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Development of an efficient solver for detailed kinetics in reactive flows

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Abstract

The use of chemical kinetic mechanisms in CAE tools for reactive flow simulations is of high importance for studying and predicting pollutant formation. However, usage of complex reaction schemes is accompanied by high computational cost in both 1D and 3D-CFD frameworks. The combustion research community has addressed such challenge via two main approaches: 1) tailor made mechanism reduction strategies; 2) pre-tabulation of the chemistry process and look-up during run-time. The present work covers both topics, although much of the methodology development and validation efforts focused on tabulation.

In the first eight months of the PhD work, an isomer lumping strategy based on thermodynamic data was developed and applied to a detailed three component reaction mechanism for *n*-decane, alpha-methylnaphthalene and methyl decanoate comprising 807 species and 7807 reactions. A total of 74 isomer groups were identified within the oxidation of *n*-decane and methyl-decanoate via analysis of the Gibbs free energy of the isomers. The lumping procedure led to a mechanism of 463 species and 7600 reactions which was compared against the detailed version over several reactor conditions and over a broad range of temperature, pressure and equivalence ratio. In all cases, very good agreement between the predictions obtained using the lumped and the detailed mechanism has been observed with an overall absolute error below 12%.

In the second phase of the PhD work, a tabulated chemistry approach was developed, implemented and validated against an on-the-fly chemistry solver across different simulation frameworks. As a first attempt, a flamelet-based tabulation method for soot source terms was coupled to the stochastic reactor model (SRM) and tested against a well stirred reactor-based approach under Diesel engine conditions. The main purpose was to assess and quantify benefits of tabulation within the 0D-SRM framework with respect to soot formation only. Subsequently, a chemical enthalpy (h_{298}) based approach was developed and implemented within the SRM model to predict both combustion and emission formation. This approach was widely validated against the detailed on-the-fly solver solutions under 0D reactor conditions as well as Diesel engine conditions for a wide range of operating points. Good agreement was found between the two solvers and a remarkable speed-up was obtained by means of computational costs of the simulation. As a last step, the same tabulated chemistry solver was coupled to a commercial CFD solver (CONVERGE v. 2.4) via user defined functions and performances were assessed against the built-in on-the fly chemistry solver (SAGE) under Diesel engine sector simulations. The tabulated chemistry solver proved to be within an acceptable level of accuracy for engineering studies and showed a consistent speed-up in comparison to the SAGE solver.

Across all the investigated frameworks, the developed tabulated chemistry solver was found to be a valid solution to speed-up simulation time without compromising accuracy of the solution for combustion and emissions predictions for Diesel engine applications. In fact, the much-reduced CPU times allowed the SRM to be included in broader engine development campaigns where multi-objective optimization methods where efficiently used to explore new engine designs.

Keywords: Detailed chemistry, Tabulated chemistry, Progress Variable, Stochastic Reactor Model

List of publications

This thesis is based on the following four appended papers.

Paper 1

Matrisciano A., Seidel L., Klauer C., Wang X., Mauss F. "An a priori thermodynamic data analysis based chemical lumping method for the reduction of large and multi-component chemical kinetic mechanisms"
Presented at the 5th International Workshop on Model Reduction in Reacting Flows (IWMRRF), 2015, Luebbenau Germany.
To be submitted to AIChe journal

Paper 2

Matrisciano A., Borg A., Perlman C., Lehtiniemi H., Pasternak M., Mauss F. "Soot Source Term Tabulation Strategy for Diesel Engine Simulations with SRM"
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Paper 3

Matrisciano A., Franken T., Perlman C., Borg A., Lehtiniemi H., Mauss F. "Development of a Computationally Efficient Progress Variable Approach for a Direct Injection Stochastic Reactor Model"
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Paper 4

Matrisciano A., Netzer C., Werner A., Borg A., Seidel L., Mauss F. "A Computationally Efficient Progress Variable Approach for In-Cylinder Combustion and Emissions Simulations"
SAE Technical Paper 2019-24-0011, 2019, doi:10.4271/2019-24-0011.

Nomenclature

Greek symbols

φ	Equivalence Ratio	[-]
λ	Lambda	[-]
ρ	Density (l for liquid, g for gas, d for droplet)	[kg/m³]

Latin symbols

C	Reaction progress variable	[-]
$\dot{C}$	Reaction progress variable source term (dC/dt)	[1/s]
h_{298}	Chemical enthalpy at reference state (T = 298 K)	[J/kg]
p	Pressure	[Pa]
R	Universal gas constant	[J/mol]
T	Temperature	[K]
T_u	Unburnt Temperature	[K]

Abbreviations

0D	Zero-Dimensional
3D	Three-Dimensional
AMN	Alpha Methylnaphthalene, $C_{11}H_{10}$
ATDC	After Top Dead Centre
BEV	Battery Electric Vehicle
BTDC	Before Top Dead Centre
BTU	Brandenburg Technical University Cottbus-Senftenberg
CAE	Computer Aided Engineering
CAD	Crank Angle Degree
CFD	Computational Fluid Dynamics
CI	Compression Ignition
CO	Carbon Monoxide
CO_2	Carbon Dioxide
CPV	Combustion Progress Variable
DI	Direct Injection
ECFM-3Z	Extended Coherent Flame Model 3 Zones
EGR	Exhaust Gas Recirculation
EOI	End of Injection
ETRF	Ethanol Toluene Reference Fuel
GHG	Green House Gases
HCCI	Homogeneous Charge Compression Ignition
ICE	Internal Combustion Engine
ICEV	Internal Combustion Engine Vehicles
KLSA	Knock Limit Spark Advance
LES	Large Eddy Simulation

LHV	Lower Heating Value
MD	Methyl Decanoate, $C_{11}H_{22}O_2$
NO_X	Nitrogen Oxides
NTC	Negative Temperature Coefficient
OEM	Original Equipment Manufacturer
PAH	Polycyclic Aromatic Hydrocarbons
PaSR	Partially Stirred Reactor
(P-)HEV	(Plug-in) Hybrid Electric Vehicle
PM	Particle Matter
PRF	Primary Reference Fuel
RoHR	Rate of Heat Release
RANS	Reynolds Averaged Navier Stokes
SAGE	Acronym of the detailed chemistry solver built-in CONVERGE
SI	Spark Ignition
SOI	Start of Injection
SRM	Stochastic Reactor Model
TCI	Turbulence Chemistry Interaction
TKI	Tabulated Kinetics of Ignition
TDC	Top Dead Centre
TRF	Toluene Reference Fuel
UDF	User Defined Function
uHC	Unburned Hydrocarbons
WLTP	Worldwide Harmonised Light Vehicle Test Procedure
WSR	Well Stirred Reactor

Contents

1

Introduction

The ever-stringent regulations on pollutants and greenhouse gases emissions have been the key drivers for research and development of propulsion systems for the automotive industry in the past decades. On the one hand, the well-known correlation between global warming and increase of GHG emissions [1] are pushing OEMs to reduce fuel consumption. On the other hand, the 2015 Diesel emission scandal, together with many other factors, intensified a heated, and sometime controversial, debate on pros and cons of traditional propulsion solutions (i.e. ICEVs) versus battery and fuel cells electric vehicles. While both scientific and legislator communities are far from reaching consensus on what should or would be the optimal path for future powertrains, numerous reports and review articles (i.e. [2], [3], [4]) tend to agree on the fact that internal combustion engines will keep playing an important role in mobility, freight, transport and mobile machinery sectors for at least the next two decades.

Within the mentioned scenario the Diesel engine has a crucial role thanks to its higher efficiency compared to spark ignited engines. Today it is applied traditionally in heavy- and medium-duty applications, but also for high-speed passenger cars. Advantages of the Diesel engine are the lean operation under high compression ratios that lead to high efficiency and less CO_2 emission per kilometer than a comparable spark-ignited engine. However, Diesel engines generally emit higher NO_X and more particle matter than spark ignition engines. Hence, in the Diesel engine development problems related to emission regulation such as the soot/NO_X tradeoff must be overcome. The diversity and complexity of the phenomena to be considered, to correctly evaluate both fuel and engine characteristics, challenge the engine development process as well as after treatment system integration.

In the Diesel engine development, experiments and simulations are going nowadays hand in hand. The use of numerical models can extend the knowledge of experimental investigations by making details such as local flow, spray formation and chemistry more understandable. In modern CAE tools, one of the main achievements is the incorporation of detailed chemical reaction mechanisms to describe fuel oxidation and emission formation. To an increasing degree the use of experiments, that demand typically expensive equipment and man power, are reduced by virtual test benches [5], design of experiments and numerical optimizations [6]. 3D Computational Fluid Dynamics analyses offer the greatest level of detail for predicting physical processes such as the turbulent flow field and the spray formation and atomization. Employing combustion models based on reaction mechanisms allows on top to predict emissions formation.

Future demands for 3D-CFD modelling require more and more fuel chemistry effect investigations, the generation of engine performance maps and the application within optimization algorithms for design exploration. Employment of high spatial and temporal discretization and depending on the turbulent combustion modeling approach (i.e. RANS or LES) and the size of the reaction mechanisms, 3D-CFD may become too computationally expensive. Further, with continuous progress in chemical reaction mechanism development, surrogate fuel models tend to contain more and more important reaction path ways, but also an increasing number of species and reactions [7]. To overcome such limits, on the one hand mechanism reduction techniques, such as the chemistry guided reduction technique with its extension to engine conditions [8], are applied.

On the other hand, the mechanisms are maintained in their full detail, but their solution is separated from the solution of the physics. Those concepts are called tabulated chemistry approaches since the chemistry is solved prior the 0D or the 3D-CFD simulation and stored in look-up tables. During run-time the combustion chemistry solver step is then reduced to a cell/zone local table look-up step where source terms are retrieved to reconstruct the chemical state. This approach avoids not only the computation of the chemistry solution on-the-fly, but also reduces the number of transported scalars. Both factors lead to a significant reduction of the run time. Thanks to these advantages tabulated chemistry-based methods have received a lot of attention by the combustion chemistry community in the past decade.

1.1 Background and previous works

For tabulated chemistry, different approaches have been proposed primarily for 3D-CFD applications but also for 0-D/1D frameworks. In most of the cases, the chemistry solution and the flow are separated, the chemistry can be solved and tabulated in one-dimensional flamelets or zero-dimensional reactor configurations [9], [10], [11], [12]. This assumption typically makes the one-time tabulation process over wide ranges of pressures, temperatures, EGR and equivalence ratios possible in reasonable computational times. For the look-up step at run-time, a progress variable to identify the correct table entry is essential. For premixed combustion, premixed one-dimensional flamelets are solved and tabulated as for example in [13] or within the flamelet-generated-manifold method [12] [14]. The flame prolongation of intrinsic low-dimensional manifolds [15] was introduced to improve the prediction at low temperatures. For non-premixed combustion, diffusion flamelets are employed for the chemistry tabulation [16], [17]. In these models the chemistry solution is stored in mixture fraction space and the usage of the scalar dissipation rate accounts for the turbulence-chemistry interaction effects. To accurately predict the premixed and non-premixed areas of a spray, premixed and diffusion flamelets have been combined as partially premixed flamelet tabulation in [18].

The use of homogenous zero-dimensional reactors for auto-ignition tabulation has also been widely explored in literature over the last years with different levels of complexity [19]. In [20], only the ignition delay time is stored in the table. This information, once retrieved from the table using cell local T, p, φ and EGR, is employed within the well-known Livengood-Wu integral [21] for knock prediction in SI engines. Such method, however, only allows to estimate the instant of the auto-ignition event with no information on the heat release rate nor its magnitude. A similar but more advanced approach has been proposed by Lafossas et al. [22] where estimation of the autoignition is done via a passive transported precursor scalar whose formulation relies on an empirical correlation dependent on fuel octane number, pressure and temperature.

The models mentioned so far lack the description of a crucial part in the auto-ignition of hydrocarbons, this is to say the low temperature combustion (also addressed in literature as the negative temperature coefficient region). To tackle such problem, Pires da Cruz et al. [23] proposed a method where both the high and low temperature ignition delay time is stored in the table. Validation was done under 0D reactor conditions (assuming constant pressure/volume) as well as under diesel engine conditions in 3D-CFD. An improved version of such model was later proposed by Colin et al. [24] where a progress variable based approach was used rather than a simple tabulation of the ignition delays. In this configuration, an additional tabulation dimension is introduced as the pre-tabulation is done for different values of the progress variable, which varies between $C = 0$ (being unburned mixture) and $C = 1$ (being fully burned mixture). Further, during run-time the progress variable source term $\dot{C}$ is retrieved for each cell/zone and it is used to reconstruct the mixture state on the given oxidation trajectory. Later improvements of such method proposed by Knop et al. [19], incorporated also a turbulence chemistry interaction term during the tabulation stage so that TCI effects could be accounted for in 3D-CFD reactive flow simulations

within the ECFM framework. The model (named TKI in [19]) has been applied to predict the ignition process of Diesel and homogeneous charge compression ignition engines and is currently implemented in various commercial CFD codes.

Also complex phenomena such as soot formation under engine conditions have been successfully predicted using flamelet library soot source terms [25], [26], [27], [28]. For the soot modelling the treatment of the polycyclic-aromatic hydrocarbons (PAH) chemistry is of special importance. In [29], the PAH formation rate is considered, whereas in [30] the PAH consumption rate is employed. The latter is beneficial since there is no need to model the consumption of PAH by soot formation on the amount of PAH in the gas phase with an additional PAH consumption feed-back model [10].

When it comes 0D/1D frameworks, the number of applications of tabulated chemistry-based methods is rather limited. Its implementation, however, is potentially very useful as it allows to preserve the details of the original complex kinetics, with a minimal impact on the computing time. In addition, tabulation and 0D/1D modeling coupling broadens the range of feasible system simulation studies such as a cylinder-to-cylinder knock estimation or emission trends prediction during transient engine operating conditions (i.e. WLTP cycles).

Mosbach et al. [31] proposed a storage/retrieval technique for Homogeneous Charge Compression Ignition (HCCI) combustion in which various quantities such as ignition timing, cumulative heat release, CO, CO_2 emissions etc., were tabulated as function of engine geometry, equivalence ratio, octane number and intake temperature using an HCCI-SRM. Their technique was based on tabulating the evolution of the engine cycle and does therefore not allow use of the same table for different engines or different engine operating points. Leicher et al. [32] proposed a table look-up approach based on mixture fraction and reaction entropy as progress variable. Their methodology was implemented in an SRM and tested under constant pressure reactor conditions. Dulbecco et al. [33] proposed a tabulated multi-zone combustion model for HCCI Diesel combustion, tracking the combustion chemistry with eight species. Bozza et al. [34] implemented the previously mentioned TKI approach [19] within a 0D-1D phenomenological combustion model for better knock prediction in spark ignited engines compared to the traditionally used Livengood-Wu [21] approach. Validation under both 0D reactors and knocking SI engine simulation at $\lambda = 1$ showed promising results when compared to the on-the-fly chemistry solution.

1.2 Thesis structure and objectives

The present work was majorly funded via a Marie-Curie FP7 action (ECCO-MATE, grant agreement number 607214 [35]) and was organized such that both mechanism reduction techniques as well as tabulation methods are investigated. During the project, and given the prior experience in tabulation at LOGE, it was decided to direct most of the efforts towards the development of a robust multi-framework method for tabulation rather than pursue advanced mechanism reduction.

In the first eight months of the PhD study, I visited the chair of thermodynamics and thermal process engineering at BTU and worked on isomer lumping. The main objective of this activity was to investigate the potential and limitations of lumping techniques when applied to large multi-component kinetic schemes. As a result of this collaboration, an isomer lumping technique was developed based on a Gibbs free energy driven analysis and it is reported in the attached Paper 1. Such methodology was later also included within the best practice steps for mechanism reduction of LOGE's chemistry guided reduction technique [8].

In the subsequent years, I worked closely with the development team of LOGE AB and investigated different tabulation/progress variable approaches for both auto-ignition and soot/NO_X emissions. In Paper 2 I coupled a flamelet based soot source term tabulation technique with the SRM framework and compared soot results to an WSR based on-the-fly chemistry solution. This work represented the first step towards a much larger development work focused on including

tabulation within the main autoignition solver step of the SRM rather than for emissions prediction only. Hence, within the scope of Paper 3, I updated the full infrastructure of the SRM to accommodate a tabulated chemistry-based solver across all sub-models (i.e. the fuel injection, heat transfer, turbulent mixing etc.). The newly developed method (noted as CPV - Combustion Progress Variable) was then compared against the on-the-fly chemistry solver based SRM solution and assessed by means of engine performance as well as computational times. This activity was in fact aligned with the main objective of the overall PhD work. Remarkable speed-ups were noted, while keeping an acceptable loss of accuracy in combustion prediction, across all investigated engine operating conditions. The newly implemented tabulated chemistry framework was later included as one of the standard models in the technological offerings from LOGE and applied in several other works where I have been involved as co-author (i.e. [6], [36]).

In conjunction with the efforts for the 0D-SRM implementation I was involved also in the coupling of the CPV solver with the commercial CFD code CONVERGE 2.4 [37]. In Paper 4 a comparison between the tabulated and the built-in on-the-fly chemistry solver is presented for different Diesel engine conditions assuming sector meshes in a 3D-CFD RANS framework. As done for the 0D framework, the objective of this work was to assess pros and cons of applying the CPV model in 3D-CFD by means of combustion and emissions predictions as well as run-times. Also in this framework, promising speed-ups were obtained and the model proved to be a feasible solution to consider especially for multi-objective 3D-CFD optimization campaigns that would normally require an unaffordable run-time with traditional on-the-fly combustion chemistry solvers.

2

Summary of papers and author contribution

Paper 1: Matrisciano A., Seidel L., Klauer C., Wang X., Mauss F. "An a priori thermodynamic data analysis based chemical lumping method for the reduction of large and multi-component chemical kinetic mechanisms" Presented at the 5th International Workshop on Model Reduction in Reacting Flows (IWMRRF), 2015, Luebbenau Germany. To be submitted to AIChe journal

Summary. This paper reports on the development and application of a lumping technique developed for the reduction of large multi-component reaction mechanisms. The lumping strategy was based on an a priori analysis of the Gibbs free energy of the isomers of a detailed mechanism having oxidation paths for three main fuel molecules (*n*-decane, alpha-methylnaphthalene and methyl decanoate) and comprising 807 species and 7807 reactions. A total of 74 isomer groups were identified within the oxidation of *n*-decane and methyl-decanoate. The lumping procedure led to a mechanism of 463 species and 7600 reactions, whose performances were compared against the detailed version over several reactor conditions and over a broad range of temperature, pressure and equivalence ratio. In all cases, very good agreement between the predictions obtained using the lumped and the detailed mechanism were observed with an overall absolute error below 12%.

Author contribution. I investigated different lumping techniques and eventually developed the Gibbs free energy-based analysis. I then implemented a series of bash scripts to automate the lumping process and apply it to the mentioned reaction mechanism, which was developed prior to my work by Wang X., Seidel L. and Mauss F. Once the lumping technique was in place, I ran all necessary calculations to validate the reduction methodology and post-processed the results. I wrote the vast majority of the paper to which Seidel L. and Mauss F. contributed with edits and fruitful comments. I presented the results at 5th IWMRRF as well as at the 3rd topical workshop: "Testing combustion models with experimental data" prior the 7th European Combustion Meeting (ECM) in 2015.

Paper 2: Matrisciano A., Borg A., Perlman C., Lehtiniemi H., Pasternak M., Mauss F. "Soot Source Term Tabulation Strategy for Diesel Engine Simulations with SRM" SAE Technical Paper 2015-24-2400, 2015, doi:10.4271/2015-24-2400.

Summary. A flamelet-based tabulation method for soot source terms was coupled to the stochastic reactor model and tested against a well stirred reactor-based approach under Diesel engine conditions. The main purpose was to assess the benefits of tabulation within the 0D-SRM framework with respect to soot formation only. A pre-existing soot source term table, obtained using an *n*-heptane kinetic scheme of 121 species and 974 reactions, was used and a look-up strategy was implemented in the SRM framework to reconstruct the contributions of the different soot formation and oxidation processes. As a validation test case, a heavy-duty Diesel engine case was used, and the tabulated chemistry-based soot predictions were compared against the regular on-the-fly (WSR based) chemistry solver.

Author contribution. The flamelet based soot source terms tabulation strategy was developed prior to my work by Borg A., Lehtiniemi H. and Mauss F for 3D-CFD applications. I implemented the mentioned methodology within the 0D-SRM code and run all the presented simulations as well as post-processing. I wrote the main parts of the paper to which Lehtiniemi H. and Mauss F. contributed with edits and useful comments. I presented the paper at the 12th international SAE-NA conference on engines and vehicles in 2015.

Paper 3. Matrisciano A., Franken T., Perlman C., Borg A., Lehtiniemi H., Mauss F. "Development of a Computationally Efficient Progress Variable Approach for a Direct Injection Stochastic Reactor Model" SAE Technical Paper 2017-01-0512, 2017, doi:10.4271/2017-01-0512.

Summary. This paper discusses the theory and application of the tabulated chemistry solver (CPV) developed during my PhD studies and applied to the 0D-SRM. After various iterations, a chemical enthalpy-based progress variable definition was assumed for the tabulation phase and implemented. Different structures and tabulation grid resolutions were tested so that both accuracy and table size are in line with typical mid-range workstation computer specifications. All sub-models of the SRM (such as fuel injection, heat transfer and mixing) were updated to comply with the new tabulated chemistry solver. One heavy-duty conditions as well as ten passenger car Diesel engine conditions were used as validation cases to assess accuracy and computational performance of the CPV solver against the on-the-fly chemistry solution. Reasonably good agreement was found between the two solvers. Further, the methodology proved to be an attractive solution to facilitates the usage of the SRM in the engine development process.

Author contribution. The actual solver for tabulation and the subsequent interpolation routines were developed by Perlman C., Borg A., Lehtiniemi H., Mauss F. and others prior the beginning of my work. I contributed to small developments of some updates/features needed to account for the new CPV table structure. On the 0D engine code side, I implemented the new coding infrastructure necessary to couple a tabulated chemistry-based solver with the SRM code which, previously, had always relied on an online chemistry-based solver. I worked on each of the sub-models present in the SRM code for online chemistry and ensured their correct functionality with the CPV solver. I then ran all simulations presented in the paper and postprocessed the results. I wrote the major parts of the paper to which Lehtiniemi H., Perlman C. and Mauss F. contributed with edits and comments. I presented the work at the 2017 SAE world congress experience.

Paper 4. Matrisciano A., Netzer C., Werner A., Borg A., Seidel L., Mauss F. "A Computationally Efficient Progress Variable Approach for In-Cylinder Combustion and Emissions Simulations" SAE Technical Paper 2019-24-0011, 2019, doi:10.4271/2019-24-0011.

Summary. The CPV solver described in Paper 2 was coupled to CONVERGE 2.4 via user defined functions designed to override the built-in detail chemistry model (SAGE). In this work three passenger car Diesel engine conditions were used as validation cases under the RANS sector mesh assumptions. The CPV solver was then compared against the SAGE solver predictions for combustion, soot and NO_X as well as for run-time performances. A two component (70% *n*-decane, 30% alpha-methylnaphthalene, by mass) Diesel surrogate, comprising 189 species was used for both the online and tabulated chemistry solver tests. Remarkable speed-ups were noted while keeping a low loss of accuracy across all the investigated conditions.

Author contribution. The main implementation work of the CONVERGE User Defined Functions was performed by my colleagues Lehtiniemi H. and Borg A. I contributed to some marginal parts of the debugging process of the mentioned UDFs and implemented some minor improvements in the look-up methodology. I then ran all presented simulations in CONVERGE 2.4 and post-processed the results. Werner A. contributed to the generation of the 3D contour plots while Netzer C. and Seidel L. contributed to the writing of the introduction and case setup description paragraphs. I wrote the results and conclusions sections and took care of all necessary edits/refinements during the rebuttal phase.

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