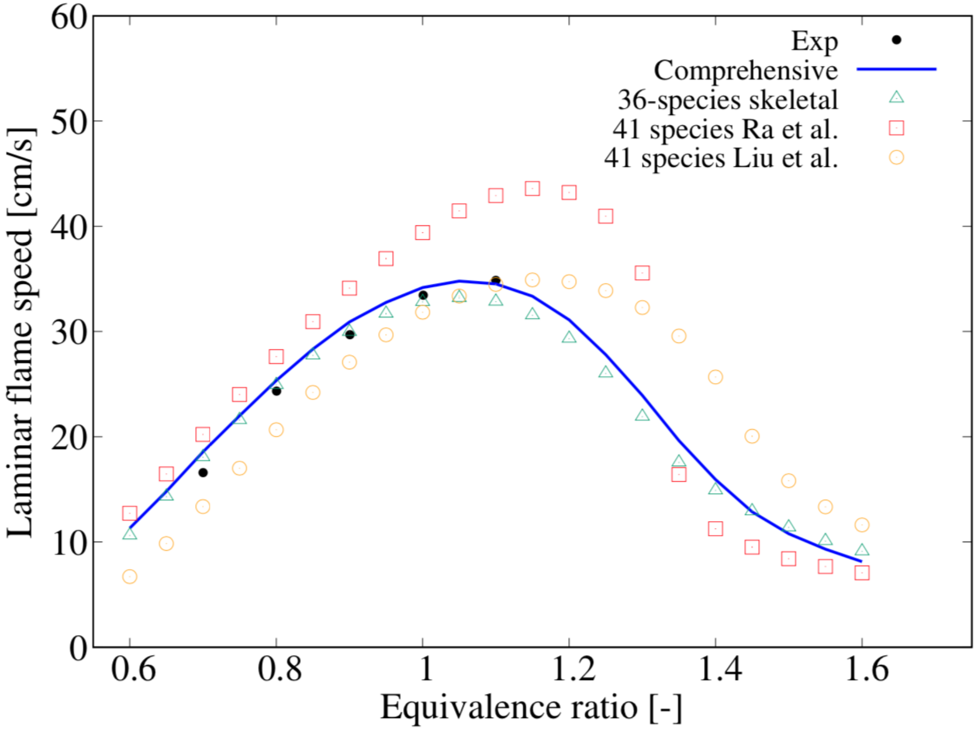
(a) 1 atm, T_r = 398 K, α = 0



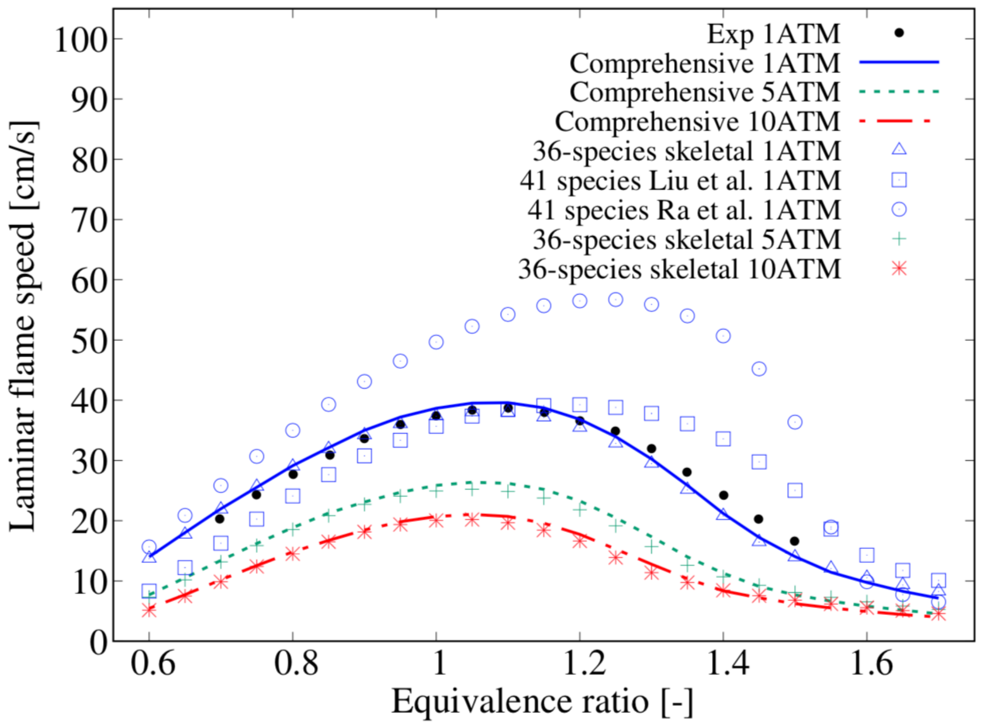
(b) 2 atm, T_r = 353 K, α = 0

T_r: *reactants temperature* α: *dilution level*

Validation: laminar flame speed



(a) 5 atm, T_r = 353 K, α = 0



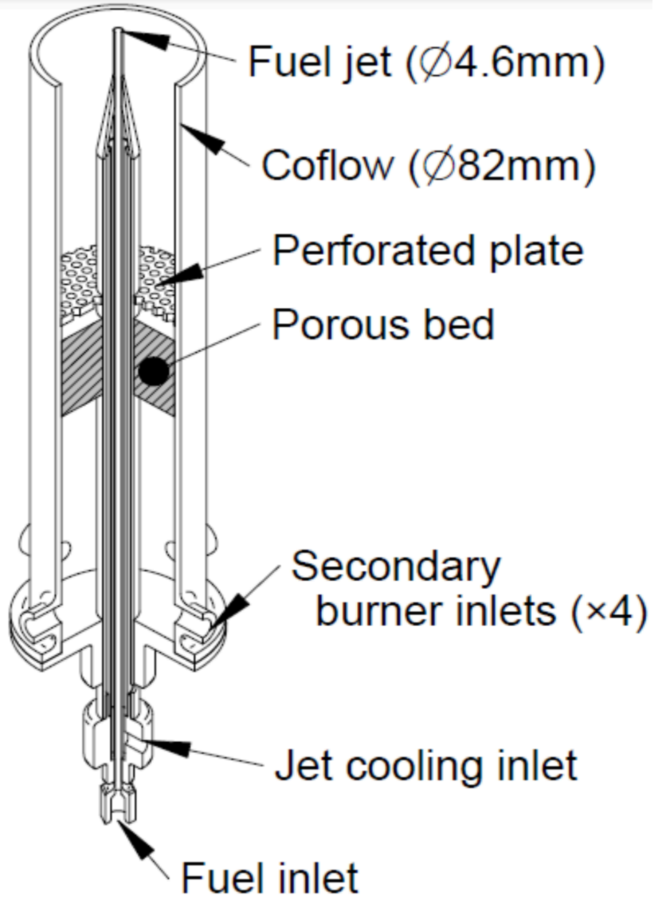
(b) 1/5/10 atm, T_r = 298 K, α = 0

T_r: *reactants temperature* α: *dilution level*

Validation: ignition delay time and laminar flame speed

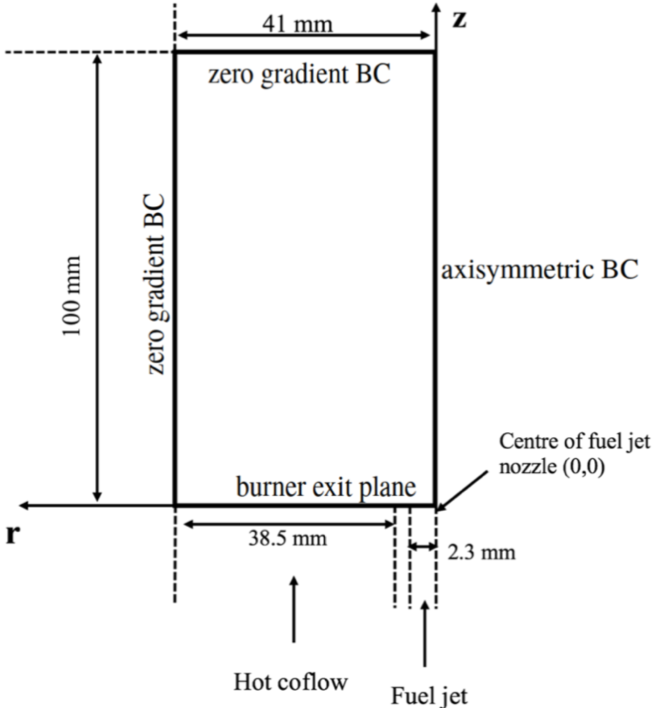
- The availability of experimental data under diluted condition is limited.
- We have compared the newly developed skeletal model with the comprehensive mechanism under wide range of **dilution levels (10% - 60%)**, **equivalence ratio (0.6-1.6)** and **reactants temperature**: good agreement is achieved.
- These results are not presented here for brevity.

Validation: CFD simulation

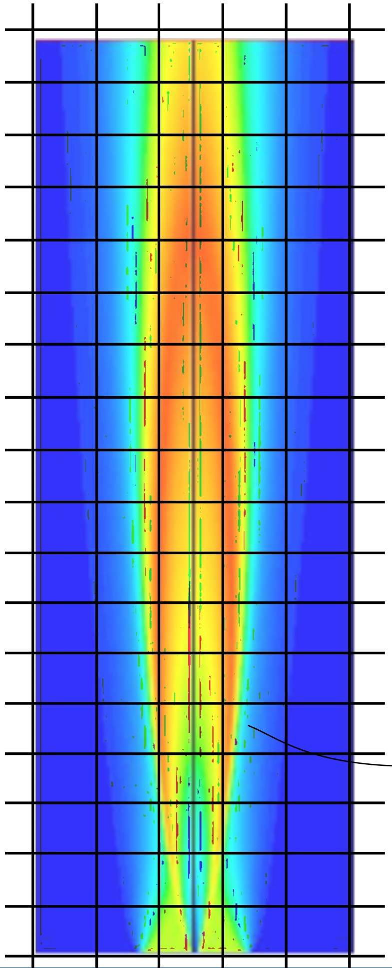


Jet in Hot co-flow burner with pre-vaporized n-heptane

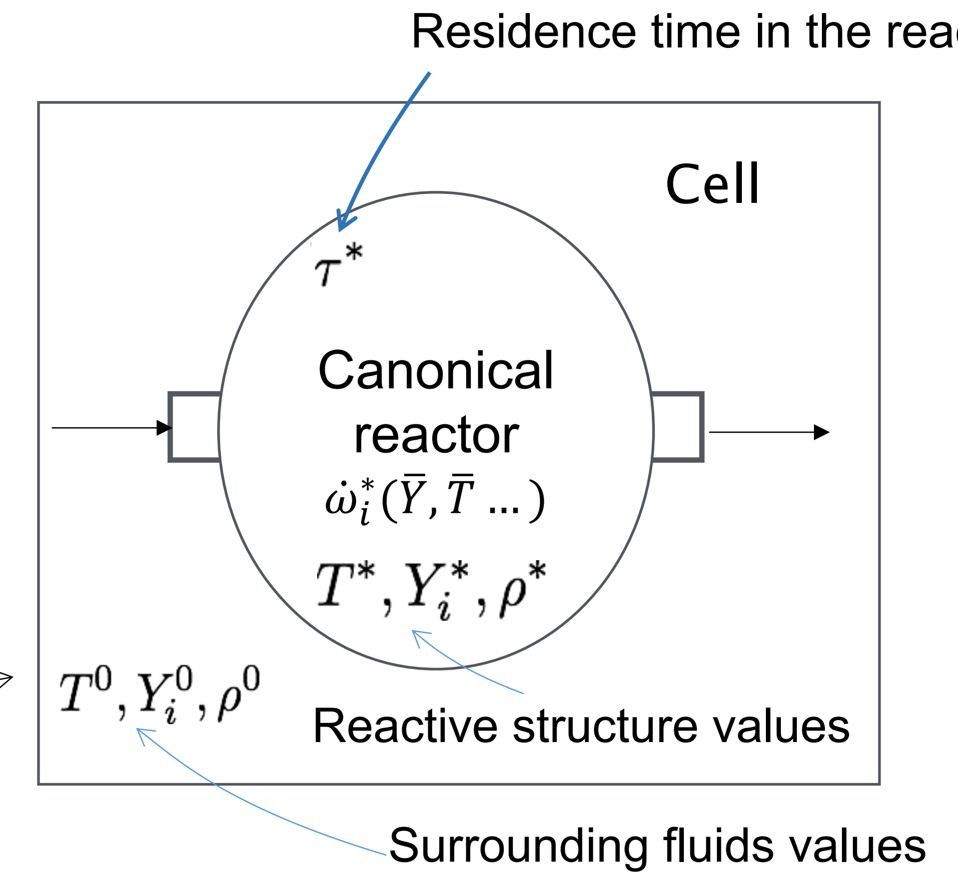
Quantities	Central jet	Hot coflow
Velocity	50 m/s	2.4 m/s
Temperature	412 K	1250 K
Reynolds number	10,000	1000



Validation: CFD simulation



URANS with Partially Stirred Reactor model



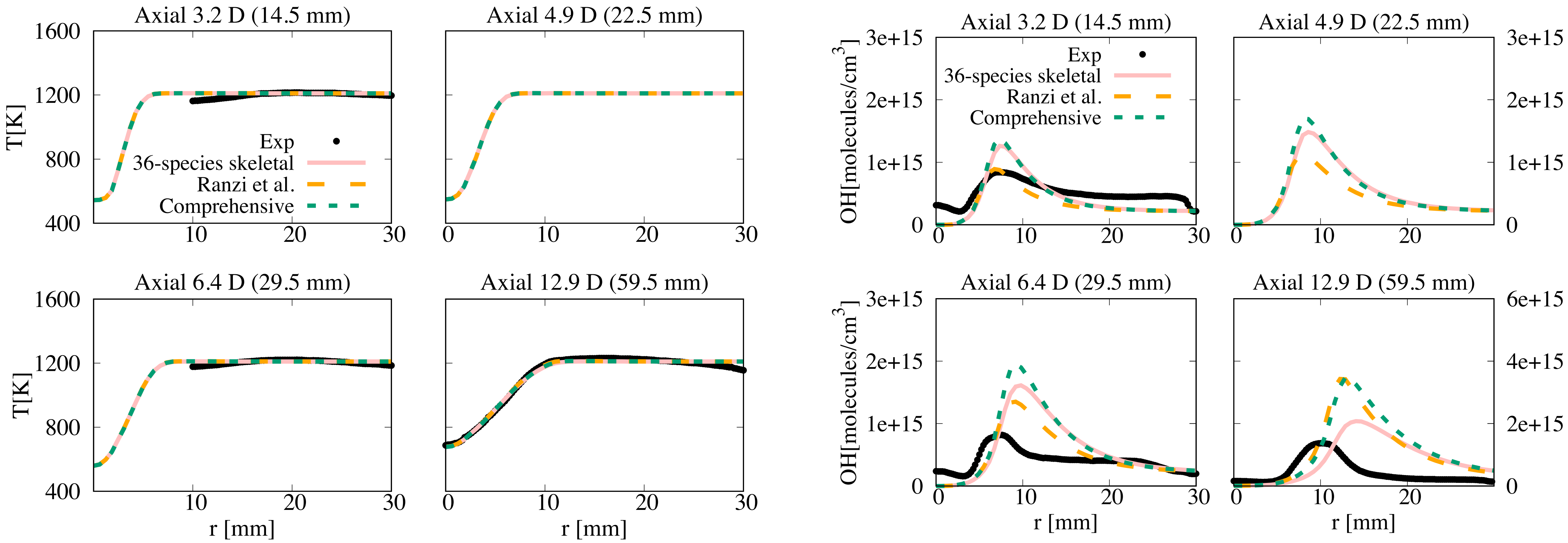
Reaction source term:

$$\overline{\dot{\omega}_i} = \kappa \dot{\omega}_i^*(\bar{Y},\bar{T}\ ...)$$

$$\kappa = \frac{\tau_c}{\tau_c + \tau_{mix}}$$

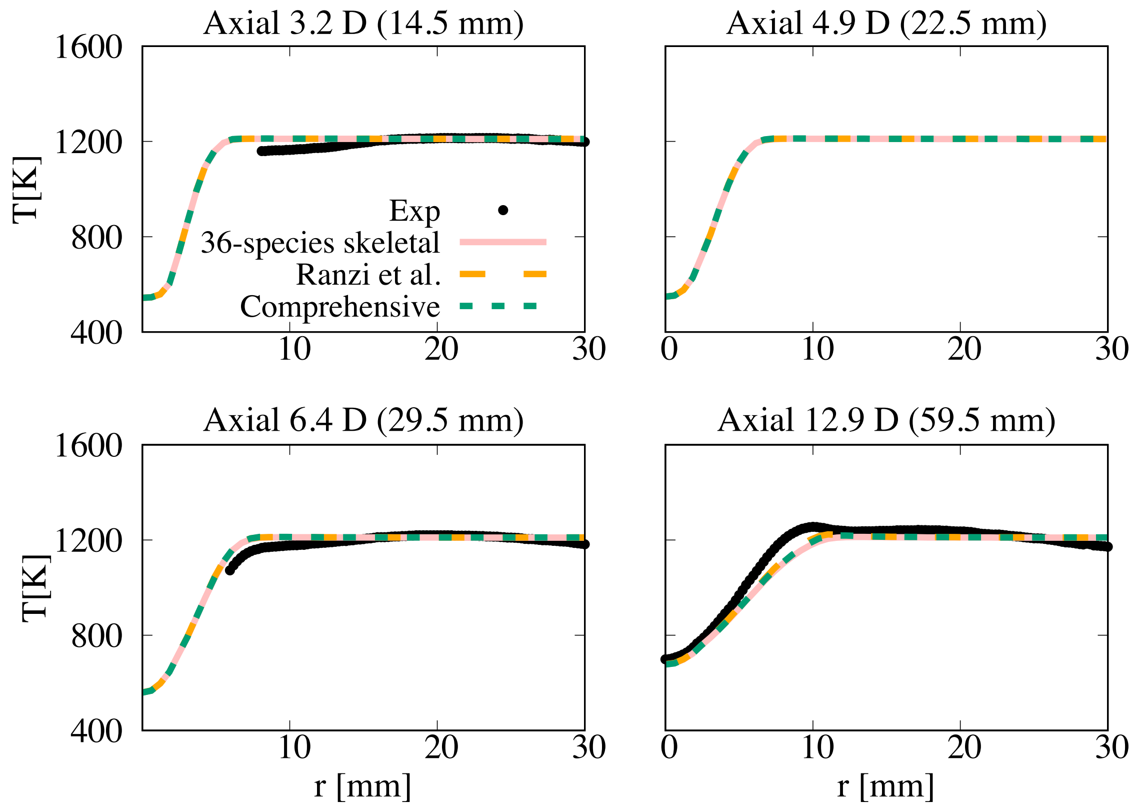
- Chemistry is solved on the fly.
- All species are transported.

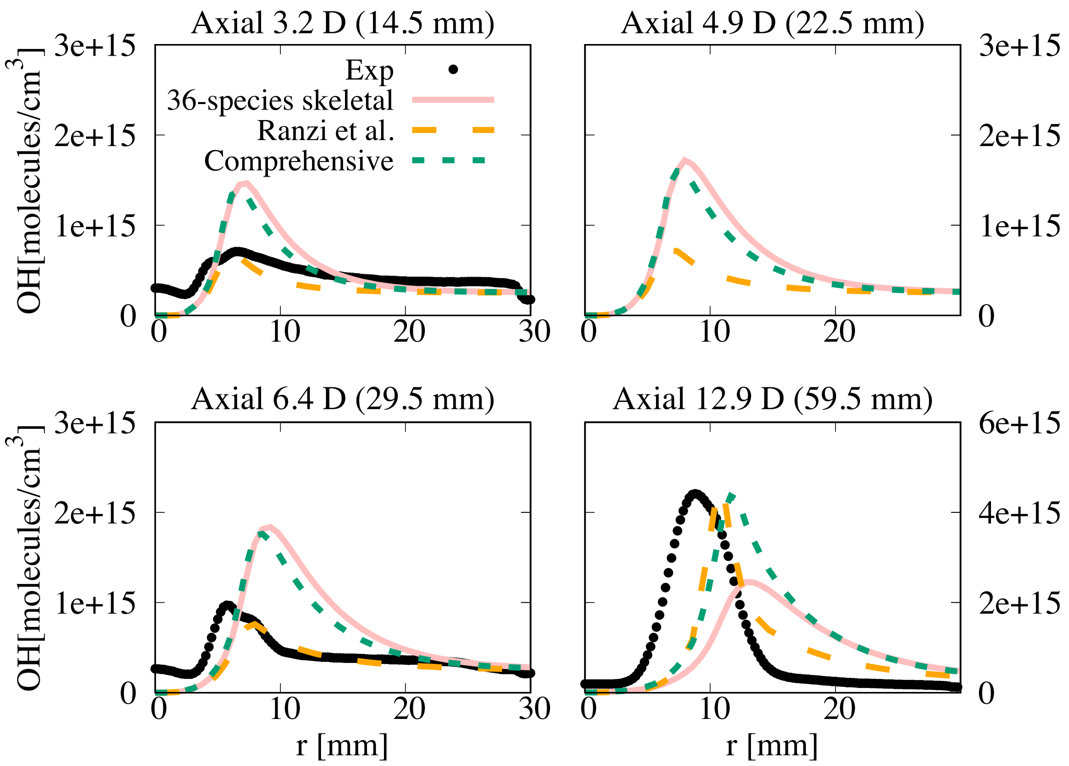
Validation: CFD simulation 3% oxygen level



Comprehensive: 1268 species Ranzi et al: 106 species

Validation: CFD simulation 6% oxygen level





Comprehensive: 1268 species Ranzi et al: 106 species

Conclusion

Chemistry reduction technique CARM is applied on the comprehensive n-heptane mechanism from Zhang et al. for the development of a skeletal mechanism (36 species) for LES/DNS study of MILD combustion with long-chain alkane fuel.

- **Ignition delay**: compared with other mechanisms with similar no. of species, the present reduced 36 species skeletal mechanism show slightly better prediction under conditions that are pertinent to MILD combustion.
- **Laminar flame speed**: much improved values are obtained compared with mechanisms reduced for engine conditions.
- **CFD simulation**: satisfactory results compared with comprehensive (1268 species) and skeletal (106 species) mechanisms with much more species & low temperature range.

References

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