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

Alexander Lebedev, Ivan Zaev, Boris Potapkin
Kintech Lab Ltd
Moscow, Russia

## 1 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. The second stage is more careful removal of the few remaining unimportant species by the genetic algorithms or other mathematical method [1]. The third stage includes quasi-steady-state assumption and/or tabulation, approximation and other mathematical means of the computational cost reduction of the computational fluid dynamics (CFD) simulations of chemically active species [3].

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), principal components analysis (PCA) and computational singular perturbation (CSP) 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), directed relation graph aided sensitivity analysis (DRGASA), directed relation graph with error propagation and sensitivity analysis (DRGEPSA), etc. appear.

The goal of the current work is to provide description of the newly developed improved version of the DRG [2] 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.

## 2 Self-consistent DRG

Correspondence to: allexandrleb@gmail.com 

The underlying idea of the proposed implementation of DRG method 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.

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 $\delta$, 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 $\delta$
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 $\delta$ allows calling the developed implementation of the DRG as self-consistent DRG.

# 2 Performance of the scDRG

The developed version of the scDRG was tested on a number of the combustion mechanism, which are usually used as a reference for testing the mechanism reduction algorithms. These include:

- n-heptane combustion mechanism [5]
- iso-octane combustion mechanism [6]
- comprehensive mechanism of n-alkane oxidation [7]

The target conditions for n-heptane combustion mechanism reduction were selected T=600-1600K, p=1-20atm, $\varphi$ =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. Kinetic reactor model with constant volume and entropy was utilized.

The performance of the scDRG was compared with the original DRG, as well as with its improved versions DRGEP [8] and DRGASA [9]. All these 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.

**Erreur ! Source du renvoi introuvable.** gives the sizes of the reduced mechanisms obtained in the range of the conditions with four DRG implementations. In last column the errors in simulation of the induction time (compared with detailed mechanism) for initial conditions T=850K, p=13.5 atm, $\varphi$ =1 is given. It is seen, that the smallest mechanism is generated with the scDRG method. The second efficient method is DRG ASA as expected. The validation of the reduced mechanism, obtained with four reduction methods, is given on Fig. 1. The mechanism obtained with scDRG procedure contains

less than 100 species which is almost half the number of species obtained with DRG [4]. Among all the considered procedures the scDRG proved to be the most effective in elimination of the redundant species and reactions.

Table 1. n-heptane reduction results

| | Number of species | Number of reactions | Induction time error, % |
|---|---|---|---|
| Detailed mechanism | 561 | 5059 | 0.0 |
| DRG | 140 | 1138 | 4.8 |
| DRGEP | 168 | 1459 | 26.8 |
| DRGASA | 126 | 994 | 7.0 |
| scDRG | 83 | 652 | 21.5 |

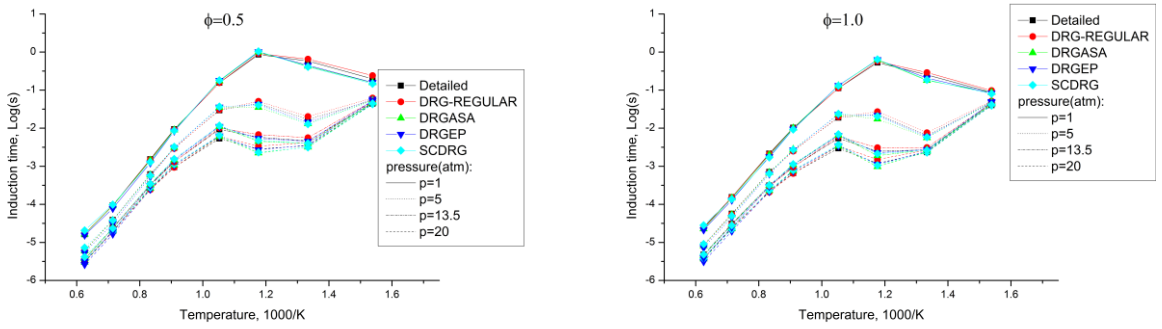


Figure 1. Temperature dependence of the induction time for the detailed and reduced mechanisms of the oxidiation of n-heptane in air

The similar test of the proposed algorithm was performed for the iso-octane [6] and n-decane [7] oxidation, presented in Table 2 and Table 3. These tables confirm the trend, found for n-heptane. The validation of the accuracy of obtained reduced mechanisms of iso-octane and n-decane oxidation in air is presented Figure 2 and Figure 3. The kinetic reactor model with constant pressure and entropy was used for iso-octane. Reactor model with constant volume and entropy was used for n-decane.

Table 2. iso-octane reduction results

| | Number of species | Number of reactions |
|---|---|---|
| Detailed mechanism | 857 | 7193 |
| DRG | 287 | 2321 |
| DRGEP | 209 | 1903 |
| DRGASA | 230 | 1673 |
| scDRG | 99 | 922 |

Table 3. n-decane reduction results

| | Number of species | Number of reactions |
|---|---|---|
| Detailed mechanism | 2115 | 15787 |
| DRG | 176 | 1547 |
| DRGEP | 197 | 1645 |
| DRGASA | 128 | 925 |

| | | |
|---|---|---|
| scDRG | 85 | 577 |

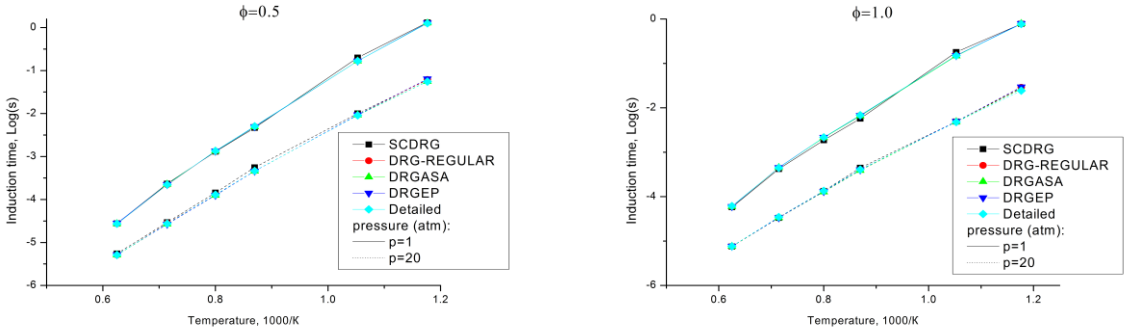


Figure 2. Temperature dependence of the induction time for the detailed and reduced mechanisms of the oxidiation of iso-octane in air

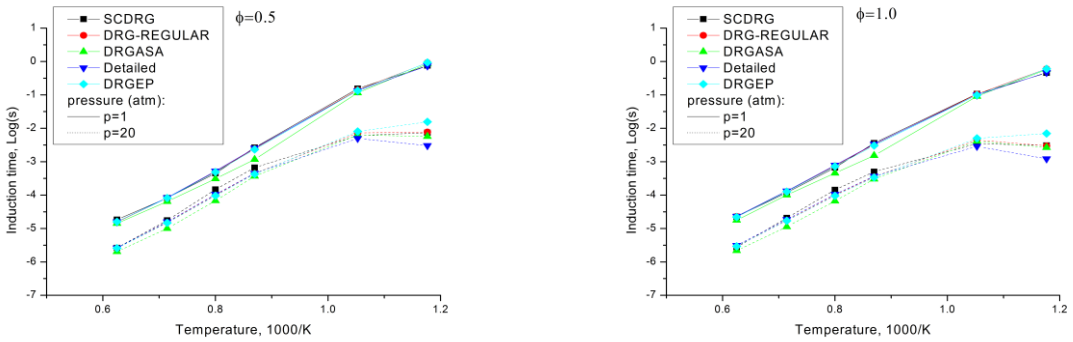


Figure 3. Temperature dependence of the induction time for the detailed and reduced mechanisms of the oxidiation of n-decane in air

# References

[1] Tomlin AS, Turanyi T, Pilling MJ. (1997). in: Comprehensive Chemical Kinetics. Elseveir. Amsterdam. 35. 293.

[2] Hernandez J.J., Ballesteros R., Sanz-Argent J. (2010). Reduction of kinetic mechanisms for fuel oxidiation through genetic algorithms. Math. Comput. Model. 52. 1185.

[3] Hiremath V., Ren Zh., Pope SB. (2011). Combined dimension reduction and tabulation strategy using ISAT-RCCE-GALI for the efficient implementation of combustion chemistry. Combust. Flame. 158. 2113.

[4] Lu T., Law CK.(2005). A Directed Relation Graph Method for Mechanism Reduction. Proc. Comb. Inst. 30. 1333.

[5] Curran HJ., Gaffuri P., Pitz WJ., Westbrook CK. (1998). A Comprehensive Modeling Study of n-Heptane Oxidation. Combust. Flame. 114. 149.

[6] Curran HJ., Gaffuri P., Pitz WJ., Westbrook CK. (2002). A Comprehensive Modeling Study of iso-Octane Oxidation. Combust. Flame. 129. 253.

[7] Westbrook CK, Pitz WJ, Herbinet O, Curran HJ, Silke EJ. (2009). A Detailed Chemical Kinetic Reaction Mechanism for n-Alkane Hydrocarbons from n-Octane to n-Hexadecane. Combust. Flame. 156. 181.

[8] Pepiot-Desjardins P., Pitsch H. (2008). An efficient error propagation based reduction method for large chemical kinetic mechanisms. Comb. Flame. 154. 67.

[9] Niemeyer KE, Sung CJ. (2010). Skeletal mechanism generation for surrogate fuels using directed relation graph with error propagation and sensitivity analysis. Combust. Flame. 157. 1760.