Skeletal Mechanism Generation for Surrogate Fuels Using Directed Relation Graph with Error Propagation and Sensitivity Analysis (DRGEPSA)

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Objectives

- Accurate prediction of fuel combustion and pollutant emissions requires comprehensive detailed chemical reaction mechanisms.
- However, detailed mechanisms for hydrocarbons of interest contain too many species/reactions and time scales to be used in practical simulations.
- Reduction of these large mechanisms is needed.

Background

Skeletal Reduction:

eliminating unimportant species and reactions while retaining important chemistry

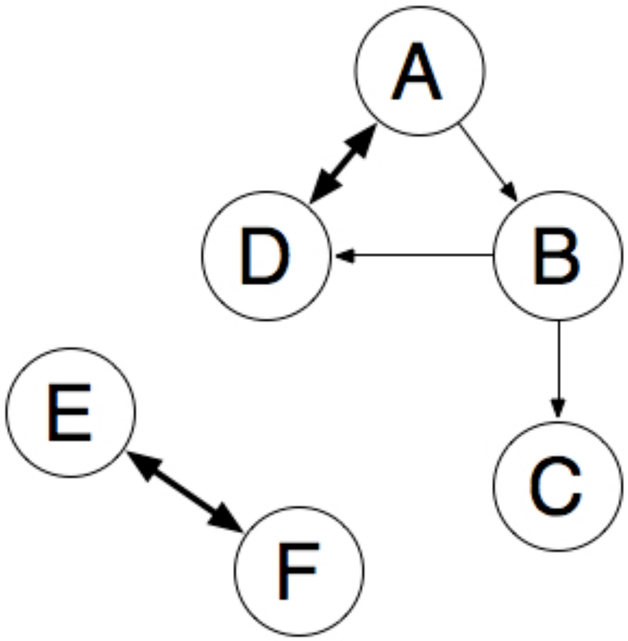
Recently Developed Skeletal Reduction Methods:

- Directed Relation Graph (**DRG**) – Lu and Law (2005)
- Directed Relation Graph with Error Propagation (**DRGEP**) – Pepiot-Desjardins and Pitsch (2005, 2008)
- DRG-aided Sensitivity Analysis (**DRGASA**) – Lu and Law (2007)

Current Approach:

- Directed Relation Graph with Error Propagation and Sensitivity Analysis (**DRGEPSA**)

DRG/DRGASA Method (1)



- Coupling of species determined by normalized contribution to overall production
- Directed arrow shows dependence of one species to another.

$$r_{AB} \equiv \frac{\left|\sum_{i=1,I} \nu_{A,i}\omega_i\delta_B^i\right|}{\left|\sum_{i=1,I} \nu_{A,i}\omega_i\right|}$$

r_{AB} – normalized interaction coefficient of species B to the production of species A

$n_{A,i}$ – stoichiometric coefficient for the i^{th} elementary reaction for species A

ω_i – production rate of the i^{th} reaction

$$\delta^i{}_B = \begin{cases} 1, & \text{if the } i^{th} \text{ reaction involves species B}, \\ 0, & \text{otherwise} \end{cases}$$

DRG/DRGASA Method (2)

- Species B where $r_{AB} < \varepsilon_{DRG}$ is removed from the dependent set for target species A (ε_{DRG} is a small value, e.g. 0.1)
- Skeletal mechanism consists of set of dependent species for designated target species (fuel, oxidizer, important pollutants, etc) based on depth first search (DFS).
- Species with $\varepsilon_{DRG} < r_{AB} < \varepsilon^*$ (e.g. 0.5) are then analyzed with sensitivity analysis to produce a minimal skeletal mechanism for a given error threshold.

DRGEP Method (1)

$$r_{AB} \equiv \frac{\left|\sum_{i=1,I} \nu_{A,i}\,\omega_i\,\delta^i{}_B\right|}{\max\left(P_A, C_A\right)}$$

$$P_A = \sum_{i=1,I} \max\left(0, \nu_{i,A}\,\omega_i\right)$$

$$C_A = \sum_{i=1,I} \max\left(0, -\nu_{i,A}\,\omega_i\right)$$

- Extension of DRG considering error propagation along species paths.
- Identifies more unimportant species for an equivalent error.
- Species B where $R_{AB} < \varepsilon_{EP}$ is removed from the dependent set for target species A.

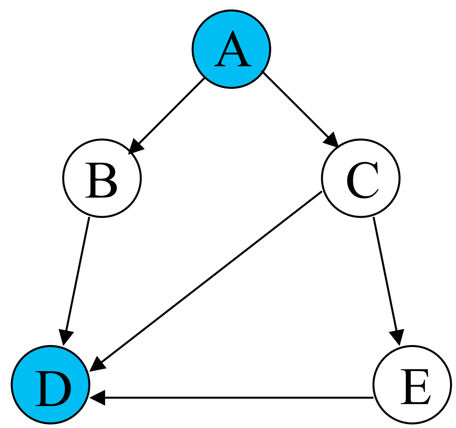
$$r_{AB,p} = \prod_{i=1}^{n-1} r_{S_i S_{i+1}}$$

$$R_{AB} = \max_{\text{all paths } p}\left(r_{AB,p}\right)$$

$r_{AB,p}$ – path-dependent interaction coefficient for path *p* between species A and B.

R_{AB} – overall interaction coefficient

DRGEP Method (2)



DRG: $R_{AD} = \max\left[\max\left(r_{AB}, r_{BD}\right), \max\left(r_{AC}, r_{CD}\right), \max\left(r_{AC}, r_{CE}, r_{ED}\right)\right]$

DRGEP: $R_{AD} = \max\left[\left(r_{AB} \cdot r_{BD}\right), \left(r_{AC} \cdot r_{CD}\right), \left(r_{AC} \cdot r_{CE} \cdot r_{ED}\right)\right]$

R_{AD} is the overall interaction coefficient of species D to the target species A

DRGEPSA vs. DRGASA

- Sensitivity analysis (SA) included to eliminate more unimportant species, but computationally expensive.
- By using DRGEP prior to SA phase, more species can be removed than with DRGASA to produce a smaller final mechanism for the same mechanism performance.
- DRGEP alone is insufficient because the relationship between interaction coefficient and induced error in global properties is unclear for some species, requiring sensitivity analysis.

DRGEPSA Method (1)

- DRGEP produces a preliminary skeletal mechanism.
  - *Removed species*: $R_{AB} < \varepsilon_{\mathrm{EP}}$
- Species are classified into two categories based on overall interaction coefficient:
  - *Limbo species:* $\varepsilon_{\mathrm{EP}} < R_{AB} < \varepsilon^*$ (e.g. 0.5)
    - analyzed with SA
  - *Retained species:* $R_{AB} > \varepsilon^*$
    - retained in mechanism without analysis

DRGEPSA Method (2)

- SA is performed by removing each species in the limbo category one at a time and calculating the induced error.
- Species are arranged in order based on the differences between induced errors and the error of the DRGEP skeletal mechanism.
  - Many species do not change the mechanism performance compared to the DRGEP mechanism, so using induced errors alone for ranking would be incorrect.
- The final skeletal mechanism is generated by removing species one at a time in order until the resulting error reaches the required tolerance level.

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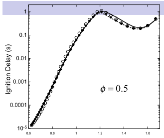
DRGEPSA Example (1)

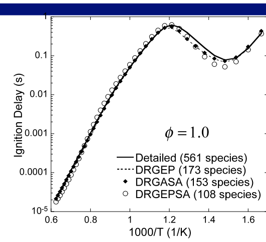
Constant volume ignition of ***n*-heptane**: initial conditions 600-1600 K, 1-20 atm, and f=0.5-1.5 from detailed mechanism of Curran *et al.* 1998:

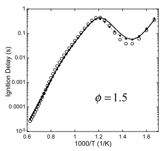
- Maximum tolerable error: 30%
- ε_{DRG}=0.16, ε_{DRGEP}=0.01
- Target species: *n*-heptane, oxygen, nitrogen, H-radical

	Detailed	DRG	DRGEP	DRGASA	DRGEPSA
Species	561	211	173	153	108
Reactions	2539	1044	868	691	406
Maximum error		21%	28%	24%	27%

DRGEPSA Example (2)







Autoignition Results (*n*-Heptane)

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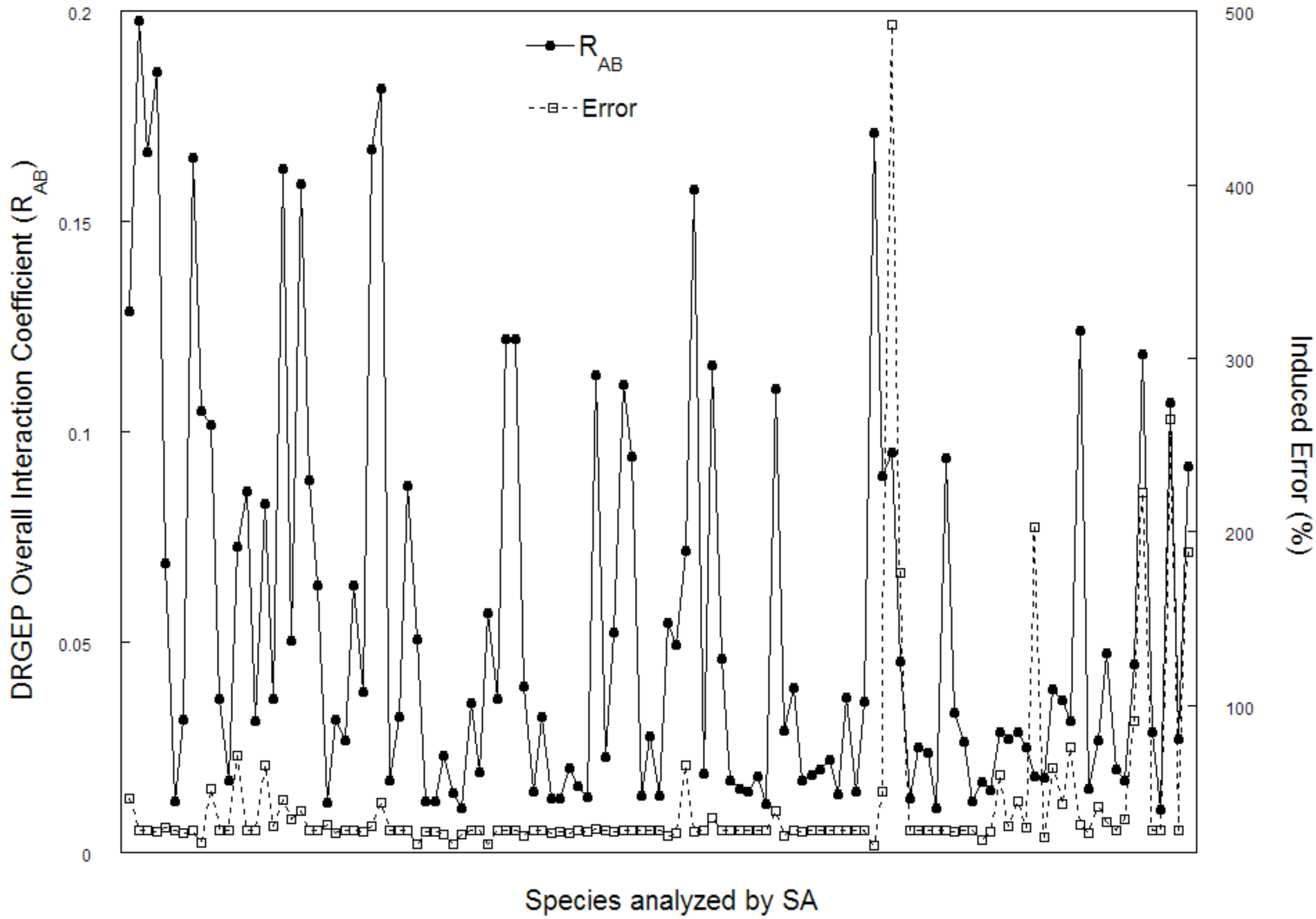
DRGEPSA Example (3)

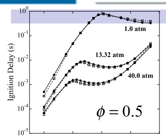


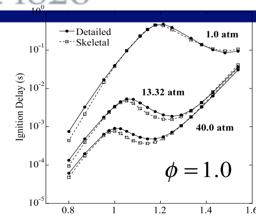
Limbo species: R_{AB} and induced error

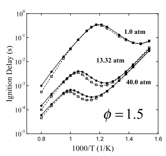
n-Decane Skeletal Mechanism (1)

- Two skeletal mechanisms generated from constant volume autoignition **n-decane** mechanism of Westbrook *et al.* 2009 (940 species, 3878 reactions):
  - Initial conditions: 650-1250 K, 13.32 atm, and $\phi = 1.0$ (*comprehensive mechanism*)
    - Skeletal mechanism: 232 species, 822 reactions
  - Initial conditions: 1000-1300 K, 1.0 atm, and $\phi = 0.5 – 1.5$ (*high-temperature mechanism*)
    - Skeletal mechanism: 50 species, 242 reactions
- Validation performed with autoignition and laminar flame speed calculations

n-Decane Skeletal Mechanism (2)



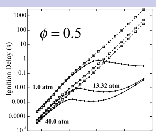


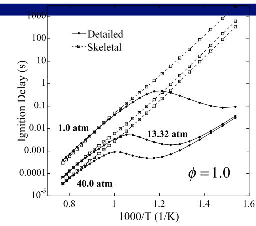


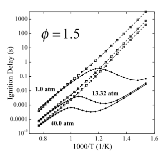
1000/T (1/K)

Autoignition Results: 232 species

n-Decane Skeletal Mechanism (3)

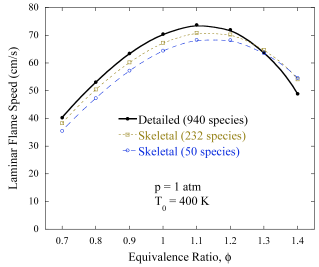






Autoignition Results:
50 species

n-Decane Skeletal Mechanism (4)



Summary

- By combining error propagation and sensitivity analysis, DRGEPSA provides greater reduction of large mechanisms with equivalent performance compared to the DRGASA and DRGEP methods.
- DRGEPSA can be used to generate skeletal mechanisms to match the performance of large reaction mechanisms in predicting autoignition and flame propagation with acceptable error.

Questions?