Toward Development of Machine Learned Techniques for Production of Compact Kinetic Models

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Introduction

- Detailed chemical kinetic models describe the actual combustion reaction mechanism of a fuel at fundamental detail.
- These models are almost completely condensable to chemical reaction theory.
- Hence, these models describe the consequent combustion phenomena and behaviour of the fuel to excellent fidelity.
- However, due to the complexity involved in reacting flow simulations, these models are of limited utility.
- Thus, to allow for rapid iterative deployment of multi-dimensional reacting flow simulations in the combustor design process, a much smaller kinetic model of reduced dimensionality is needed.
- This model must retain a predictive fidelity in the computation of key quantities of interest, to the detailed model calculations.

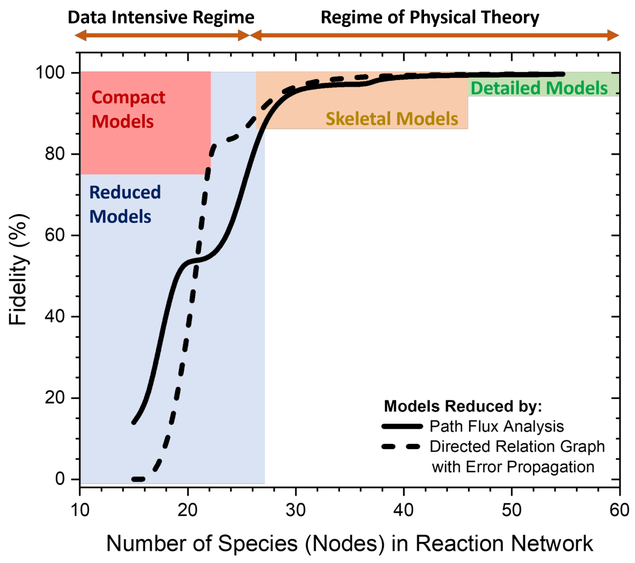

Figure 1. Dependence of the fidelity of model calculation for methane combustion on complexity of reaction network, for models produced by PFA and DRGEP to detailed model calculations of ignition delay times at: 1-40 atm, 1100-2000 K, methane/air mixture fractions 0.5 – 1.5.

Concept – "Compact Models"

- *Compact models:* Overly-reduced and optimised kinetic models.
- These provide an attractive compromise between accuracy and computational cost.
- Compact kinetic model production (or compaction) involves:
  1. Generating a virtual reaction network using a minimal number of nodes (species).
  2. Optimisation of input parameters (virtual reaction rate constants and/or network nodes' thermomolecular properties) to a set of combustion calculations.
- As the construct is entirely virtual, model descriptors are not constrained to obey chemical reaction theory or confined to experimental measurements.

Result: A minimally-sized kinetic model (in ChemKin reaction format) that is highly accurate across a defined set of combustion calculations.

Automated Compaction Algorithm – "MLOCK"

- **M**achine **L**earned **O**ptimisation for **C**hemical **K**inetics (**MLOCK**) is a compute intensification automated compaction methodology.
- **MLOCK** makes use of modern computing power to perform a large number of simulations quickly.
- A series of error functions are then used to analyse the data generated and to learn which discreet combination of kinetic model parameters result in an accurate replication of the target set of combustion kinetic calculations.

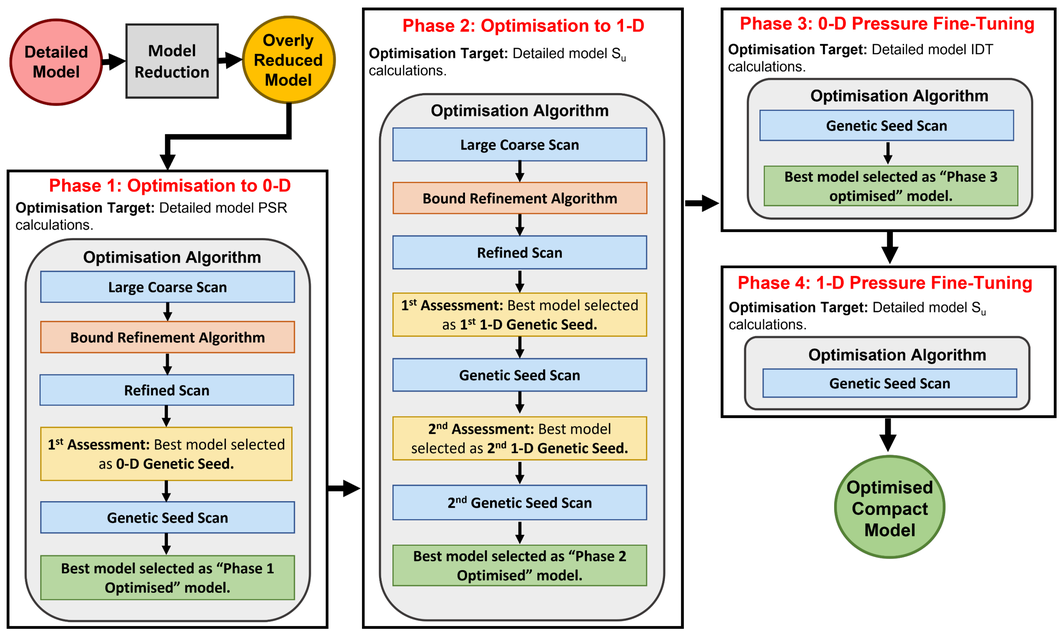

Figure 2. Process flow of the MLOCK1.0 algorithm which allows for the definition of any set of variables of interest to the user.

- The virtual reaction rate constants (k_v) of important connections (reactions) are optimised to detailed model 0-D (Phase 1 & 3) and 1-D (Phase 2 & 4) calculations.
- Phases 1 and 2 process flow:
  1. Coarse grid-like scan of large k_v range – produces representation of each connections error function topology.
  2. Bound refinement algorithm uses this information to perform binomial and Z-tests to score each region of k_v, for every connection undergoing optimisation, based on the probability that a good model is produced there.
  3. Refined scan is constrained to high scoring (low Z-score) regions of k_v.
  4. Narrow scan centred on best model (Genetic Seed) from the Coarse and Refined scans.

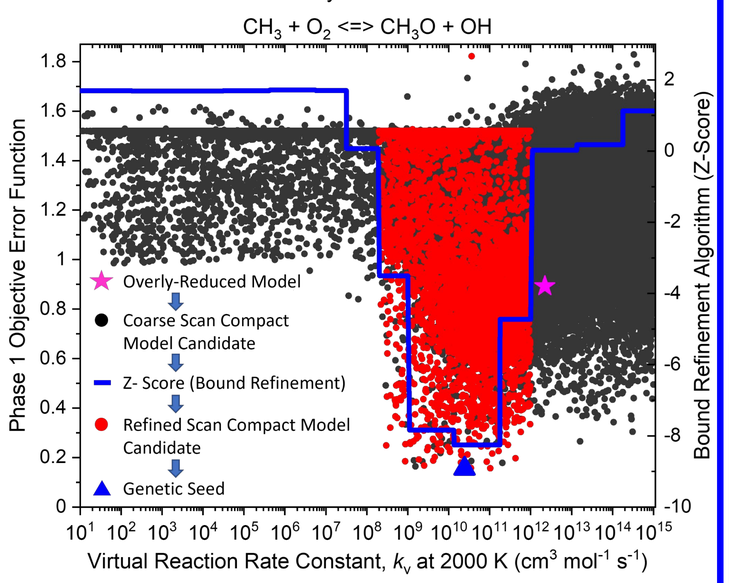

Figure 3. Phase 1 error function of compact model candidates produced in the Phase 1 Coarse and Refined Scans as a function of the virtual reaction rate constant of the connection $CH_3 + O_2 <=> CH_2O + H$, during 15-node methane compaction.

Compact Model for Methane/Air Combustion

- MLOCK was applied to methane/air combustion using two separate detailed models as starting points.
- Path flux analysis [7] was applied to the detailed model.
- The overly-reduced model was then optimised in 4 Phases (Figure 1).
- This performed to produce a 15- and 19-node compact model.
- These models were shown to outperform the state-of-art overly-reduced models (Table 1) in terms of PSR, IDT and Su across wide temperature, pressure and mixture fraction conditions.

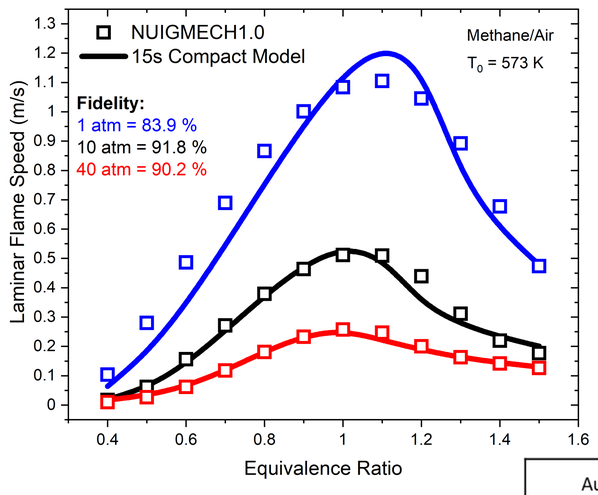

Table 1. Comparison of state of art models for methane/air combustion to respective detailed model calculations.
Fidelities were calculated at;
IDT: 1 – 40 atm, 1100 – 2000 K and equivalence ratios 0.5 – 1.5;
Su: 1 – 40 atm, 473 – 673 K and equivalence ratios 0.4 – 1.5;
PSR: 1 - 40 atm, 1000 – 2000 K and equivalence ratios 0.7 – 1.4 for errors in CO, CO_2, OH and H_2O maximum and equilibrium mole fractions.

Author	No. of Nodes	IDT Fidelity	S_u Fidelity	PSR Fidelity	Parent Mechanism
Benchmarking Model					
DRM22 [1]	24	98.1 %	94.5 %	98.1 %	GRI 1.2
State-of-art Models					
Lytras et al. [2]	14	18.6 %	65.4 %	81.8 %	USC Mech II
Leylegian [3]	15	39.3 %	83.6 %	74.9 %	USC Mech II
Leylegian et al. [4]	15	16.3 %	85.9 %	93.0 %	USC Mech II
MLOCK Compact Models					
This Work [5]	15	87.1 %	88.8 %	87.2 %	NUIGMECH1.0
Kelly et al. [6]	15	75.0 %	83.4 %	93.9 %	NUIG18_17_C3
Kelly et al. [6]	19	93.6 %	94.9 %	95.1 %	NUIG18_17_C3

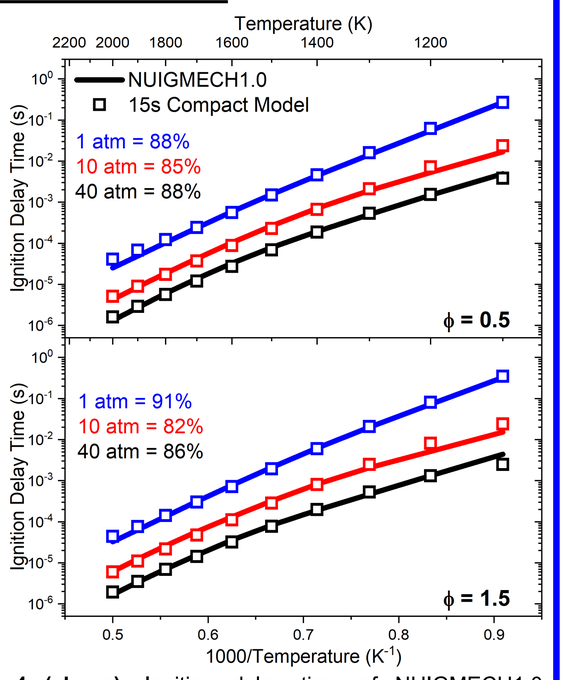

Figure 4 (above). Ignition delay time of NUIGMECH1.0 detailed model and the 15-node compact model produced by MLOCK algorithm as a function of temperature, at a range of pressure and methane/air fuel mixtures.

Figure 5 (left). Laminar flame speed of NUIGMECH1.0 detailed model and the 15-node compact model produced by MLOCK algorithm as a function of equivalence ratio, at an unburned gas temperature of 573 K and at 1, 10, and 40 atm.

Compact Model for NO_X Formation

- An adapted version of MLOCK1.0 was used for NO_X modelling.
- A NO_X virtual reaction network of minimal complexity with three nitrogen-containing nodes (N, NO & NO_2) was created using a Latin Square combinatorics method.
- This reaction network was then added to the 15-node methane compact model presented above.
- The virtual reaction rate constants of the NO_X virtual reaction network were optimised to NUIGMECH1.0 NO_X mole fractions in PSR and flame calculations.
- Series of 18-node compact models were produced that exhibit good fidelity to NUIGMECH1.0 NO_X calculations at ranges of equivalence ratios.

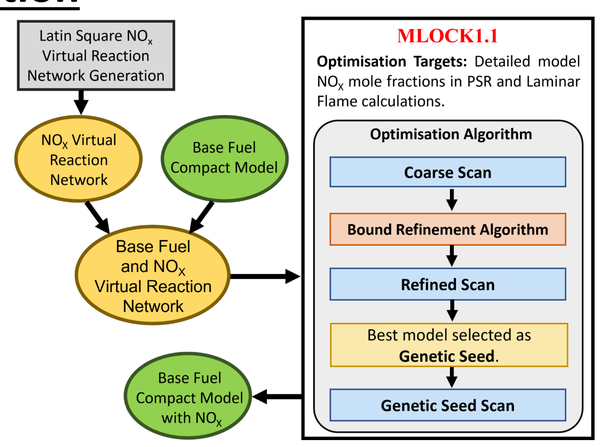

Figure 6. Process flow of MLOCK1.1 algorithm for NO_X compaction. Base fuel was methane in this study

- These compact models were found to out-perform the state-of-art NO_X formation models [8].
- However, this 3-node virtual reaction network does not possess sufficient degrees of freedom to manipulate the reaction fluxes in a way that one set of rate constants can replicate NO_X in flame calculations at both lean and rich conditions.

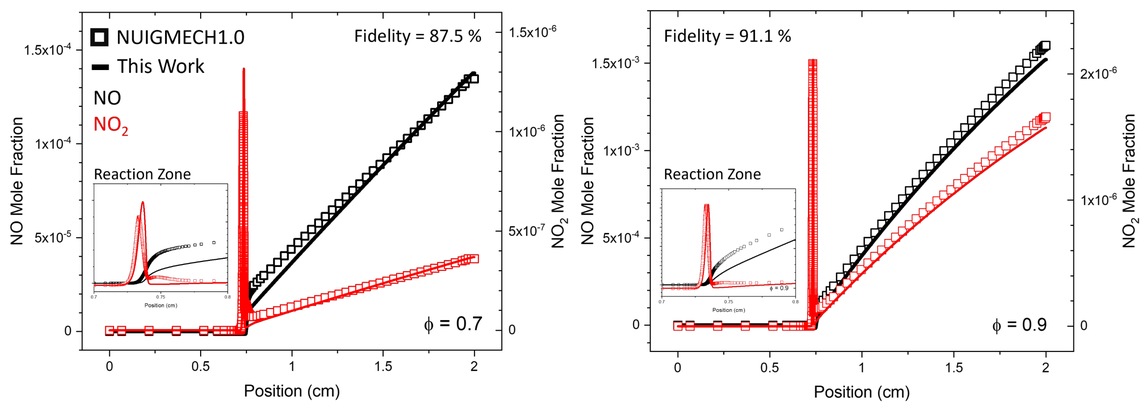

Figure 7. NO and NO_2 mole fractions in laminar flame calculations using NUIGMECH1.0 (symbol) and a 18-node compact model (line) at 573 K, 10 atm and fuel/air equivalence ratios 0.7 and 0.9. INSET: Expanded view of reaction zone.

Conclusions

- A novel compute intensification automated compaction methodology has been created: The MLOCK coded algorithm.
- MLOCK produces compact models that use the ChemKin form of reaction description (no additional subroutines or modification of solver required).
- MLOCK was used to produce state-of-art 15- and 19-node compact models for methane combustion.
- MLOCK was used to produce a series of 18-node compact models for NO_X formation during methane/air combustion using a Latin Squares approach to construct the NO_X virtual reaction network.
- MLOCK is currently being extended to liquid fuel combustion.

Acknowledgements

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