

Systematic Mechanism Reduction for Engine Applications

Lars Seidel*, Christian Klauer†, Michał Pasternak*, Andrea Matriciano†‡, Corinna Netzer†, Martin Hilbig*
Fabian Mauss*

*Brandenburg University of Technology, Cottbus, Germany

†Lund Combustion Engineering, Lund, Sweden

‡Chalmers University of Technology, Göteborg, Sweden

Abstract—In this work we apply various concepts of mechanism reduction with a PDF based method for species profile conservation. The reduction process is kept time efficient by only using 0D and 1D reactors. To account for the expansion phase in internal combustion engines a stochastic engine tool is used to validate the reduction steps.

I. INTRODUCTION

In the last decades the use of computational tools became an inherent part of engine design. Even though the available computers and algorithms became faster over the years full CFD calculations with detailed reaction schemes are time consuming. Therefore the reduction to a minimal size (species and reactions) with a good agreement against the detailed scheme is one solution to the problem. A major demand on the reduction procedure is that is applicable to any size of mechanism, for any kind of mixtures (single / multi component fuel) and for a wide parameter range. Furthermore the reduction methods shall preserve certain features depending on the application and shall not introduce artefacts such as quenching in the expansion phase. In addition users are often limited to the use of mechanisms in standard format since it is often not possible to validate and reduce the detailed mechanism in CFD for a wide range of engine conditions. To overcome this problem we suggest to use a combination of 0D/1D reactors and stochastic engine tools for the mechanism reductions.

A. Proposed tool chain

The proposed tool chain consists of two major strains: the main reduction is carried out in 0D and 1D reactors and each reduction step is compared against the detailed solution. To assure that the performance under engine conditions is within the defined error range a stochastic engine model is used to compare intermediate reaction steps against the detailed mechanism [1].

II. MECHANISM REDUCTION STEP BY STEP

A. Definition of Parameter Range

Since the species and reaction removal is carried out in 0D reactors (constant volume / pressure) or flame configurations, it is essential to define a range of inlet parameters which well represents typical engine conditions. Therefore a matrix in mixture compositions, temperature, pressure and

fuel equivalence ratio is defined as a first step. Afterwards a set of targets and the acceptable deviation against the detailed model predictions needs to be defined. Such constrains define the validity of the reduced mechanism.

B. Horizontal Lumping

The first reduction step consists of horizontal lumping of isomeric species as introduced by Ahmed et al. [2]. A simple tool was developed in order to automatically suggest the list of species to lump based on a set of *n* a priori assumptions. The thermodynamic data of the pseudo species are averaged over the isomers involved in the lumped group and the main reaction hierarchy is maintained.

C. Species Removal

The species removal follows the concept of Chemical Guided Reduction introduced by Zeuch et al. [3]. Species will be removed based on a necessity analysis and the most conservative value over all reactors and targets is chosen. The necessity I of a species i is calculated iteratively from

$$\bar{I}_i = \max(I_j f_{i,j}^a, I_j c_{i,j}^a, I_i; \quad j = 1, N_s, a = 1, N_a)$$

where the first value for I_i is calculated as

$$I_{i,0} = \max\left(\frac{S_{j,i}^S}{\max_{k=1, N_s}(S_{j,k}^S)}, B_i\right)$$

N_s and N_a are the total number of species and atoms respectively, k denotes a species and B_i is 1 or 0 depending on if i is set as a necessary species or not. $f_{i,j}^a$ is the weighted formation of species i from species j by atom flow from species j to species i ;

$$f_{i,j}^a = \frac{\int_{t=0}^{t_1} \left(\sum_{R=1}^{N_r} r_R(t) n_i^a \nu'_{jR} \nu''_{iR} \frac{1}{\Delta n_R^a} \right) dt}{\int_{t=0}^{t_1} \left(\sum_{R=1}^{N_r} r_R \nu'_{jR} \right) dt}$$

Similarly, $c_{i,j}^a$ is the weighted consumption of atoms from species i to species j ;

$$c_{i,j}^a = \frac{\int_{t=0}^{t_1} \left(\sum_{R=1}^{N_r} r_R(t) n_i^a \nu'_{iR} \nu''_{jR} \frac{1}{\Delta n_R^a} \right) dt}{\int_{t=0}^{t_1} \left(\sum_{R=1}^{N_r} r_R \nu''_{jR} \right) dt}$$

The species profiles of the detailed and reduced reaction scheme are mapped to probability density functions (PDF).

Moments of the PDF are used to compare the profiles against the detailed solution. Furthermore the maximum and the equilibrium values are evaluated. This way the position and shape of target species profiles are kept in a given error range. Validation of the ignition delay time is simply based on the evaluation of the maximum temperature slope. If all targets (ignition delay time, species profile) over all reactors in the matrix are within the given tolerance the reduction is considered as valid and the necessity analysis will be repeated to account for a change in flow. All species which could not be removed are regarded as removable after a successful reduction step.

D. Reaction Removal

Reaction removal is done in the same manner as species removal. Due to the control of species profiles the major pathways are preserved. Furthermore we remove all slow and unimportant reverse reactions of those which are formulated in equilibrium.

E. Vertical lumping

The idea of vertical lumping or chemkin type steady state can be expressed with a theoretical reaction chain:

... $\rightarrow [A] \rightarrow [B] \rightarrow [C] \dots$ where $[A] \cdot k_1 - [B] \cdot k_2 = 0$ can be written as: $[B] = \frac{[A] \cdot k_1}{k_2}$. The production rate of [C] can be calculated as: $\frac{\partial C}{\partial t} = [B] \cdot k_2 = \frac{[A]k_1 \cdot k_2}{k_2} = [A]k_1$. In order to identify species which can be set to a steady state we carry out a life time analysis. The chemical lifetime can be expressed as

$$\tau_i = \frac{1}{\frac{\partial \omega_i}{\partial c_i}} = \frac{c_i}{\sum_{k=1}^{N_r} (\nu'_{i,k} - \nu''_{i,k}) \nu'_{i,k} r'_k}$$

where ω_i represents the species source term in terms of concentrations, c_i , $\nu_{i,k}$ is the stoichiometric coefficient (prime - reactant and double prime - product values) and r_k is the reaction rate for reaction k . Unfortunately not every species with a short life time can be removed by this assumption. This is often the case for reactions which involve the formation or consumption of major radicals such as H or OH, hence this step is not automated.

F. Further reduction

It is possible to reduce the mechanism even more by applying non standard format, lumping fuel molecules, solver based QSSA reduction or introducing global reactions.

III. APPLICATION ON N-HEPTANE AS DIESEL REFERENCE FUEL

The proposed tool chain is applied to a published n-heptane mechanism [4] with 349 species. The main target is to reduce the mechanism for typical Diesel engine conditions without affecting prediction for major emissions (NOx, CO, CO₂, H₂O and unburned hydrocarbons) and correctly cover a broad range of fuel equivalence ratios (0.3 - 4.0). Following the steps proposed above the mechanism was reduced as follows (species / reactions): Detailed (349/3686) \rightarrow Lumping

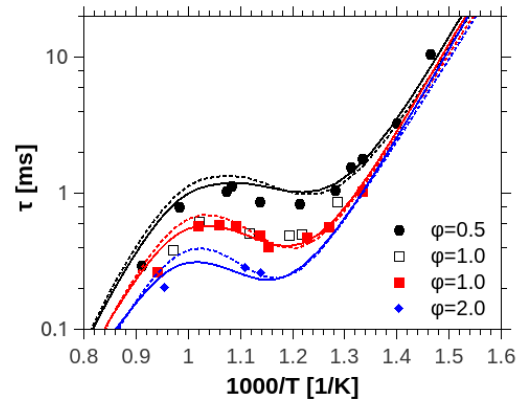


Fig. 1. Comparison predicted ignition delay time (solid lines - detailed scheme; dotted lines - 56 species scheme) against experimental values. For references see [4].

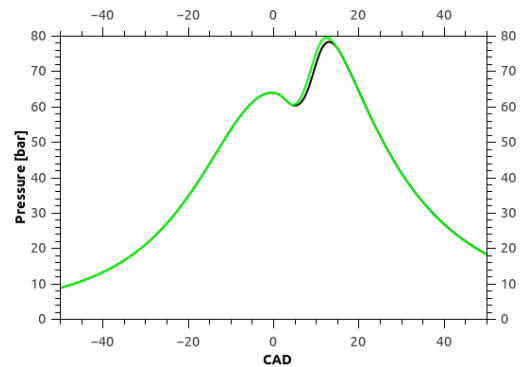


Fig. 2. In cylinder pressure trace with detailed (red) and 56 species scheme (green)

(305/3668) \rightarrow Species removal (84/772) \rightarrow Reaction removal (84/329) \rightarrow Vertical lumping (56/206). Predicted speciation of major species in burner stabilized flames [4] and ignition delay times (figure 2) are close to the detailed scheme. The CPU time for a calculation of 30 engine cycles in the stochastic DI model was improved by factor 28 to 64s for the smallest mechanism. Average exhaust out emissions (NOx and unburned HC) were compared in a sample case and differ less than 10%. The predicted in cylinder pressure shows excellent agreement (see figure 2).

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