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Development of skeletal chemical mechanisms with coupled species sensitivity analysis method

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1. Background and Motivation

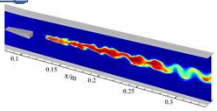
◆ Chemical kinetic is useful and important

- Laminar Buring Velocity
- Ignition Delays
- Species Fraction

Chemical Reaction Model

Combustion Modeling

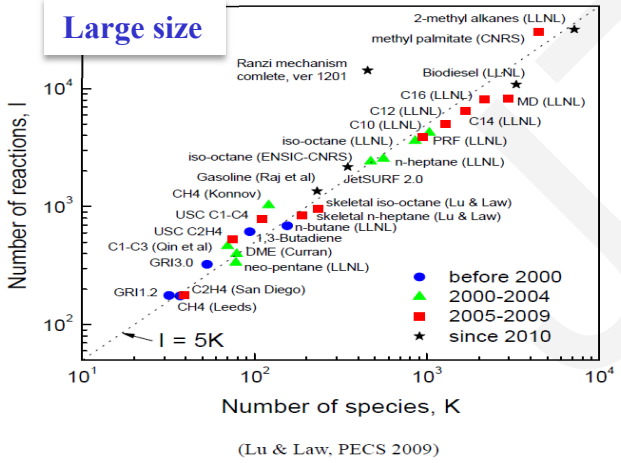
- RANS, LES, DNS
- Turbulence/Chemistry



Elementary Reaction

- Quantum Chemistry
- Molecular Modeling

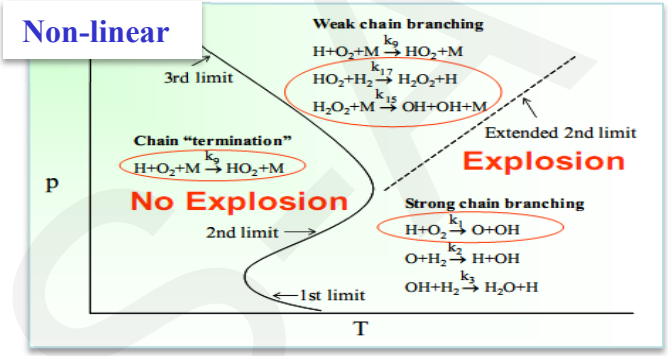
Large size



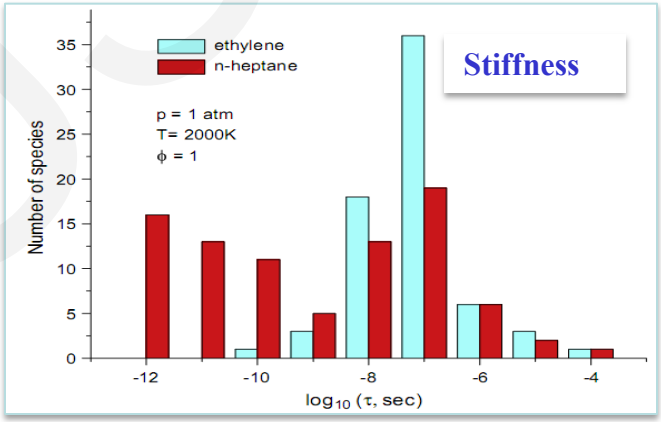
(Lu & Law, PECS 2009)

◆ Detailed chemical kinetic is copmplex

Non-linear



Stiffness



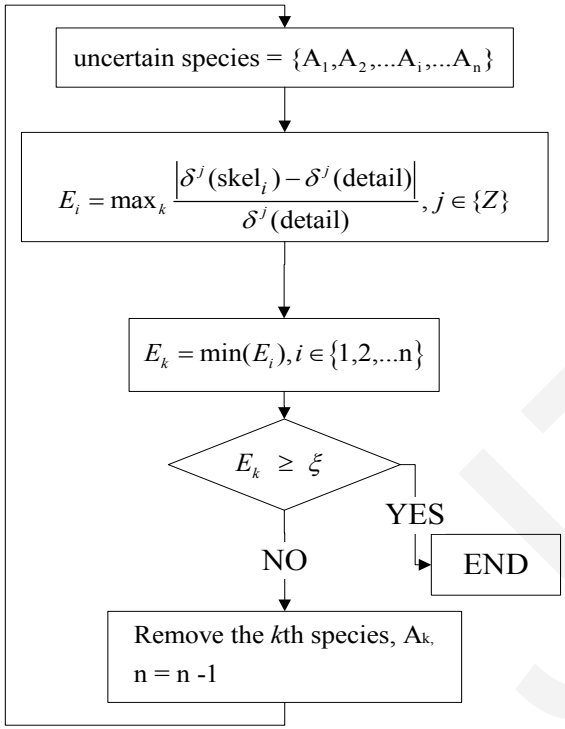
- ✓ Detailed reaction models are large
- ✓ Transportation fuels: ~10^3species,~10^4 reactions
- ✓ Flame simulations with detailed chemistry are time-consuming or unaffordable
- ✓ Time of CFD ~ N^2 (N: number of species)

2. Reduction Method: CSSA

◆ CSSA: Coupled Species Sensitivity Analysis

Make the species coupled in the uncertain set: redundant species are removed in a two-at-a-time and one-by-one way

$$E_i = \max_j \frac{\left|\delta^j(\text{skel}_i) - \delta^j(\text{detail})\right|}{\delta^j(\text{detail})}, j \in \{Z\}$$



Flowchart and concept of CSSA method

$$R_{AB} = r_{AB}^{DRG} + r_{BA}^{DRG}$$

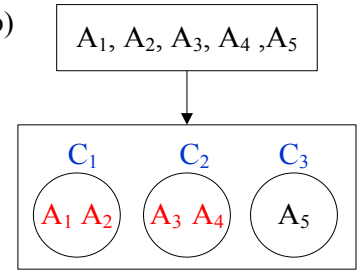
$$r_{AB}^{DRG} = \frac{\sum_{i=1,I} \left|v_{A,i}\omega_i\varphi_B^i\right|}{\sum_{i=1,I} \left|v_{A,i}\omega_i\right|}, \quad r_{BA}^{DRG} = \frac{\sum_{i=1,I} \left|v_{B,i}\omega_i\varphi_A^i\right|}{\sum_{i=1,I} \left|v_{B,i}\omega_i\right|}.$$

(a)

coupled species	R_{AB}
A_1, A_2	1.70
A_1, A_3	1.60
A_2, A_4	1.50
A_3, A_4	1.40

A_1, A_2	1.70
A_3, A_4	1.40

(b)



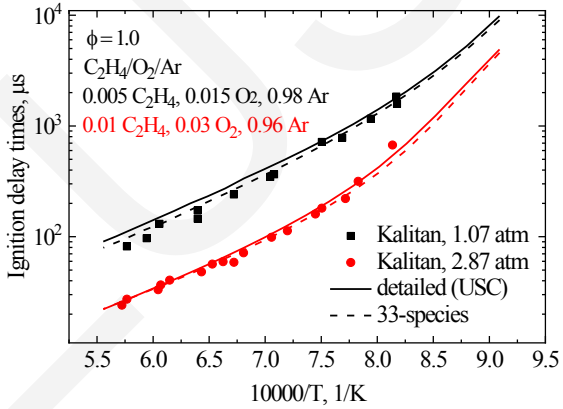
Definition of the coupled species

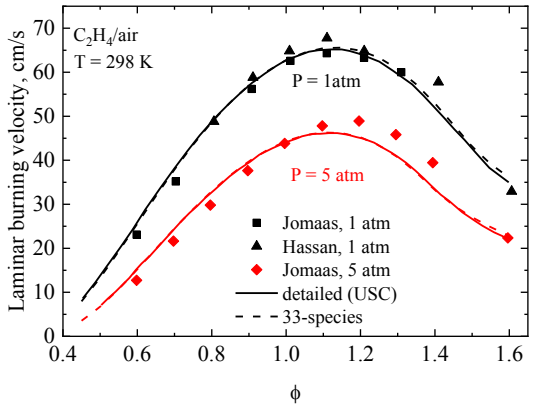
3. Skeletal mechanisms development: C_2H_4 (1)

- Detailed reaction models: USC 2.0 model (111-species, 784-reaction)
- Reduction target conditions: Φ = 0.5~2.0, P = 1atm~30atm}, and T = 1000K~2000K
- Reduction method: CSSA
- Finally, skeletal mechanism containing 33-species and 211-reactions for ethylene combustion was obtained. The maximum error of the ignition delay time was about 10%

Coupled species of the uncertain set in ethylene reduction

Coupled species		R_{AB}	Uncoupled
aC_3H_5	C_3H_6	1.57	C_2O
HCCO	C_2H_2	1.53	CH_2OCH
C_3H_8	nC_3H_7	1.50	CH_2*
C_3H_3	aC_3H_4	1.41	C_2H_6
$C_4H_{8-}1$	C_4H_7	1.32	H_2O_2
C_4H_4	C_4H_6	1.31	CH_2CO
CH_3OH	CH_3O	1.20	CH_4
C_2H	C_4H_2	1.17	
CH	pC_3H_4	1.14	



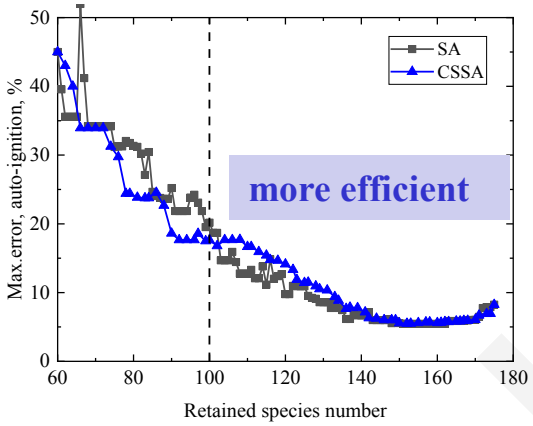


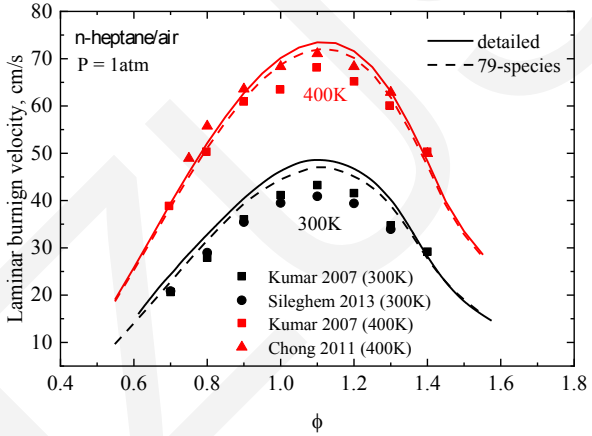
Validation: auto-ignition delays **Validation: laminar flame speeds**

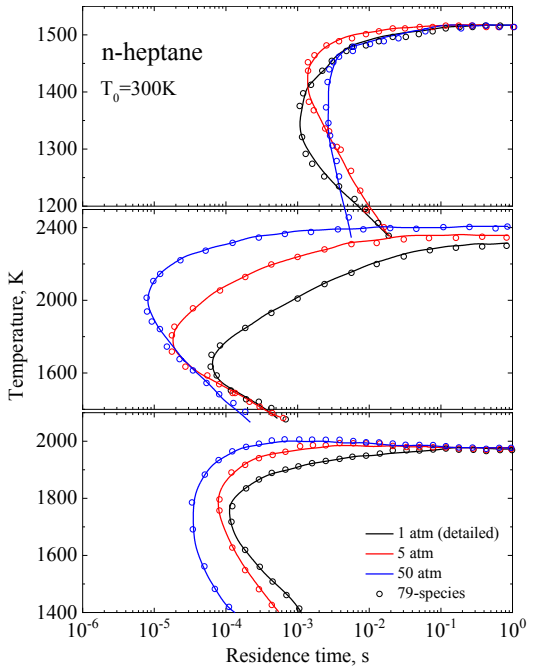
✓ The achieved 33-species ethylene reaction model with CSSA method can afford auto-ignition and laminar flame

3. Skeletal mechanisms development: n-C_7H_{16} (2)

- Detailed reaction models: LLNL model (561-species, 2539-reaction)
- Reduction target conditions: Φ = 0.5~1.5, P = 1atm~50atm}, and T = 1000K~1800K (NTC)
- Reduction method: CSSA
- Finally, skeletal mechanism containing 79-species and 339-reactions for n-heptane combustion was obtained. The maximum error of the ignition delay time was about 22%







- ✓ The reduction time of the CSSA method was 55 CPU hours, less than half that of the conventional SA method (136 h)
- ✓ The achieved 79-species ethylene reaction model with CSSA method can afford auto-ignition, laminar flame and PSR validation

4. Conclusion

- A new chemical reaction reduction method, CSSA is introduced. Two species having a large interaction coefficient are regarded as one coupled unit and removed together.
- A 33-species skeletal reaction model for ethylene combustion was generated. The conditions for model validation covered ϕ = 0.5–2.0, temperature 1000–1800 K, and pressure 1–30 atm.
- A skeletal mechanism of n-heptane with 79 species was achieved. Ignition delay times, laminar flame speeds, PSR modeling, temperature-time profiles and brute-force sensitivity coefficients were in good agreement with those of the detailed mechanisms.
- The CSSA method is less time-consuming than the conventional SA method, and the achieved skeletal chemical mechanisms are suitable for combustion modeling.