Self-consistent DRG: new implementation of directed relation graph mechanism reduction procedure

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***Abstract*— The self-consistent procedure for the mechanism reduction based on physical criteria of mechanism accuracy was elaborated and applied for the reduction of hydrocarbon fuel combustion mechanism. The procedure developed uses an optimal approach to utilization of a given reduction technique. Comparison of the several reduction procedures on the n-heptane oxidation detailed mechanism consisting of 561 species and 2539 reversible reactions were performed. The reduction was performed for auto-ignition simulations with the induction time as a target physical parameter. The comprehensive range of initial conditions was studied including high pressures, atmospheric pressures, lean and rich mixtures, low and high temperatures, region of negative temperature coefficient. The final reduced mechanism obtained using the self-consistent procedure contains 90 species and 782 irreversible reactions. The mechanism is describing the induction time of auto-ignition within the error tolerance of 30%. The procedure developed was shown to provide superior performance compared to DRG, DRGEP and DRGASA.**

I. Introduction

Development and design of the new automotive and aerospace propulsion technology requires the development of complex kinetic models of physical and chemical processes occurring in combustive mixtures. Excessive number of equations in the kinetic models for the combustion of complex hydrocarbon fuels hinders incorporation of these models into the hydrodynamic simulations. In order to overcome this obstacle the reduced kinetic models are being used instead [1]. Usually the reduced kinetic model is obtained in a sequence of steps [1]. The reduction of the kinetic mechanism of a chemical process is a complex and multi-stage process itself with the first stage being the removal of redundant species and reactions from the model. On the final stage the global reaction mechanism is obtained which can be used in the computational fluid dynamics (CFD) simulations.

In this work we focus on the first stage of the reduction since it is the most general stage which does not require a deep insight into the peculiarities of the kinetic scheme at hands and provides the greatest degree of reduction in terms of number of species/reactions eliminated.

The primary disadvantage of all original automatic mechanism reduction procedures like directed relation graph (DRG)[2], principal components analysis (PCA)[3] and computational singular perturbation (CSP)[4] is not yet the optimal size of the reduced mechanism for a given accuracy of the simulation. After application of these basic reduction techniques the remaining unimportant species and reactions can be identified in the mechanism. That is why until now the active research is performed on improvement of these methods and algorithms like directed relation graph with error propagation (DRGEP)[5], directed relation graph aided sensitivity analysis (DRGASA)[6], directed relation graph with error propagation and sensitivity analysis (DRGEPSA)[7], etc. appear.

The goal of the current work is to provide description of the newly developed improved version of the DRG method, which is called Self-Consistent DRG (scDRG). This finely tuned automatic reduction procedure provides the reduced mechanism of significantly smaller size, than all known alternative versions of DRG.

II. Self-consistent DRG

The underlying idea of the proposed implementation is the automatic adjustment of the DRG parameters during the iterative reduction process, which is guided by the reduced mechanism validation against the detailed one. The new idea of the method is to consider the set of important species (species, which are the roots of the directed relation graph) as variable parameters of the method.

TABLE I
Sizes of mechanisms obtained by each procedure

	Number of species	Number of reactions	Worst case induction time error
detailed	561	5059	0
DRG-REGULAR	222	2115	0.282
DRGEP	139	1277	0.259
DRGASA	164	1437	0.283
scDRG	90	782	0.298

TABLE II
Time spent on the reduction with each procedure, in minutes

	DRG-REGULAR	DRGEP	DRGASA	SCDRG
n-heptane	612	492	2631	1174

The reduced mechanism validation is performed after every run of the DRG for a target mechanism. A set of accuracy criteria can be identified and include for 1D problems (ignition, plug flow, laminar or diffusion flames):

- Equilibrium temperature
- Ignition delay time
- Species and temperature profile

The automatic reduction procedure includes

1. the kinetic simulations with the detailed mechanism and storage of these data for further comparison with generated reduced mechanisms
2. reduction of the mechanism with DRG with certain set of important species and variable numeric parameter δ, which defines the threshold to keep/remove the species from the graph and mechanism
3. simulations with the reduced mechanism obtained after DRG with a predefined set of important species and variable δ
4. comparison of the results obtained with the detailed and reduced mechanisms,
5. an iterative search for the new set of important species and re-run of DRG for the reduced mechanism, which did not pass the accuracy check
6. comparison of the results of simulations with the detailed mechanism and the reduced mechanism, obtained after step 5
7. for the new set of important species, which can provide a desired accuracy of the simulation, go to step 2.

This process is continued until the parameter set is exhausted.

The simultaneous iterative search for list of the important species and adjustment of the numerical parameter δ allows calling the developed implementation of the DRG as self-consistent DRG.

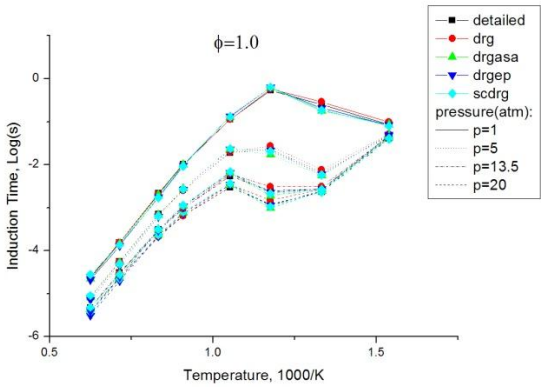

Fig. 1. Validation of the reduced mechanisms

III. Performance of the scDRG

The developed version of the scDRG was tested on the n-heptane combustion mechanism [8]. The target conditions for n-heptane combustion mechanism reduction were selected T=600-1600K, p=1-20atm, fuel-air equivalence ration φ =0.5-1.5. All the reduced mechanisms were demanded to fit into the 30% error tolerance for the induction time and 0.2% tolerance for the final temperature.

The performance of the scDRG was compared to the original DRG and modifications, namely DRGEP and DRGASA. All the methods had the same implementation of the core DRG method, thus the presented results provide performance assessment of the proposed algorithm itself, not the specific implementation of the DRG.

TABLE I gives the sizes of the reduced mechanisms obtained in the range of the conditions with four DRG implementations. The last column gives the worst case errors of the mechanisms measured against the detailed mechanism. The smallest mechanism consisting of less than 100 species was generated with the scDRG method. The validation of the reduced mechanisms obtained is given in Fig. 1. Only the results corresponding to simulations with stoihiometric mixtures are presented. For the atmospheric pressures the low-temperature region corresponds for the most significant error, especially for the mechanisms obtained with DRG and DRGASA. For the elevated pressures, the NTC region is the most troublesome, especially for the DRG mechanism. The TABLE II presents the comparison of the procedures performance. In all cases the bulk of the time was mostly spent in the kinetic simulations and minor time was spent on the reduction of the mechanism. Despite performing a lot more iterations the scDRG procedure works only twice slower than DRG-REGULAR and more than twice faster than DGRASA while providing the smallest reduced mechanism.

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