



CASE WESTERN RESERVE
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Skeletal Mechanism Generation of Surrogate Fuels Using Directed Relation Graph with Error Propagation and Sensitivity Analysis (DRGEPSA)

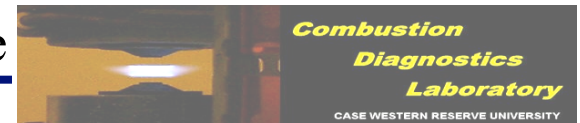
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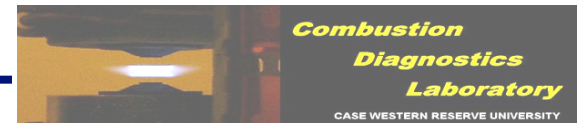


Objectives

- 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.



- Developing mechanism reduction software package: **Mechanism Automatic Reduction Software (MARS)**
- Package contents:
 - Skeletal reduction via DRGEPSA (*current focus*)
 - QSS-based time-scale reduction (*in progress*)
 - Unimportant reaction removal (*future work*)
 - Isomer lumping (*future work*)
 - Diffusive species bundling (*future work*)
- Goal of package: limited user interaction
 - Inputs: Autoignition initial conditions, maximum error limit





Skeletal Reduction:

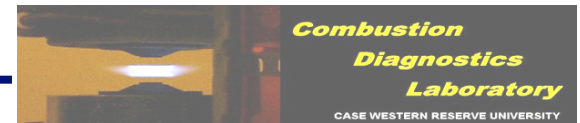
eliminating unimportant species and reactions while retaining important chemistry

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)

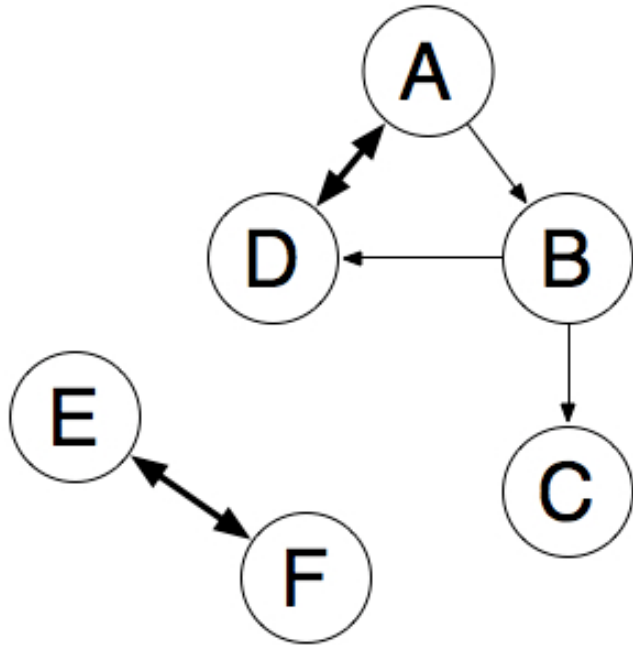
Current Approach:

- 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.

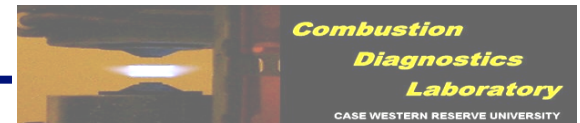
$$r_{AB} \equiv \frac{\left| \sum_{i=1,I} \nu_{A,i} \omega_i \delta_B^i \right|}{\left| \sum_{i=1,I} \nu_{A,i} \omega_i \right|}$$

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

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

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

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





- Species B where $r_{AB} < \epsilon_{DRG}$ 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 $\epsilon_{DRG} < r_{AB} < \epsilon^*$ (e.g. 0.5) are then analyzed with sensitivity analysis to produce a minimal skeletal mechanism for a given error threshold.



DRGEP Method (1)

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

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

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

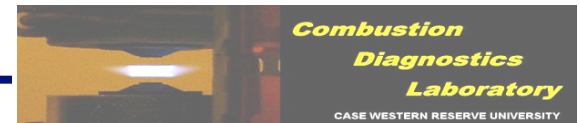
$$r_{AB,p} = \prod_{i=1}^{n-1} r_{S_i S_{i+1}}$$

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

- 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.

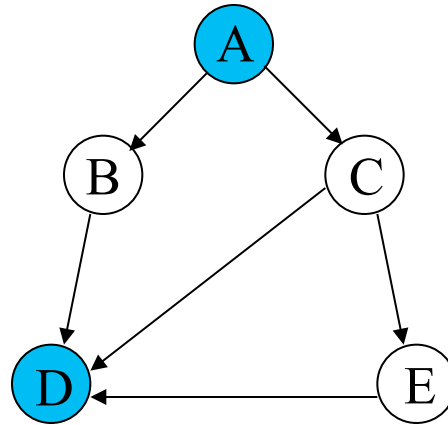
$r_{AB,p}$ – path-dependent interaction coefficient for path p between species A and B.

R_{AB} – overall interaction coefficient





DRGEP Method (2)



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

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

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



- 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.

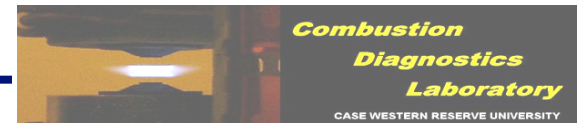


- DRGEP produces a preliminary skeletal mechanism.
 - *Removed species*: $R_{AB} < \epsilon_{EP}$
- Species are classified into two categories based on overall interaction coefficient:
 - *Limbo species*: $\epsilon_{EP} < R_{AB} < \epsilon^*$ (e.g. 0.2 - 0.4)
 - analyzed with SA
 - *Retained species*: $R_{AB} > \epsilon^*$
 - 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.





DRGEPSA Example (1)

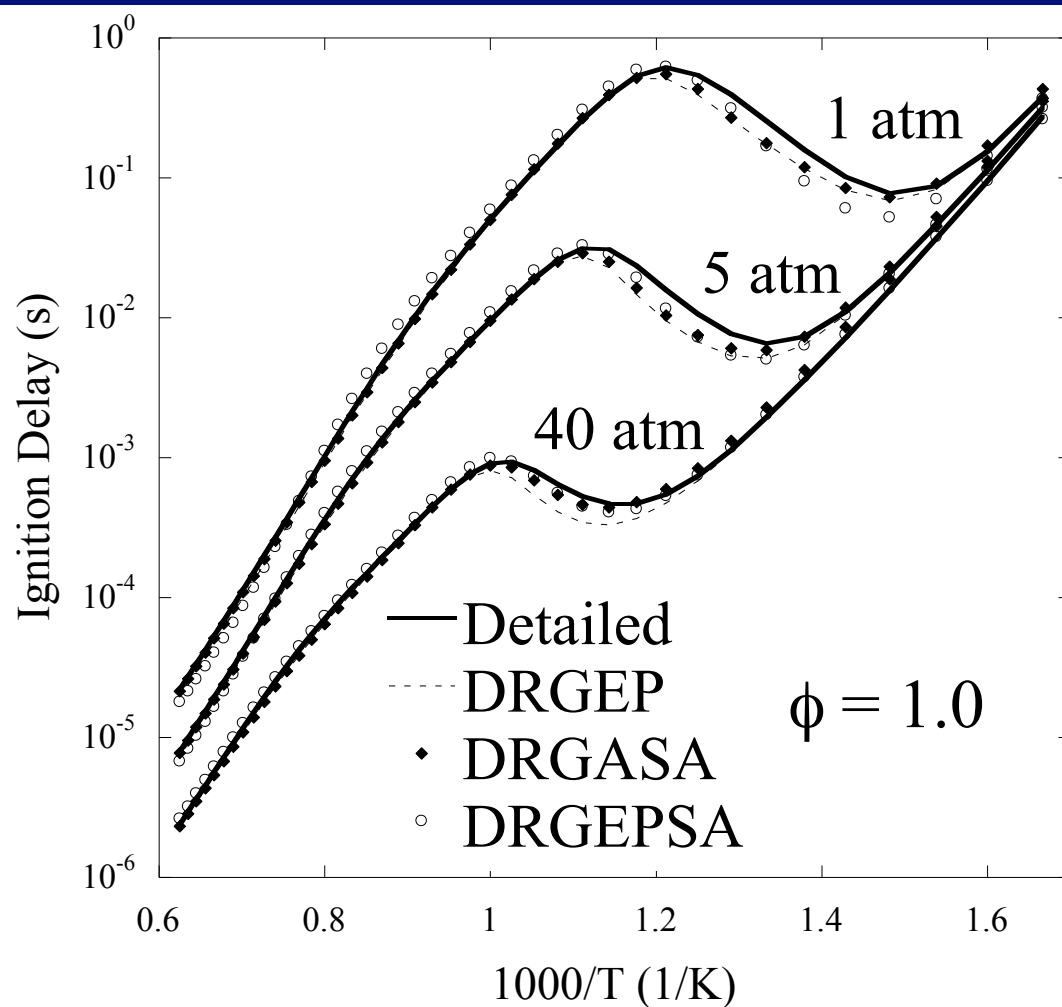
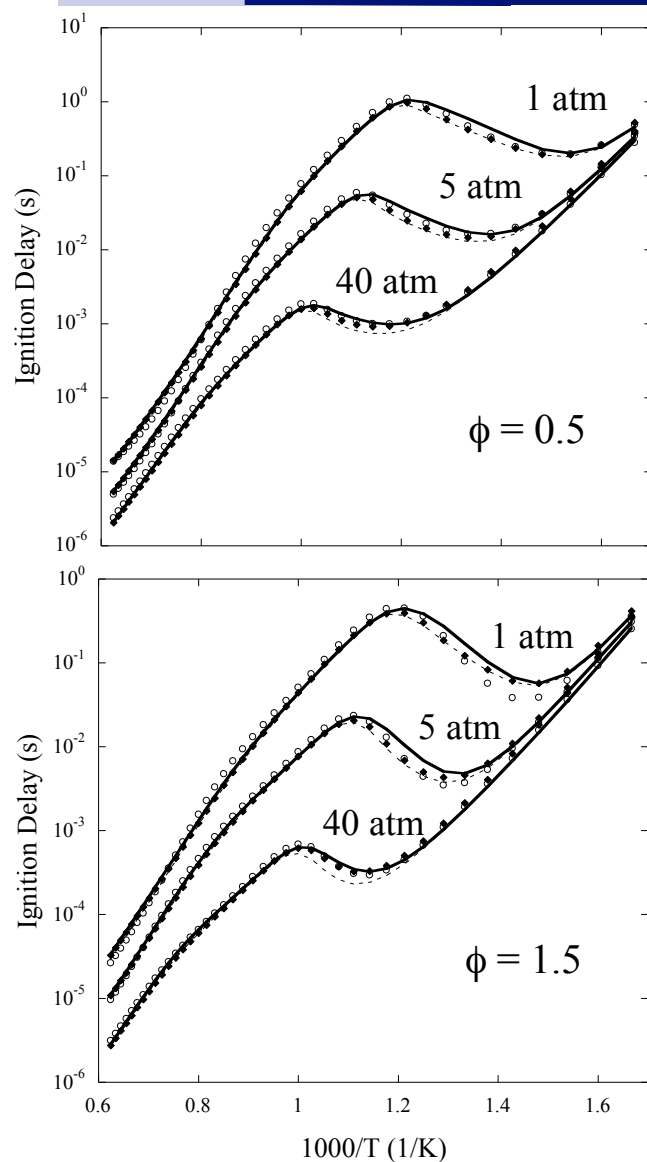
Constant volume ignition of ***n*-heptane**: initial conditions 600-1600 K, 1-20 atm, and $\phi=0.5$ -1.5 from detailed mechanism of Curran *et al.* 1998:

- Maximum tolerable error: 30%
- $\varepsilon_{\text{DRG}}=0.16$, $\varepsilon_{\text{EP}}=0.01$
- 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)

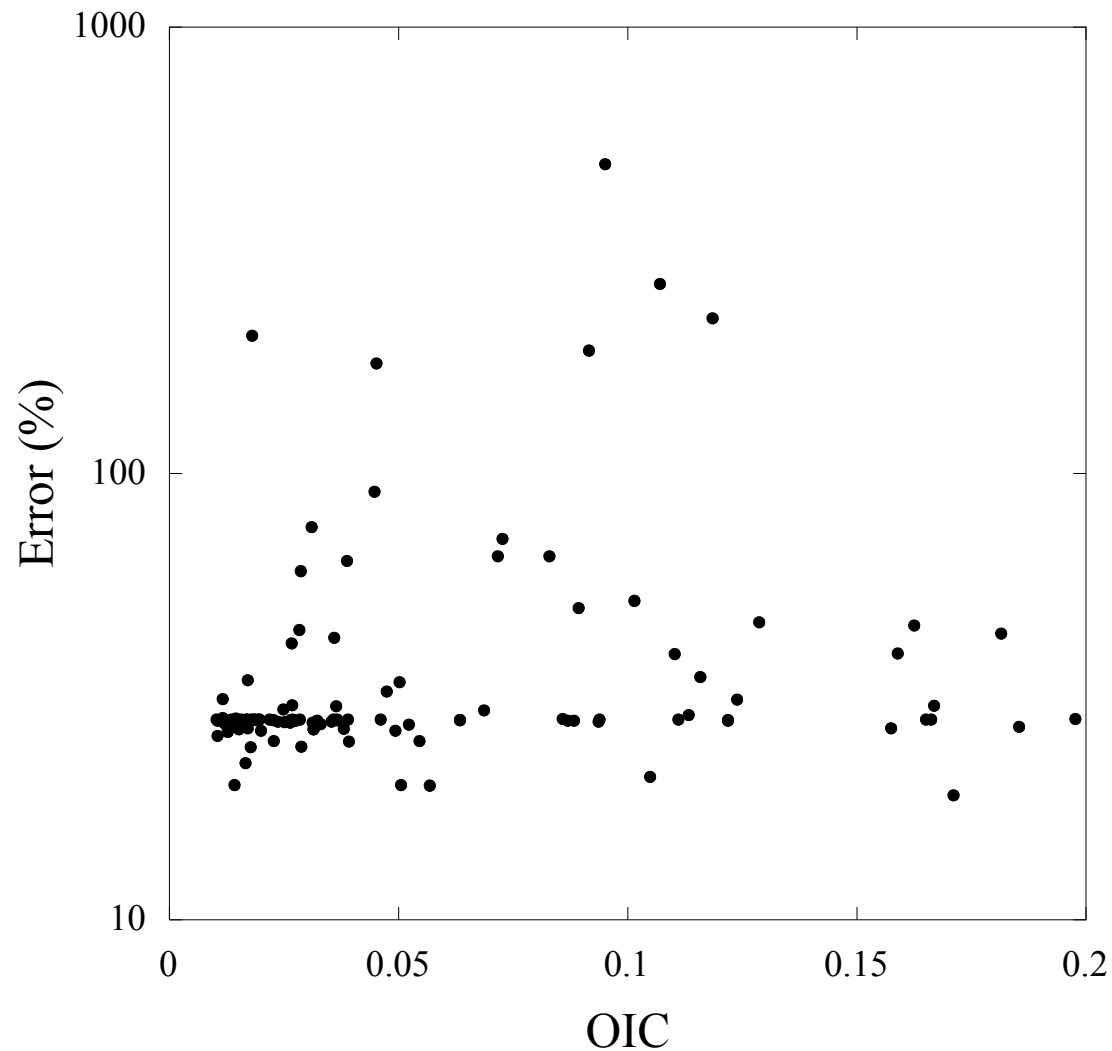


Autoignition Results (*n*-Heptane)





DRGEPSA Example (3)



Limbo species: Max induced error vs. R_{AB}





DRGEPSA Example (4)

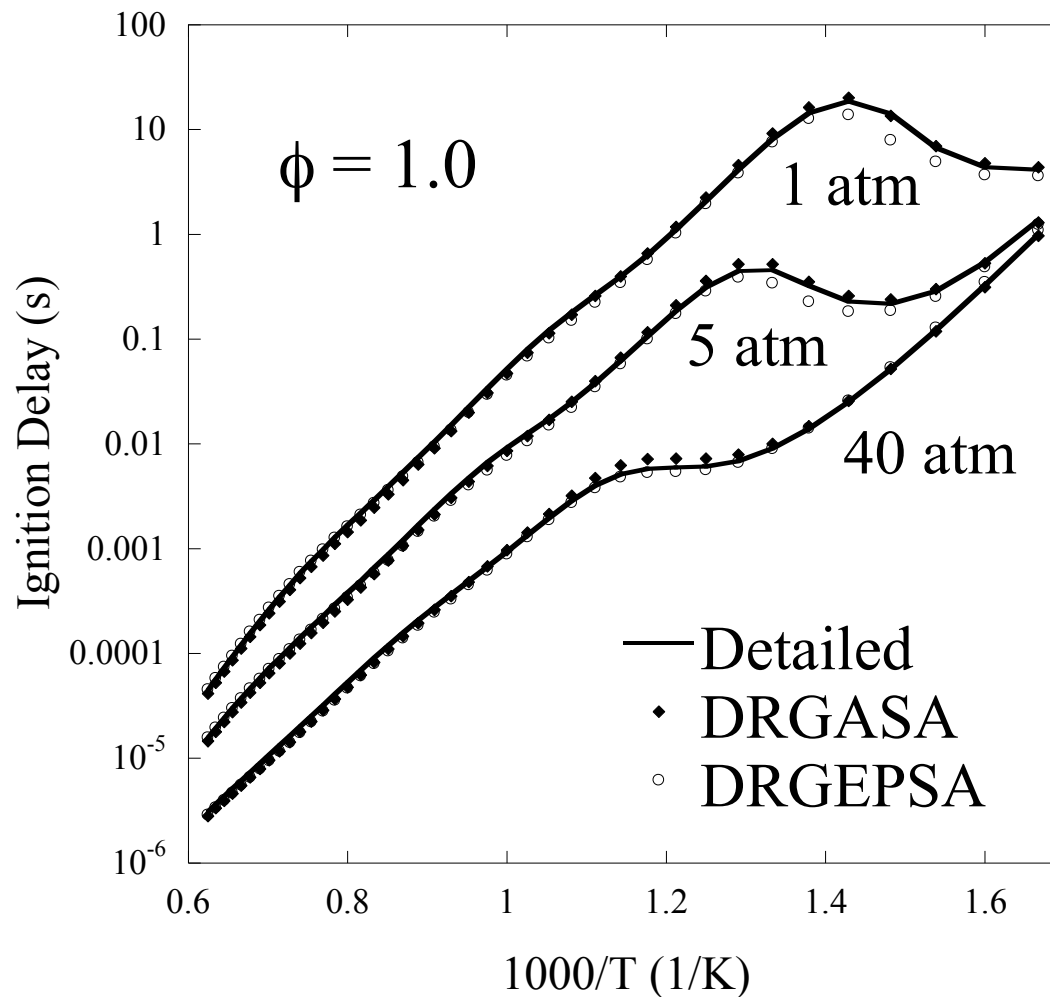
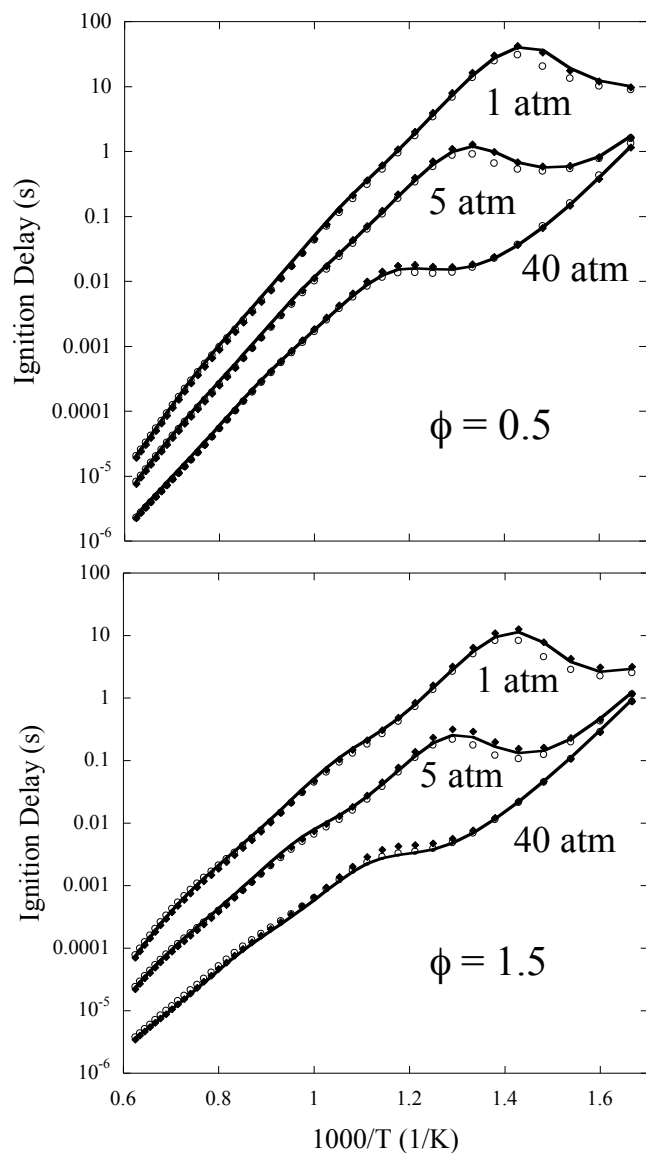
Constant volume ignition of *iso*-octane: initial conditions 600-1600 K, 1-20 atm, and $\phi=0.5$ -1.5 from detailed mechanism of Curran *et al.* 2002:

- Maximum tolerable error: 30%
- $\varepsilon_{\text{DRG}}=0.15$, $\varepsilon_{\text{EP}}=0.004$
- Target species: *iso*-octane, oxygen, nitrogen, H-radical

	Detailed	DRG	DRGEP	DRGASA	DRGEPSA
Species	857	275	232	211	165
Reactions	3606	722	1140	885	779
Maximum error		13%	15%	26%	19%



DRGEPSA Example (5)



Autoignition Results (*iso*-Octane)





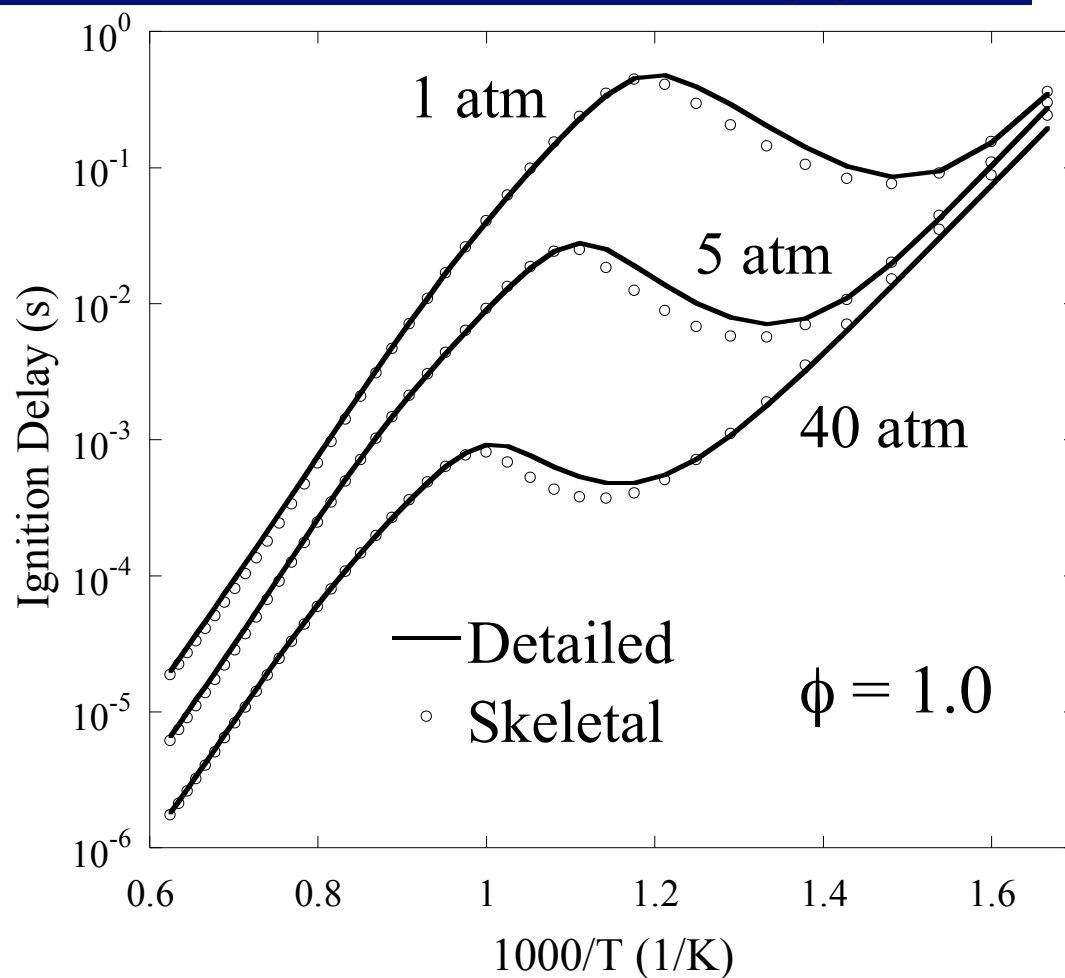
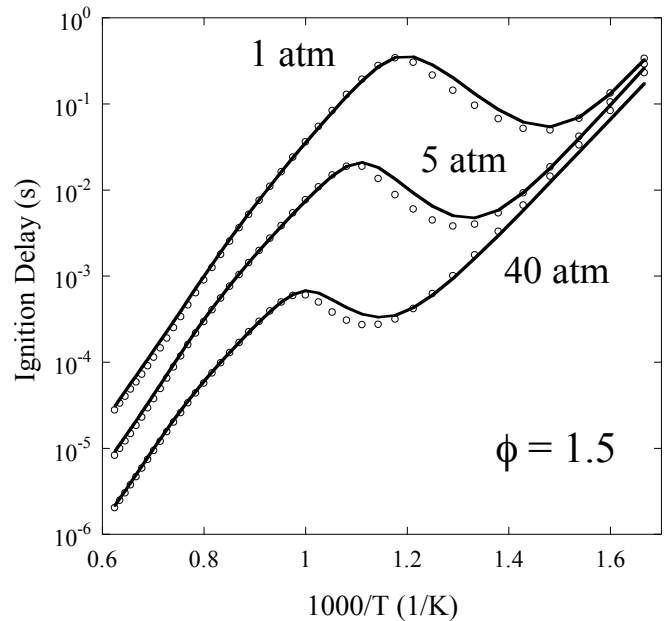
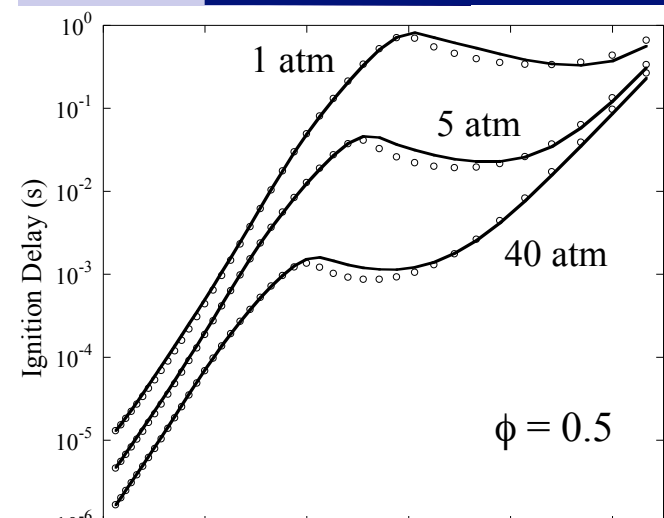
n-Decane Skeletal Mechanism (1)

- Two skeletal mechanisms generated from constant volume autoignition **n-decane** from mechanism of Westbrook *et al.* 2009 (2115 species, 8157 reactions):
 - Initial conditions: 600-1600 K, 1-20 atm, and $\phi = 0.5-1.5$ (*comprehensive mechanism*)
 - Skeletal mechanism: 202 species, 846 reactions
 - Initial conditions: 1000-1300 K, 1.0 atm, and $\phi = 0.5-1.5$ (*high-temperature mechanism*)
 - Skeletal mechanism: 45 species, 190 reactions
- Validation performed with autoignition





n-Decane Skeletal Mechanism (2)

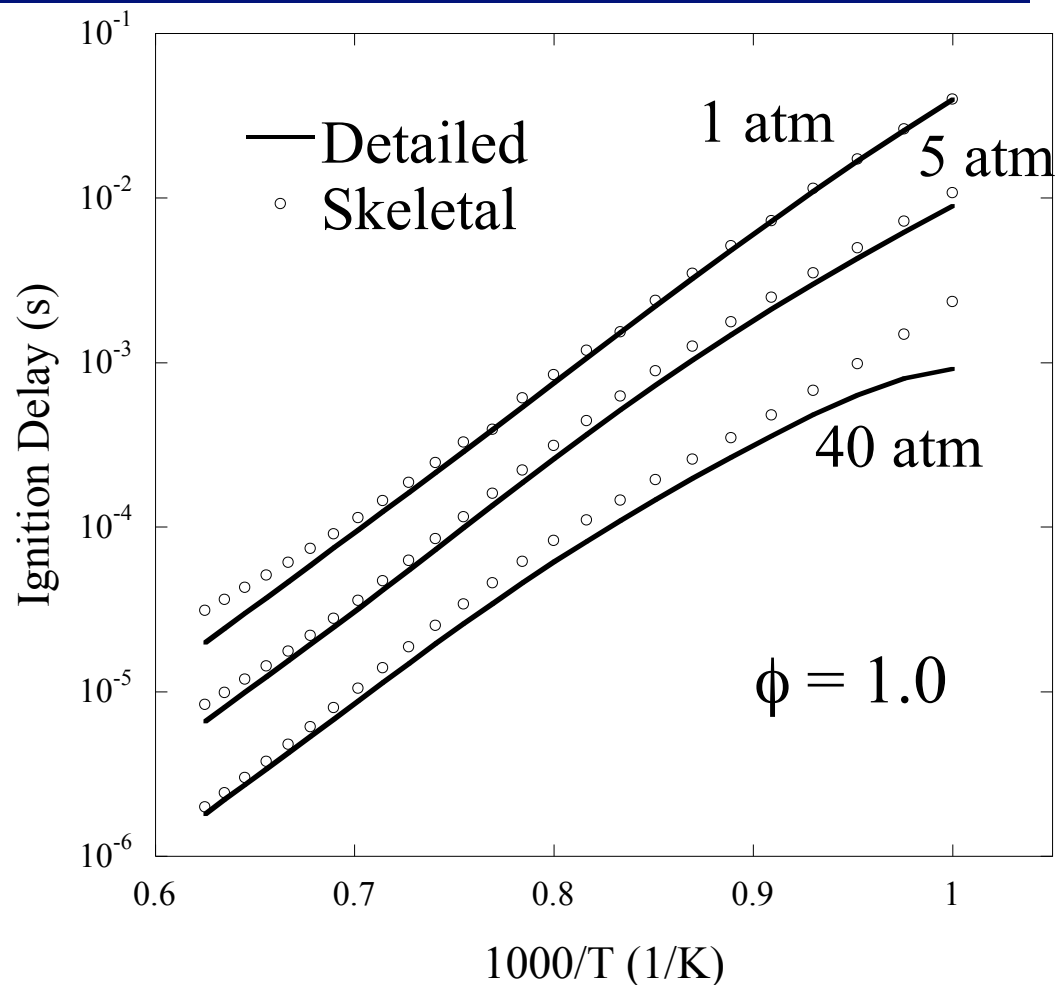
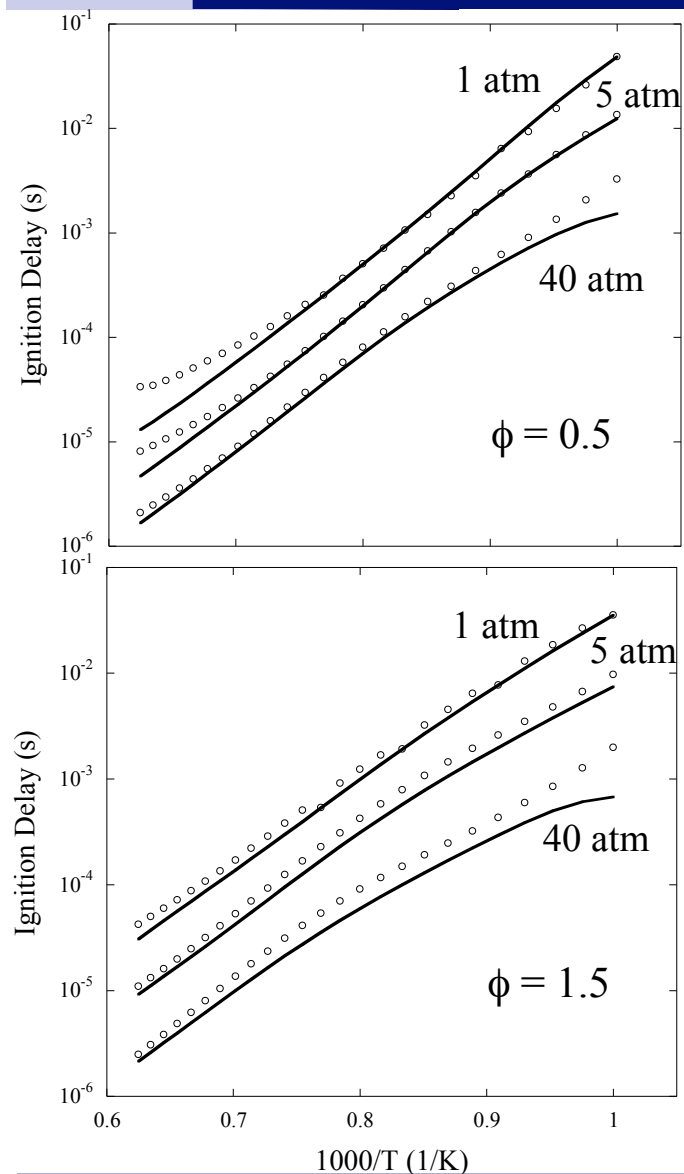


Autoignition Results:
202 species





n-Decane Skeletal Mechanism (3)



Autoignition Results:
45 species





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 with acceptable error.
 - By limiting the range of validity to that desired, skeletal mechanisms for use in large-scale simulations can be developed.
- As one component of MARS package, DRGEPSA provides simple and automated method to generate skeletal mechanism.





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Thank you

Questions?

