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Tailor-made reduction of a chemical kinetic reaction mechanism for the combustion of C_2H_4 / N_2O mixtures

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Abstract

Within this work a recently developed optimised chemical kinetic model DLR SynNG + NO v0.2 for mixtures of C_2H_4 / N_2O was reduced for boundary conditions relevant for combustion processes in satellite thrusters. The application of the rapid reduction method of the linear transformation model allowed a significant reduction of the number of modelled species from 165 to 35. Due to the post optimisation of this highly efficient chemical kinetic model, the predictive capability of the detailed, validated model was kept. Specifically, quantities of interest like ignition delay times, laminar flame speeds and species profiles in homogeneous reactors and laminar reactive flows are in excellent agreement between the detailed and reduced model. A special focus was set on the accurate prediction of O and H species profiles, which are required in the numerical model e.g. to simulate OH chemiluminescence. This allows the extended comparison with experimental values, for which OH chemiluminescence is typically observed to localise and characterise the combustion processes. The newly developed reduced model is applicable in CFD simulations and directly supports the efficient and effective design of novel in-space thrusters using advanced green propellants.

1. Introduction

Hydrazine is the a commonly used monopropellant for space propulsion applications, positioning control systems for satellites. It offers many advantageous features such as long-term stability and high specific impulse, but is known to be highly toxic and is included in the list of "substances of very high concern" by the framework legislation of the "European Commission for the Registration, Evaluation, Authorization and Restriction of Chemicals" (REACH). Taking possible restrictions into account, the handling of hydrazine will become expensive and impractical on a short to medium time scale.

Mixtures of ethylene and nitrous oxide—so called green propellants—are promising replacements of carcinogenic hydrazine as propellants for in-space propulsion systems.[18,23] The design of next generation thrusters, using these propellants, requires experimental testing with the support of sophisticated numerical CFD simulations. For the numerically expensive reactive flow simulations, accurate and efficient chemical kinetic mechanisms for the combustion of these green propellants are inevitable for a time and cost-effective design. For reactive CFD simulations the main driver for the computational costs is the number of species in the reaction scheme, for which the costs increase exponentially. The main objective for creating accurate and efficient chemical kinetic models is the reduction of the simulated species.

Various strategies have been applied for the reduction of chemical kinetic mechanisms. The directed relation graph (DRG) method established by Lu and Law[8] lay the ground for further method extensions. The DRG was extended with an analysis of the error propagation (DRGEP)[15] and a DRG-aided sensitivity analysis (DRGASA) was developed.[24] Other established reduction approaches are the application of the principal component analysis (PCA),[21] the simulated error minimization connectivity method (SEM-CM)[13] or the method using multi path-flux analysis and sensitivity analysis (MPFASA).[22] Also genetic algorithms (GA) have been successfully applied to reduce chemical kinetic mechanisms.[1,16,19] All these methods tend to find a minimum number of species and reactions, for which the model predictive capability is kept within certain error margins compared to experimental or numerical reference data. It is possible to go below this minimum number, when post-optimisation of the model parameters of the reduced mechanism is applied.[10,16] The reduced mechanism is optimised on the experimental or numerical reference data, to allow

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the targeted error margins to be in the desired limits. This was achieved with GA[16] or in our previous work with the highly efficient optimisation method of the linear transformation model (linTM).[2,5,10,12,23]

In prior work, we applied the linTM to generate reduced chemical kinetic mechanisms for the combustion of mixtures of N_2O with C_2H_4[23] and C_2H_6.[5] For the work of C_2H_4 modelling, the reduced model was based on updated version of the detailed GRI 3.0 mechanism.[14,20] In the subsequent work on the C_2H_4 and C_2H_6 modelling,[6] the base model was changed due to recent advancements in the chemical kinetic modelling of C_2H_x species combustion[11] and nitrogen chemistry.[3] The new base model was created by merging the chemical kinetic model DLR SynNG[9,11] with the nitrogen submodel from Glarborg et al.[3] As a key step N_2O decomposition reactions were updated in the mechanism with rates from Powell et al.[17] and optimised to form the model DLR SynNG + NO v0.2.[6] The substantial change of the base model enables numerical chemical kinetic simulations of high accuracy, being a major advantage in the numerically design of sophisticated, modern space propulsion systems by CFD.

In this work the generation of a reduced chemical kinetic mechanisms for the combustion of mixtures of N_2O with C_2H_4 is revisited, by applying the modern chemical kinetic mechanism DLR SynNG + NO v0.2 as the basis of this study. The model is reduced by applying the rapid reduction approach of the linTM.[10] The reduced model is tailor-made to be applicable for combustion boundary conditions within a satellite thruster model combustor.[23] A focus of the model generation is put on a reproduction capability of species involved in the generation of OH chemiluminescence. This feature allows an improved comparability between typical experimental observations and the numerical prediction of OH chemiluminescence. The predictive capability is compared between the detailed and the reduced, post-optimised model for the global combustion characteristics of the laminar burning velocities and the ignition delay times. Additionally, the performance of the models is compared for the detailed chemical kinetic reaction process given by species profiles from zero- and one-dimensional reaction systems. The reduced, post-optimised chemical kinetic model is designed to consist of a relatively small number of species to allow the cost-efficient use of the model in CFD simulations.

2. Model reduction approach

For the generation of the reduced chemical kinetic model, the rapid reduction method[10] of the linear transformation model (linTM) was applied. With the linTM[10] approach, species profiles from zero- and one-dimensional reaction systems as well as laminar flame speed profiles are analysed by means of characteristic points on the profiles. Examples for these characteristic points are the coordinates of the maximum of the curve or the point where one third of the curve maximum is reached. The relation between these coordinates and normalised chemical kinetic model parameters τ—e.g. transformed Arrhenius coefficients[10]—is approximated linear in the linTM. Hence, these points are analysed by sensitivity analyses (SA) of their x and y coordinates in dependence from the model parameters τ with a brute-force approach to estimate $\partial x/\partial\tau$ and $\partial y/\partial\tau$. In the linTM framework, these derivatives are utilised for global SA of extensive combustion systems and model parameter optimisations targeting experimental or numerical x and y values. The combination of the global SA with the optimisation methods leads to the rapid reduction scheme of chemical kinetic mechanisms.[10]

The first step of the rapid reduction, is the numerical generation of initial species profiles from zero- and one-dimensional reactive systems with a detailed chemical kinetic model for user given boundary conditions, e.g. satellite thruster conditions. As the second step, the global SA is applied to identify important reactions. Subsequently, reactions with a low sensitivity are removed from the mechanism—simultaneously reducing the numbers of species. In the last step, the reduced model is post-optimised on the initially created species profiles and flame speed profiles, to match the model predictability of the detailed chemical kinetic model. The rapid reduction scheme is highly automatable and was implemented with python[10] utilising the open-source package Cantera[4] for the chemical kinetic simulations.

In this work, the initial species profiles were generated for various isobaric conditions with the chemical kinetic model DLR SynNG + NO v0.2.[6] The combustion boundary conditions of the multiple simulations selected for ranges of the equivalence ratio φ, the initial temperature T_0 and the pressure p given in Tab. 1. These ranges were designed to be representative for testing conditions of a satellite thruster model.[23] Secondly, the selected boundary conditions cover a broad range of φ, T and p to increase the validity range of the reduced model. Species profiles were considered in the procedure, when their maximum molefraction exceeded at least 0.5% during the reaction time. To allow an extended comparability of CFD simulations and experiments, main species that are involved in chemiluminescence reactions were targeted additionally. OH chemiluminescence is the photon emission from exited OH(A) radicals, relaxing to the ground state. The main production of OH(A) comes from the radical radical recombination:[7]

$$\mathrm{O} + \mathrm{H} + \mathrm{M} \rightleftharpoons \mathrm{OH(A)} + \mathrm{M} \tag{R1}$$

Therefore, the species O, H, and OH are included to the targeted species profiles. 4842 characteristic points were automatically created to describe the initial species profiles.

For the post-optimisation, the model parameters of reduced mechanism were optimised within their 3σ uncertainty. The parameter uncertainties were taken from prior work.[11] A OH chemiluminescence scheme, e.g. from Kathrotia et al.,[7] was not considered in the reduced mechanism. Such schemes could be added posterior to the reduced model, in case it is required for the comparison with experimental results from OH chemiluminescence data. All simulations were performed with the open-source software package Cantera.[4]

Table 1: Simulation boundary condition ranges of the targeted numerical data of C_2H_4 / N_2O combustion

Domain	φ	p / Pa	T_0 / K
0D	0.5–2.0	1–16	1300–2600
1D	0.8–1.4	1–4	298–450

3. Results and discussion

In the first step of the rapid reduction scheme, the SA was performed and the reactions—or species respectively—with lower global sensitivity coefficients were removed. Here the chemical kinetic mechanism was reduced from 165 to 35 species and the number of reactions was reduced from 1510 to 249. Therefore, the reduced model can be efficiently applied in CFD simulations, offering a high potential of lowering calculation costs.

With the initially reduced model, the reproducibility of the coordinates of the characteristic points on the targeted species profiles from the detailed model was significantly reduced. The average absolute error between these coordinates from the initial reduced mechanism to the detailed mechanism was 20%. With the post-optimisation this average error was significantly reduced to below 3%. Thus, the reproducibility of species profiles from the detailed model is almost identical by the drastically reduced, post-optimised chemical kinetic model.

The model analysis is described in the following section by comparing the results for the detailed, reduced and post-optimized models. Examples of the excellent model performance of the post-optimised model are given in Figs. 1–10. For the discussion in this section two reference cases were selected from the comprehensive set of simulation cases in Tab. 1. Figures 1–8 compare targeted species profiles for a zero-dimensional and a one-dimensional reference case. The zero-dimensional case is representative for the chemical kinetic self-ignition model performance at relatively low temperatures. On the other hand, the one-dimensional case represents the chemical kinetic model performance at higher temperatures.

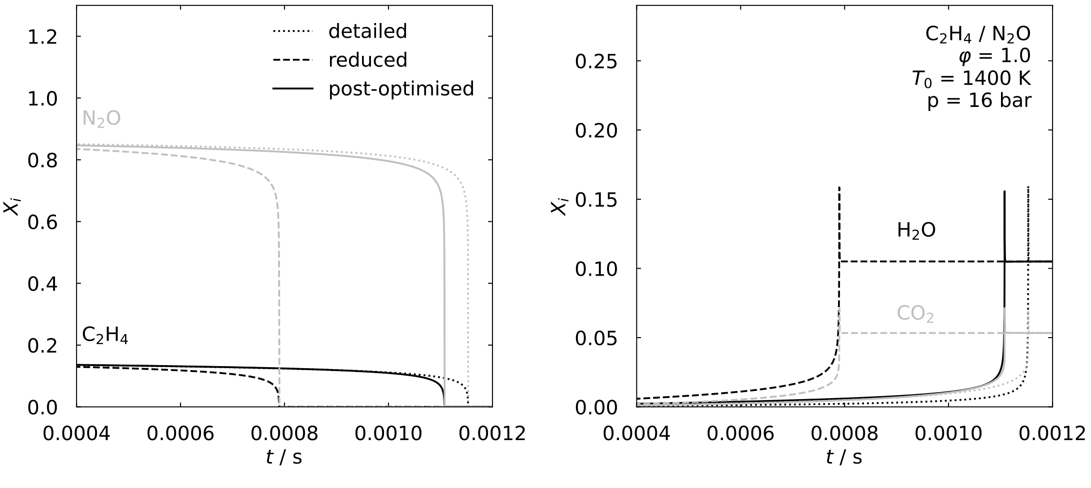

Figure 1: Homogeneous reactor results of species profiles for the reactants C_2H_4 and N_2O (left) and main products CO_2 and H_2O (right)

Figure 1 demonstrates the effect of the extensive reduction on initial main decomposition of the reactants and the subsequent generation of main products for a homogeneous reactor simulation. The not optimised model shows a significant temporal shift of approximately 30% of the initiation of the reactant decomposition. With the optimisation of this reduced model, the post-optimised model is in good agreement with the initial detailed model. For the high temperature case in Fig. 2 the detailed, reduced and post-optimised model are all in good agreement. The overall good

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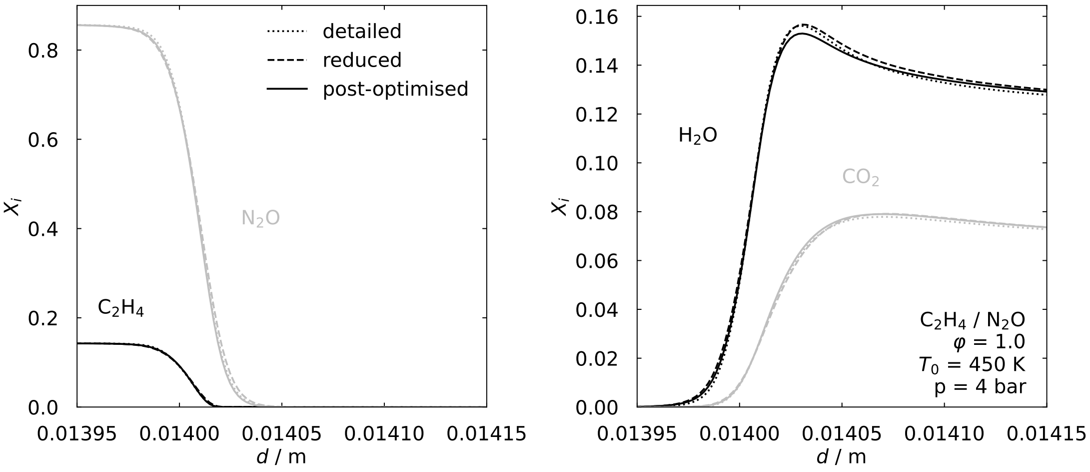

Figure 2: Laminar reactive one-dimensional flow results of species profiles for the reactants C_2H_4 and N_2O (left) and main products CO_2 and H_2O (right)

prediction of the destruction and formation of main species is important for predicting right heat releases in reaction systems. Therefore, the model predictability of the main species is substantial when designing new combustion systems like satellite thrusters. For instance, this allows the accurate simulation of flame positions and heat loads to walls, which is an essential information when designing the cooling system of combustion applications.

Figures 3–5 compare the model performance for targeted major intermediate species. Also, the formation of major intermediate species during reaction processes is of high importance to the heat release, as their heat of formation impacts the local temperatures. For the selected species in Figs. 3–5, the simply reduced model is not able to capture the maximum concentrations compared to the initial detailed model. In Fig. 3 (left), Fig. 4 (left) and Fig. 5 (left) the reduced model underpredicts the formation of methane and formaldehyde by approximately a factor of two, for both the zero- and one-dimensional reference case. In Fig. 3 (right), Fig. 4 (right) and Fig. 5 (right) the reduced model significantly overpredicts the formation of HCN, for both reference cases. With the successful optimisation process, the results of the post-optimised model are in very good agreement with the results of the initial detailed model. Hence, the similar prediction of the maximum concentrations of the major intermediate species, is a further demonstration of the accurate heat release prediction of the post-optimised model.

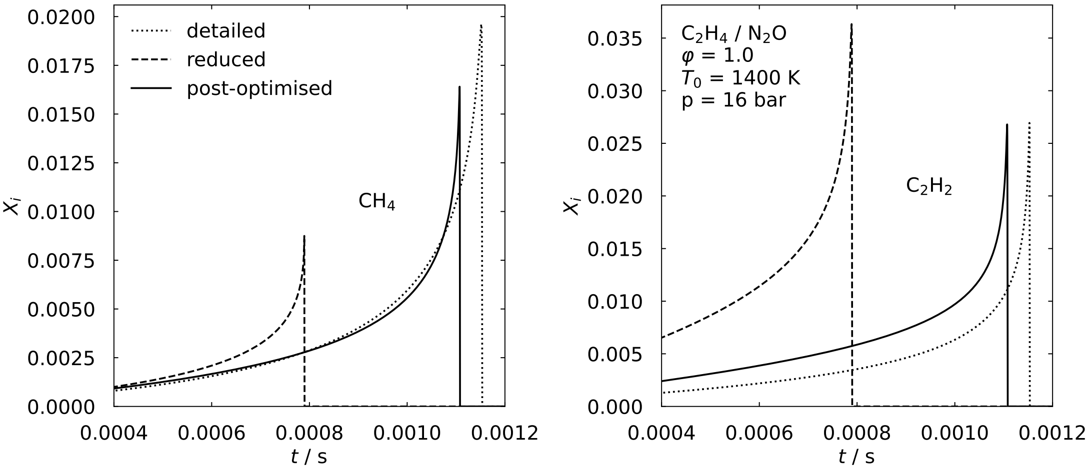

Figure 3: Homogeneous reactor results of species profiles for the main intermediates CH_4 (left) and C_2H_2 (right)

Figures 6–8 compares the numerical results of the species OH, H and O, relevant for the accurate prediction of OH chemiluminescence, e.g. for the comparison with experimental data. Also, for the simulation of these species profiles, the substantial reproducibility is demonstrated for the numerical data from the detailed chemical kinetic model

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by the post-optimised model for the low-temperature conditions in Fig. 6, for fuel rich high temperature conditions in Fig. 7 as well as for the high temperature reactive flow conditions in Fig. 8.

Figure 6 shows a remarkable improvement of the post-optimised model. Under these boundary conditions, the detailed chemical kinetic model predicts local concentration maxima for the species OH, H and O. After the maximum, all concentrations decrease to their corresponding equilibrium concentrations. This phenomenon can be related to the following reactions:

$$N_2O + H \rightleftharpoons N_2 + OH \tag{R2}$$

$$CO + OH \rightleftharpoons CO_2 + H \tag{R3}$$

$$H_2 + OH \rightleftharpoons H_2O + H \tag{R4}$$

Reaction R2 has a relatively high reaction rate[17] and H radicals are instantly consumed by this reaction with the presence of N_2O. Due to stronger bond energies of N_2O compared to C_2H_4, N_2O decomposes slower than C_2H_4, which is also clearly shown in Fig. 2. Consequently, significant amounts of N_2O are still present when C_2H_4 is decomposed, while species like H_2, CO, OH and H are already produced. In the pool of produced species, the H radical is directly consumed by R2. Due to the absence of H radicals, reactions R3 and R4 are shifted towards the product side, producing the main products CO_2 and H_2O. Due to this shift, CO_2 and H_2O exceed their expected concentration in the thermodynamic equilibrium. As soon as N_2O is consumed, the net production of H increases significantly, as shown

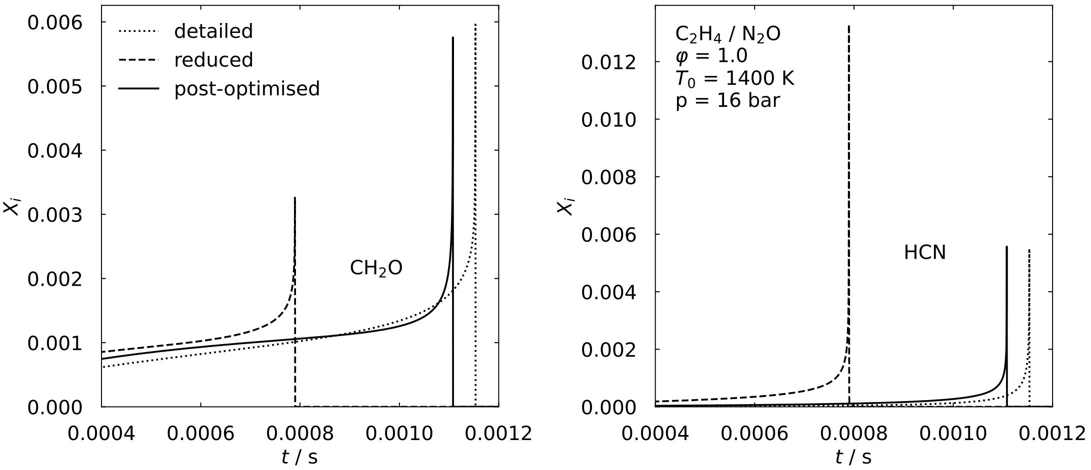

Figure 4: Homogeneous reactor results of species profiles for the main intermediates CH_2O (left) and HCN (right)

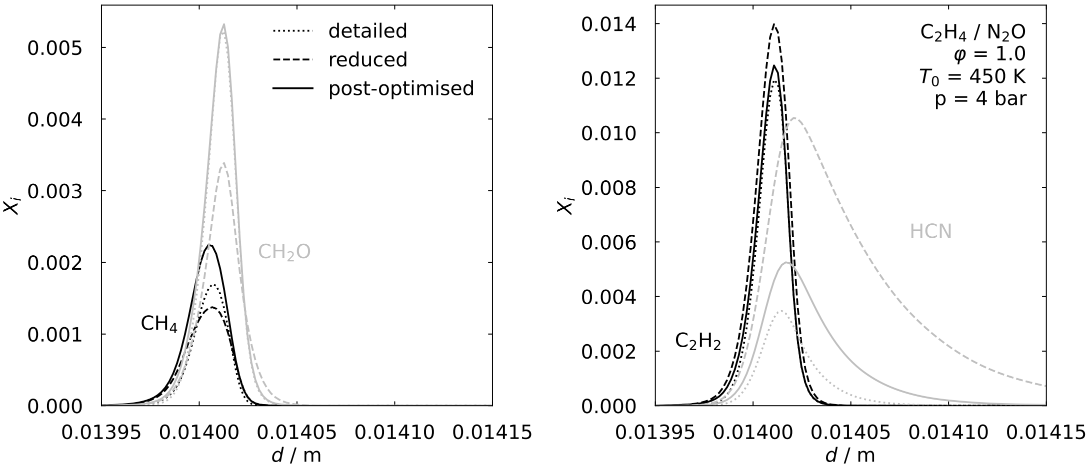

Figure 5: Laminar reactive one-dimensional flow results of species profiles for the main intermediates CH_4 and CH_2O (left) as well as C_2H_2 and HCN (right)

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in Figs. 6–8. With the abundant presence of H radicals, the complete reaction system can reach the thermodynamic equilibrium.

The simply reduced chemical kinetic model is not able to reproduce the feature of the local maxima of the investigated OH, H and O species profiles in Fig. 6. The concentrations of all three species are constantly increasing until equilibrium concentrations are reached, so no local maxima of the species profiles are apparent. With the optimisation the post-optimised model is able to reproduce this feature of the local maximum, predicted by the detailed model. This is of utmost importance when comparing experimental and numerical data of chemiluminescence. The detection of OH chemiluminescence is performed by line of sight measurements, impeding a calibration of the signal strength or quantification of species concentrations, respectively. This becomes even more difficult for the measurement in turbulent flows. As a consequence, experimental and numerical data from chemiluminescence is usually compared to normalised values. Thus, the good agreement between the numerical results from the detailed and the post-optimised model is required for the comparison with experimental data—especially for species profiles with local maxima.

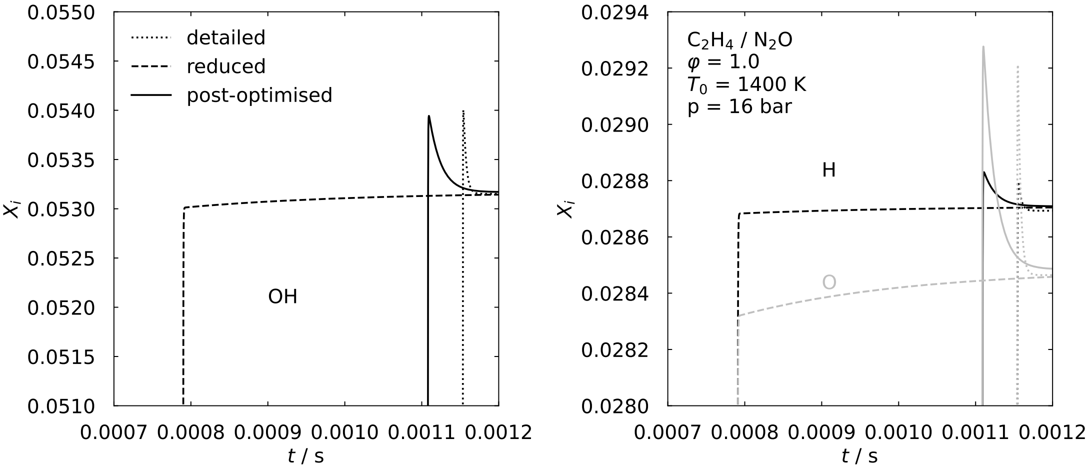

Figure 6: Homogeneous reactor results of species profiles for the intermediates OH (left) as well as H and O (right)

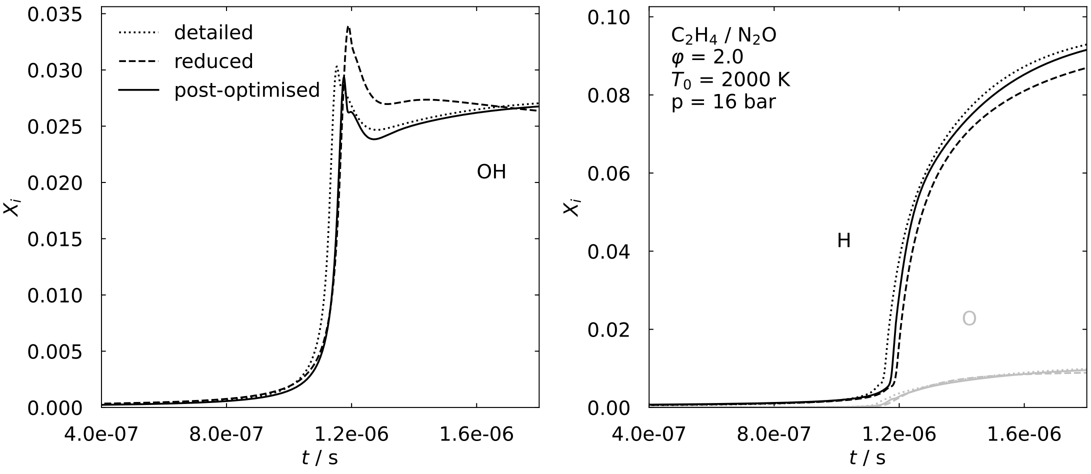

Figure 7: Homogeneous reactor results of species profiles for the intermediates OH (left) as well as H and O (right) for fuel rich conditions

The accurate modelling of global combustion characteristics like laminar burning velocities u_l^0 and ignition delay times t_{ign} are of vast importance for turbulent, reactive CFD simulations. The laminar burning velocity is an indicator of the heat release within the flame zone and is influencing the flame position in the combustor. Ignition delay times are an indicator for the general ignition behaviour and characterise the initial chemical decomposition of the fuel and oxidiser.

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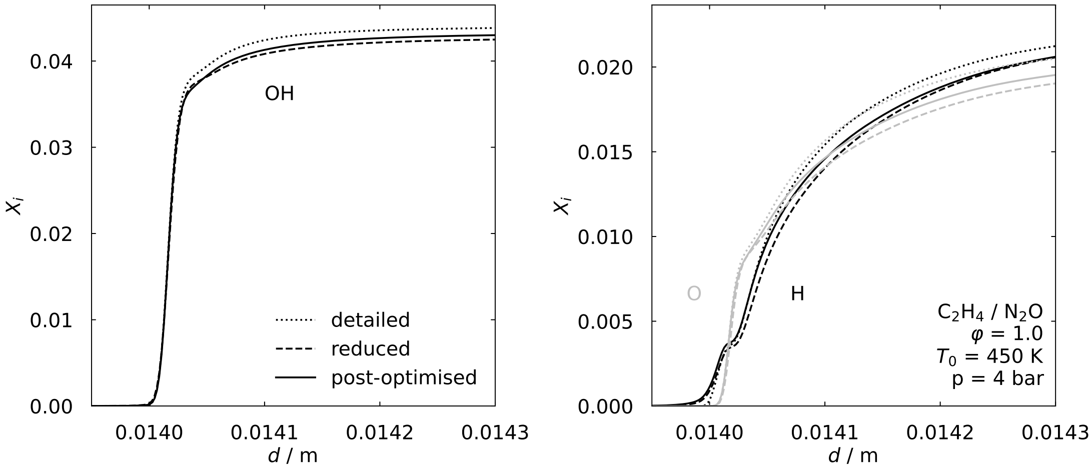

Figure 8: Laminar reactive one-dimensional flow results of species profiles for the intermediates OH (left) as well as H and O (right)

Figure 9 (right) shows that the laminar burning velocities—that were targeted by the optimisation—are in very good agreement between the detailed base model and the post-optimised model. The experimental data[6] in Fig. 9 (left) were not targeted by the optimisation because the experimental conditions are not representative for the conditions in the applied combustion. Nevertheless, the post-optimised model is capable to correctly reproduce the experimental data, which is a further validation of the applied reduction approach. For all flame speed boundary conditions in Fig. 9, the improvement of the laminar flame speed results from the reduced to the post-optimised is significant.

Figure 10 (right) demonstrates that the ignition delay times are in very good agreement between the detailed base model and the post-optimised model, for the targeted boundary conditions. Note that the experimental data[6] in Fig. 10 (left) were not targeted by the optimisation and the good agreement between the numerical and experimental results serves as an additional model validation. Consistent with the prior observations, the model predictability was improved for the ignition delay times, when comparing the results from the reduced to the post-optimised model.

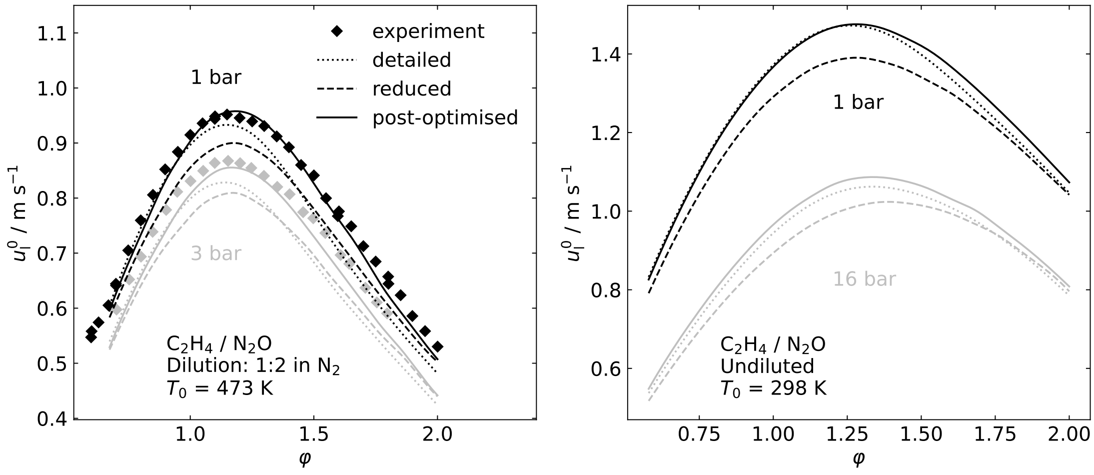

Figure 9: Laminar burning velocities for experimental data[6] (left) and for targeted numerical data of the applied combustion conditions (right)

Overall, the post-optimised model is able to accurately reproduce the predicted combustion characteristics of the detailed chemical kinetic model. The post-optimised model is capable of reproducing ignition processes as well as the general heat release in reactive flows. Consequently, this reduced chemical kinetic model can be applied for the given boundary conditions in CFD simulations with the same accuracy as the detailed model. Thus, allowing efficient and accurate numerically aided design of space propulsion systems for green propellant mixtures of C_2H_4 and N_2O.

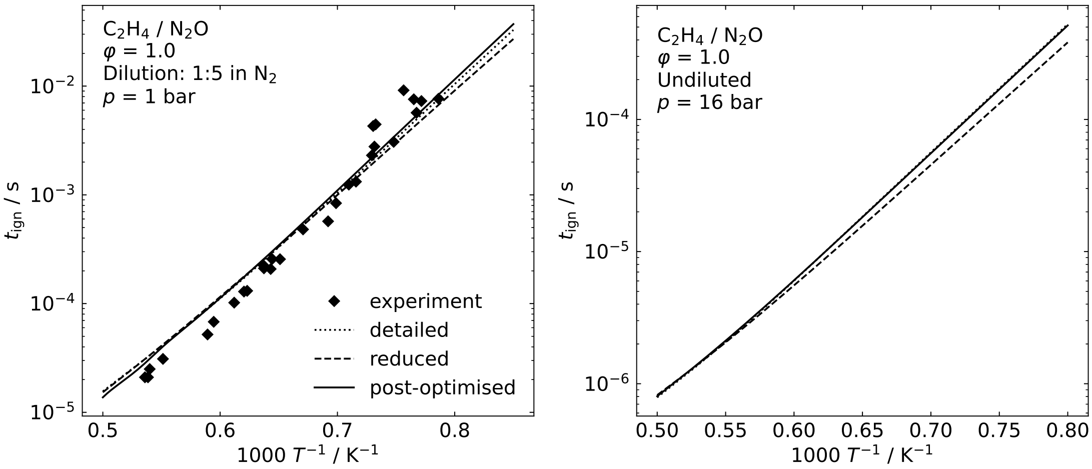

Figure 10: Ignition delay times for experimental data[6] (left) and for targeted numerical data of the applied combustion conditions (right)

4. Conclusions

A new reduced chemical kinetic model for the combustion of mixtures of C_2H_4 and N_2O, was created by applying the rapid reduction approach of the linear transformation system. This model is based on the state-of-the-art detailed chemical kinetic mechanism DLR SynNG + NO v0.2 for the combustion of C_2H_x including a detailed nitrogen chemistry submodel. With the reduction process the size of the chemical kinetic model was significantly reduced from 165 to 35 species. By post-optimising the reduced model, the predictive capability of various combustion properties by the optimised model is significantly improved and is almost identical to the ones of the detailed model. This reduced model is in good agreement with the laminar burning velocities as well as the ignition delay times, demonstrating the capability of modelling accurate heat release and ignition behaviour. Also, the species profiles in zero- and one-dimensional simulations of main and intermediate species are in very good agreement between the results from the initial detailed model and the post-optimised, reduced model. The reduced model for the C_2H_4 / N_2O combustion is particularly designed for an accurate prediction OH chemiluminescence to enable a further comparableness of numerical data with experimental results. Here, the radicals OH, H and O—being main species involved in chemiluminescence—are reproduced with high precision by the post-optimised, reduced model.

Mixtures of C_2H_4 and N_2O are proposed as green propellants, for replacing toxic hydrazine and its derivatives as rocket fuels. The tailor-made, reduced chemical kinetic mechanism can be efficiently and effectively applied in CFD simulations, facilitating the development and design of reliant and safe novel space propulsion applications.

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References

[1] K. Edwards, T. Edgar, and V. Manousiouthakis. Kinetic model reduction using genetic algorithms. *Computers and Chemical Engineering*, 22(1):239–246, 1998.

[2] Q. Fradet, M. Braun-Unkhoff, and U. Riedel. A sectional approach for the entrained-flow gasification of slurry fuels. *Energy & Fuels*, 32(12):12532–12544, 2018.

[3] P. Glarborg, J. A. Miller, B. Ruscic, and S. J. Klippenstein. Modeling nitrogen chemistry in combustion. *Progress in Energy and Combustion Science*, 67:31–68, 2018.

DOI: 10.13009/EUCASS2022-6125

[4] D. G. Goodwin, H. K. Moffat, I. Schoegl, R. L. Speth, and B. W. Weber. Cantera: An object-oriented software toolkit for chemical kinetics, thermodynamics, and transport processes. `https://www.cantera.org`, 2022. Version 2.6.0.

[5] C. Janzer and T. Methling. Ethane / nitrous oxide mixtures as green propellants substituting hydrazine: reduction of optimized reaction mechanism for CFD simulations. In *Proc. 10th European Combustion Meeting (ECM)*, number Paper 16, 2021. 14.-15.04.2021.

[6] C. Janzer, S. Richter, C. Naumann, and T. Methling. "Green propellants" as a hydrazine substitute: experimental investigations of ethane/ethene-nitrous oxide mixtures and validation of detailed reaction mechanism. *CEAS Space Journal*, 14(1):151–159, 2022.

[7] T. Kathrotia, M. Fikri, M. Bozkurt, M. Hartmann, U. Riedel, and C. Schulz. Study of the H+O+M reaction forming OH*: Kinetics of OH* chemiluminescence in hydrogen combustion systems. *Combustion and Flame*, 157(7):1261–1273, 2010.

[8] T. Lu and C. K. Law. A directed relation graph method for mechanism reduction. *Proceedings of the Combustion Institute*, 30(1):1333–1341, 2005.

[9] T. Methling, M. Braun-Unkhoff, and U. Riedel. DLR SynNG mechanism. `http://www.dlr.de/vt/mechanisms/`, 2017.

[10] T. Methling, M. Braun-Unkhoff, and U. Riedel. A novel linear transformation model for the analysis and optimisation of chemical kinetics. *Combustion Theory and Modelling*, 21(3):503–528, 2017.

[11] T. Methling, M. Braun-Unkhoff, and U. Riedel. An optimised chemical kinetic model for the combustion of fuel mixtures of syngas and natural gas. *Fuel*, 262:116611, 2020.

[12] T. Methling, S. Richter, T. Kathrotia, M. Braun-Unkhoff, C. Naumann, and U. Riedel. An Investigation of Combustion Properties of Butanol and Its Potential for Power Generation. *Journal of Engineering for Gas Turbines and Power*, 140(9), 2018. 091505.

[13] T. Nagy and T. Turányi. Reduction of very large reaction mechanisms using methods based on simulation error minimization. *Combustion and Flame*, 156(2):417–428, 2009.

[14] C. Naumann, T. Kick, T. Methling, M. Braun-Unkhoff, and U. Riedel. Ethene/nitrous oxide mixtures as green propellant to substitute hydrazine: Reaction mechanism validation. *International Journal of Energetic Materials and Chemical Propulsion*, 19(1):65–71, 2020.

[15] P. Pepiot-Desjardins and H. Pitsch. An efficient error-propagation-based reduction method for large chemical kinetic mechanisms. *Combustion and Flame*, 154(1):67–81, 2008.

[16] F. Perini, J. L. Brakora, R. D. Reitz, and G. Cantore. Development of reduced and optimized reaction mechanisms based on genetic algorithms and element flux analysis. *Combustion and Flame*, 159(1):103–119, 2012.

[17] O. A. Powell, P. Papas, and C. Dreyer. Laminar burning velocities for hydrogen-, methane-, acetylene-, and propane-nitrous oxide flames. *Combustion Science and Technology*, 181(7):917–936, 2009.

[18] T. Pregger, G. Schiller, F. Cebulla, R.-U. Dietrich, S. Maier, A. Thess, A. Lischke, N. Monnerie, C. Sattler, P. L. Clercq, B. Rauch, M. Köhler, M. Severin, P. Kutne, C. Voigt, H. Schlager, S. Ehrenberger, M. Feinauer, L. Werling, V. P. Zhukov, C. Kirchberger, H. K. Ciezki, F. Linke, T. Methling, U. Riedel, and M. Aigner. Future fuels-analyses of the future prospects of renewable synthetic fuels. *Energies*, 13(1), 2020.

[19] N. Sikalo, O. Hasemann, C. Schulz, A. Kempf, and I. Wlokas. A genetic algorithm-based method for the automatic reduction of reaction mechanisms. *International Journal of Chemical Kinetics*, 46(1):41–59, 2014.

[20] G. P. Smith, D. M. Golden, M. Frenklach, N. W. Moriarty, B. Eiteneer, M. Goldenberg, C. T. Bowman, R. K. Hanson, S. Song, W. C. Gardiner Jr., V. V. Lissianski, and Z. Qin. GRI 3.0 mechanism. `http://combustion.berkeley.edu/gri_mech/`, 1999.

[21] S. Vajda, P. Valko, and T. Turányi. Principal component analysis of kinetic models. *International Journal of Chemical Kinetics*, 17(1):55–81, 1985.

DOI: 10.13009/EUCASS2022-6125

[22] W. Wang and X. Gou. A mechanism reduction method integrating path flux analysis with multi generations and sensitivity analysis. *Combustion Science and Technology*, 189(1):24–42, 2016.

[23] L. K. Werling, T. Hörger, K. Manassis, D. Grimmeisen, M. Wilhelm, C. Erdmann, H. K. Ciezki, S. Schlechtriem, S. Richter, M. Torsten, E. Goos, J. Corina, C. Naumann, and U. Riedel. Nitrous oxide fuels blends: Research on premixed monopropellants at the german aerospace center (DLR) since 2014. In *AIAA Propulsion and Energy 2020 Forum*. American Institute of Aeronautics and Astronautics, 2020.

[24] X. Zheng, T. Lu, and C. Law. Experimental counterflow ignition temperatures and reaction mechanisms of 1,3-butadiene. *Proceedings of the Combustion Institute*, 31(1):367–375, 2007.