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ChemCheck: A Cantera Tool For Debugging Chemical and Syntax Errors In Combustion Models

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Abstract: Detailed kinetic models are widely used in combustion modeling, and their size has been significantly increasing over the past decades. With the increasing size and varied data sources, there is need to detect chemical and syntax errors in the model to prevent the simulation from failure. In this work, we present a new open-source web based tool —ChemCheck, to help identify the incorrect data format, inappropriate pressure-dependent and duplicate reaction rate parameters, visualize the thermodynamic inconsistencies and the violations of collision limit. The main goal of this tool is to help Cantera, an open-source suite of tools for problems involving chemical kinetics, thermodynamics, and transport processes, debug the possible errors during computation, so a workflow about coupling Cantera and ChemCheck to improve a detailed kinetic model is demonstrated.

Keywords:* *detailed kinetic model, thermodynamic inconsistencies, collision violation, Cantera

1. Introduction

Detailed kinetic modeling is a way to model the reaction mechanisms taking place during a chemical process by describing all the essential elementary reactions, with thermodynamic data for all the intermediate species. It is a widespread technique used in different engineering fields which include complex chemical processes with a large number of intermediates, for example, combustion simulation [1], and design of molecular catalysts [2]. The simulation results for the chemical kinetics, transport, and thermodynamic processes highly depend on the quality of detailed kinetic models. The data of a detailed kinetic model is typically arranged in CHEMKIN format [3] which is composed of data to describe the reaction mechanism in detail, so obtaining an accurate CHEMKIN file is a prerequisite of a successful simulation. CHEMKIN files can be acquired from computational software, manually building from scratch, and published papers, etc., so the quality of the data varies. It is not rare that some CHEMKIN files have syntax errors or bugs that prevent them from being interpreted by other simulation software, especially with the increasing size in the past decade[4, 5]. Chen et al.[6] investigated 20 models published in 5 consecutive issues of Combustion and Flame in 2015 and 2016. Of these models, 15 were found to be contain reaction rates above the collision limit, with some exceeding it by up to 73 orders of magnitude. Since the simulation of a detailed kinetic model (DKM) requires solving a series of stiff ordinary differential equations (ODEs) by numerical integration, the ultra-fast timescales observed in reactions with collision limit violations could keep the solver from converging or extend the time required to converge. Therefore, simulation software with the ability to detect and report the collision limit violations in a DKM will be helpful for modelers to conduct a better analysis of their model. Yalamanchi et al.[7] developed a web tool to screen the rate constants of bi-molecular reactions in the DKM to filter out the reactions which have rate constants exceeding the collision limit, and they illustrate a procedure to identify the ultra-fast time scales using the computational singular perturbation algorithm. Similar work is done by Killingsworth et al. [8].

Given the aforesaid context, we present ChemCheck, an open-source web-based software available at `https://github.com/comocheng/ChemCheck/`, to help combustion researchers debug syntax errors, thermodynamic discontinuities, inappropriate Arrhenius parameters of pressure-dependent and duplicate reactions, and collision limit violations in their CHEMKIN files. ChemCheck is powered by Cantera [9], an open-source software to model kinetic, transport, and thermodynamic processes, and the graphic user interface (GUI) is built with the Django [10] framework. The tool is aimed at providing a comprehensive and thorough inspection of a model when the simulation in Cantera fails.

2. Methods

2.1 Syntax Error Diagnostic

Cantera can be used for combustion simulations in different reactors, sensitivity analysis, mechanism reduction, etc. The first step is converting a CHEMKIN file into a Cantera input file, which is written in YAML format. However, many cases have been reported where the input file cannot be successfully converted due to syntax errors in the CHEMKIN file. Debugging the syntax errors in a DKM needs extra efforts because there could be a lot of species and reactions involved in the model. Even if the CHEMKIN-to-YAML parser reports the error position, one could still be confused about how to fix the file. Therefore, ChemCheck makes suggestions about possible solutions to common syntax errors reported by the converter in Cantera. For example, it has been reported that the thermodynamic data of a species with extensive elemental composition (more than three digits) such as $C_{1250}H_{249}$

```
BIN7BJ                  C 1250H 249         G    300.00   3500.00 1390.00      1
 2.12942777e+03 2.10904362e+00-5.90181843e-04 4.95662128e-08 1.60771953e-12    2
-6.31142548e+05-1.14103717e+04-1.08227805e+03 1.13513625e+01-1.05639073e-02    3
 4.83312758e-06-8.58745044e-10 2.61711671e+05 5.14187909e+03                   4
```

cannot be properly parsed due to the fixed-width format of the CHEMKIN syntax, and this prevents the software from splitting and parsing the string correctly. A special data arrangement shown below should be applied in that circumstance.

```
BIN7BJ                  C    0H    0         G    300.00   3500.00 1390.00      1&
C 1250    H 249
 2.12942777e+03 2.10904362e+00-5.90181843e-04 4.95662128e-08 1.60771953e-12    2
-6.31142548e+05-1.14103717e+04-1.08227805e+03 1.13513625e+01-1.05639073e-02    3
 4.83312758e-06-8.58745044e-10 2.61711671e+05 5.14187909e+03                   4
```

This error diagnosis code is added into the Cantera parser to detect the inappropriate format for the thermo data of the species with extensive elemental composition, and provide a tip to check the Cantera Website about debugging instructions. The sample data arrangement for the thermodynamic data of big molecules is added in the instructions on the website as a reference to users.

This is just one example of the syntax errors that can be detected and diagnosed in ChemCheck. The syntax error diagnosis has been tested on over 50 published models, and suggestions are made for common mistakes found in these models, but special care should be taken for some rare syntax errors. Automatically diagnosing *all* the possible syntax errors is a challenge, so work will continue as other syntax errors are found. A series of published CHEMKIN models are used to test the syntax check performance of ChemCheck. In Table 1, 15 published kinetic models with various syntax errors detected by ChemCheck are shown. The 15 kinetic models are selected from the test DKMs for ChemCheck, which were randomly selected from the kinetic models database maintained by our research group.

Table 1: Syntax error found in published models.

Kinetic Models	**Syntax Errors**
Myles D. Bohon et al. [11]	Missing line index in some thermodynamic entries
Zhanjun Cheng et al. [12]	1.Indent error in thermodynamic data of "c6h5ch2oo"; 2.Redundant letter "e" at the last line
Mariam J. Al Rashidi et al. [13]	1. Indent error in thermodynamic data of some species; 2. Index out of position for thermodynamic data of some species
Nicole Labbe et al. [14]	PLOG reaction parameters are assigned to a three-body reaction
Matteo Pelucchi et al. [15]	Only 4 parameters for the SRI reaction is given
Luc-Sy Tran et al. [16]	Index out of position in thermodynamic data of some species
Nour Atef et al. [17]	Missing transport data for some species
Hanfeng Jin et al. [18]	Incorrect element sign
Paul Marshall et al. [19]	Suitable temperature range is not specified thermodynamic data
Amruta Nawdiyal et al. [20]	Some reactions have species having mixed capital and lower case letters
Weijing Wang et al. [21]	Index out of position for thermodynamic data of some species
Xiaoyuan Zhang et al. [22]	Missing magnitude sign E in some pre-exponential factors (A)
S. Mani Sarathy et al. [23]	Missing line index in some thermodynamic entries
Marina Schenk et al. [24]	1. A set of Falloff parameters is assigned to a three-body reaction; 2. Suitable temperature range is not specified at the start of thermo data
Darshan M.A. Karwat et al. [25]	1. Missing magnitude sign E in some pre-exponential factors (A); 2. Missing line index in some thermodynamic entries; 3. Index out of position for thermodynamic data of some species

2.2 Thermodynamic Discontinuity Check

One possible source of collision limit violations in a DKM is unrealistic thermodynamic parameters, so ChemCheck screens the thermodynamic properties of all species and report the suspicious

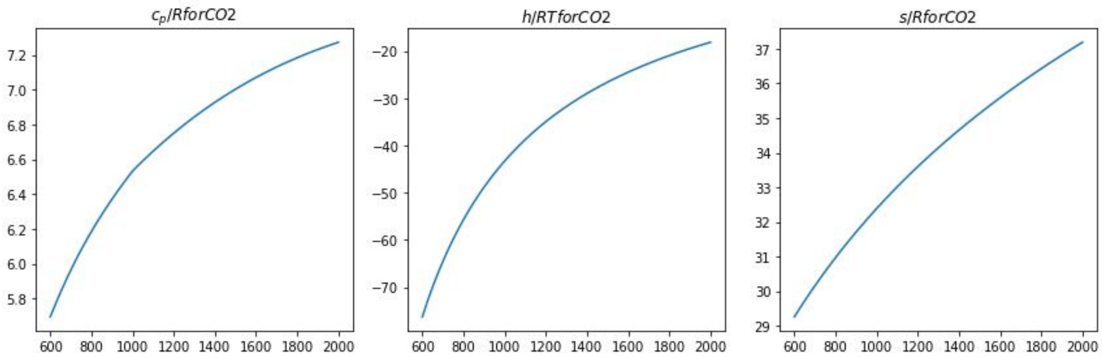


Figure 1: Plots of thermodynamic properties of CO_2

species. Thermodynamic data of a species are usually written in NASA 7-coefficient polynomial parameterization which takes up to 7 coefficients to calculate the thermal properties of a species with respect to the temperature at constant pressure. The expression is:

$$\frac{Cp}{R} = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \tag{1}$$

$$\frac{H}{RT} = a_1 + \frac{a_2}{2}T + \frac{a_3}{3}T^2 + \frac{a_4}{4}T^3 + \frac{a_5}{5}T^4 + \frac{a_6}{T} \tag{2}$$

$$\frac{S}{R} = a_1 \log T + a_2T + \frac{a_3}{2}T^2 + \frac{a_4}{3}T^3 + \frac{a_5}{4}T^4 + a_7 \tag{3}$$

where Cp is the heat capacity, H is the enthalpy, and S is the entropy. The NASA polynomial expression is applied in two temperature ranges with two sets of parameters. An example data entry is shown above for $C_{1250}H_{249}$. The first line defines the elemental composition of the species and three temperature points where the first is the lower boundary, the second is the upper boundary, and the last one is the middle temperature point. The next 7 parameters starting from the second line of the entry are the polynomial coefficients for the high temperature range. The remaining 7 parameters are the polynomial coefficients for the low temperature range.

Based on the NASA polynomial parameterization, the equilibrium constant is calculated so that the reverse reaction rate constant can be estimated. Incorrect NASA coefficients could result in a very high equilibrium constant, which leads to a high reverse rate constant causing trouble to the integration solver. A common sign of a mistake is an inconsistent value calculated from low-temperature coefficients and high-temperature coefficients at a midpoint temperature. ChemCheck screens thermodynamic parameters of all the species and plots the thermodynamic properties of the species with inconsistencies at the midpoint temperature. Figure 1 demonstrates the continuous curve of thermodynamic properties of CO_2.

An example of a species with discontinuous thermo from a model [26] plotted by ChemCheck is shown in figure 2. It is obvious that a spike occurs at mid temperature in the heat capacity plot. The discontinuities are also seen in the enthalpy and entropy plots with small discrepencies.

2.3 Inappropriate Pre-exponential Factor Check for Pressure-dependent Reactions

One kind of pressure-dependent reaction in DKM is also called PLOG reaction because it takes logarithmic interpolation of Arrhenius rate constants at various pressure points. Given two Arrhe-

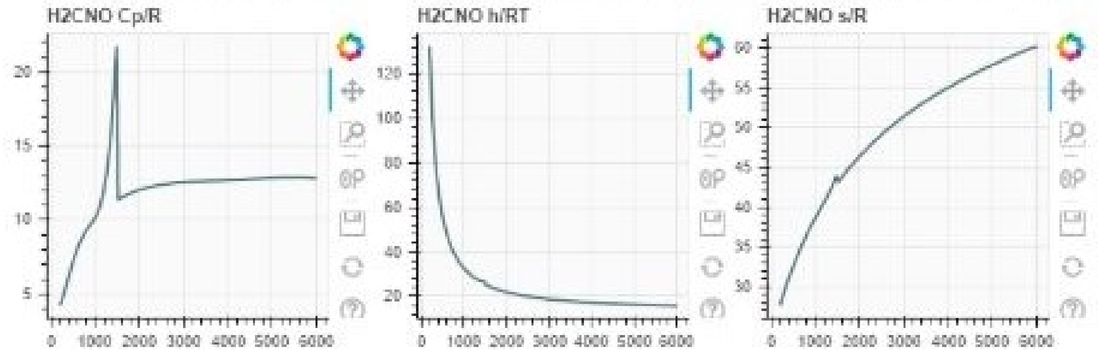


Figure 2: ChemCheck plotted thermodynamic discontinuity of H_2CNO from a published kinetic model [26]

nius rate constants at pressure P_1 and P_2:

$$P_1 : k_1(T) = A_1 T^{b_1} \exp -E_1/RT$$
$$P_2 : k_2(T) = A_2 T^{b_2} \exp -E_2/RT$$

The constant at an intermediate pressure $P_1 < P < P_2$ is computed as:

$$\log k = \log k_1 + (\log k_2 - \log k_1)\frac{\log P - \log P_1}{\log P_2 - \log P_1}. \tag{4}$$

The pressure points and the Arrhenius rate parameters associated with the pressure points are given in CHEMKIN file in the format as below:

```
CH2CHOO=CO+CH3O           1.16E-01         3.16    18420.0
 PLOG/3.160E-01    1.80E+33       -7.27    33760.0/
 PLOG/3.160E-01    8.69E-50       16.63    -3900.0/
 PLOG/1.000E+00    3.83E+33       -7.20    35100.0/
 PLOG/1.000E+00    1.19E-39       13.61    -1317.0/.
```

The first parameter on every line is the pressure point, and the next three parameters are Arrhenius parameters. When a pressure is repeated the Arrhenius rate constants are added before the interpolation. The pre-exponential factor for one expression could be negative, but the sum of the two rate constants at the same pressure has to be positive for the logarithmic interpolation to be valid. The reaction rate constants for duplicate reactions are also added to give the rate of that reaction, so a problem similar to the one for PLOG reactions could happen to duplicate reactions. ChemCheck goes through the Arrhenius parameters for each PLOG reaction and duplicate reaction at each given pressure point and at 7 temperature points from 200 K to 10000 K, to ensure a positive total k. The rate parameters, the relative pressure, and the temperature leading to the negative reaction rate are reported. This allows users to screen PLOG reaction rate parameters beforehand to avoid possible errors during computation.

2.4 Collision Limit Violation Check

For a reaction to happen, the reactants must collide with each other at proper orientation with enough energy. A reaction rate only represents the rate of collisions which are effective, so the reaction rate cannot be higher than the collision rate. As described in section 2.2, thermodynamic errors leading to a high reverse reaction rate are among the reasons why a reaction may violate the collision limit. Another reason is inaccurate rate parameters resulting in a high forward reaction rate that exceeds the limit. A specific check for bi-molecular reactions is provided by ChemCheck by comparing the reaction rate constant and the collision limit of each reaction involving two reactants. The collision limit can be calculated by the method proposed by Chen et al.[6] as Eq. 5:

$$k_{coll} = \sqrt{\frac{8\pi k_B T}{\mu_{AB}}}\sigma_{AB}^2\Omega^{(1,1)^*}N_A, \tag{5}$$

where k_B is the Boltzmann constant, T is the temperature, σ is the collision diameter, and $\Omega^{(1,1)^*}$ is the collision integral. The superscripts are the exponents used in the collision integral [27]. The collision integral is simplified by Neufeld et al. [28] as the reduced integral in Eq. 6:

$$\Omega^* = 1.16145T^{*-0.14874} + 0.52487\mathrm{e}^{-0.7732T^*} + 2.16178\mathrm{e}^{-2.437887T^*}, \tag{6}$$

where T^* is the reduced temperature calculated from Eq. 7:

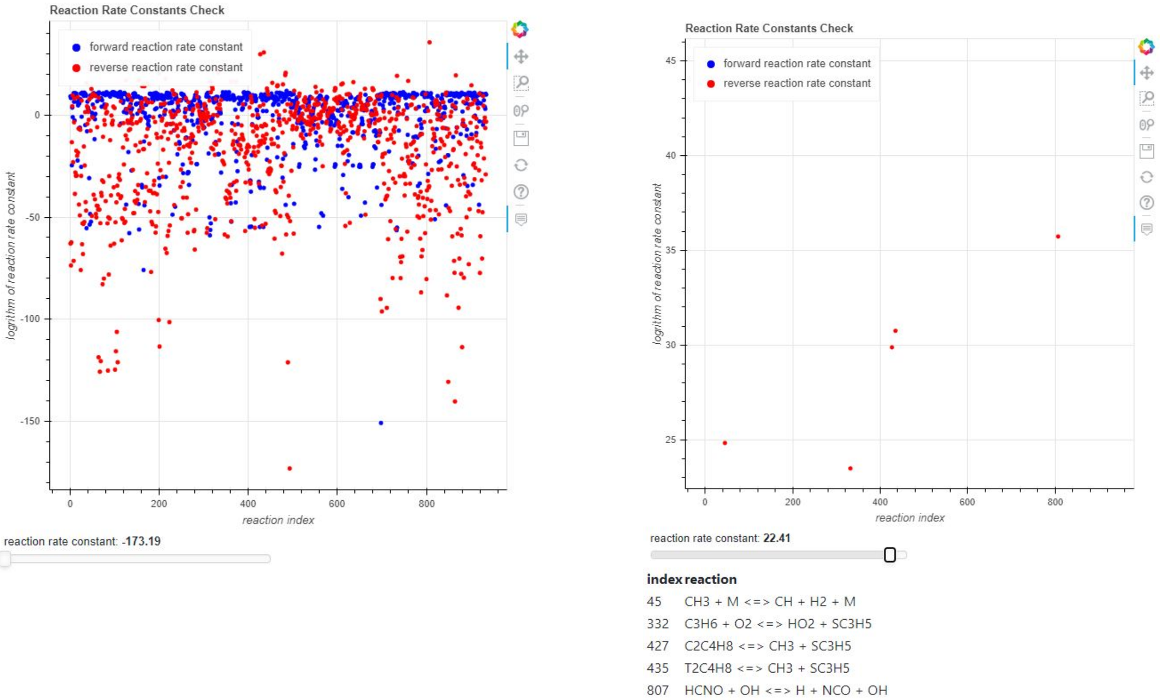
$$T^* = \frac{k_B T}{\varepsilon}, \tag{7}$$

where ε is the Lennard Jones potential well depth. The reaction rates are calculated by Cantera at a user-specified pressure and temperature. If a rate is higher than the collision limit, the reaction equation will be shown in the report associated with the reaction rate, the collision limit of that reaction, and the violation factor which describes how much the rate constant violates the collision limit. However, Lennard Jones potential and collision diameter are written as transport data of DKM which could be missing, so the collision limit cannot be calculated in those circumstances. Besides, the collision limit of a reaction involving more than two reactants is not able to be calculated by the aforesaid formula. To help in these situations, a figure showing the logarithm of the reaction rates plotted with respect to the reaction indices allows the suspicious reaction rate constants to be identified visually. For illustration purpose, figure 3 is generated from a natural gas oxidation mechanism combined with the "NOMecha2.0" sub-mechanism [29] at 300 *K*, 1 *atm*. There are a few outliers seen in figure 3a, which means that the reaction rate constants for these reactions are much higher than other reactions and further investigation is needed. The tool bar at the bottom is introduced for users to decide the cutoff and only keep the suspicious reaction rate constants on the figure. Figure 3b is an example of the plot with the magnitude of the collision limit specified as 22.41 on the tool bar. Six reactions with reaction rate coefficients greater than the threshold are regarded as reactions that are suspiciously fast and are shown at the bottom.

This method can help users make an initial guess about potentially problematic reactions, then check the database or run quantum chemistry to correct the rate parameters.

3. Results and Discussion

As discussed above, ChemCheck is able to achieve a syntax check, a thermodynamic properties check, a collision limit violation check, and an invalid PLOG and duplicate reaction rate coefficient check. The current syntax check is already able to help users detect and diagnose many common



index	reaction
45	CH3 + M <=> CH + H2 + M
332	C3H6 + O2 <=> HO2 + SC3H5
427	C2C4H8 <=> CH3 + SC3H5
435	T2C4H8 <=> CH3 + SC3H5
807	HCNO + OH <=> H + NCO + OH

Figure 3: Logarithmic plot of reaction rate coefficients in a natural gas mechanism [29]. Left: full mechanism. Right: filtered for $\log_{10}(k) > 22.41$.

errors in a model, but it is a functionality that needs to keep improving as more cases of syntax errors are discovered. Aside from the collision limit violations, a reaction that has a very high rate constant without exceeding the collision limit could also result in a very long computational time or a solver crash. The CSP algorithm described in Yalamanchi et al.'s work[7] and Jacobian analysis introduced in [8] are effective methods to visualize the time scales of reactions in a DKM, so the future work of ChemCheck would be adding time scale analysis to filter out the reactions with ultra-fast time scales.

Overall, ChemCheck and the modifications made to Cantera provide combustion researchers with a convenient suite of tools to rapidly detect and correct many common errors in detailed kinetic models of combustion. This reduces the barrier to researchers using these detailed modeling tools, and reduces the the probability of incorrect modeling simulations.

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References

[1] M. E. Fuller, R. H. West, and C. F. Goldsmith, A computational investigation into the combustion byproducts of a liquid monopropellant, Proc. Combust. Inst. 37 (2019) 5671–5677. DOI: `10.1016/j.proci.2018.05.175`.

[2] M.-H. Ho, R. Rousseau, J. A. S. Roberts, E. S. Wiedner, M. Dupuis, D. L. DuBois, R. M. Bullock, and S. Raugei, Ab Initio-Based Kinetic Modeling for the Design of Molecular Catalysts: The Case of H2 Production Electrocatalysts, ACS Catalysis 5 (2015) 5436–5452. DOI: `10.1021/acscatal.5b01152`.

[3] R. J. Kee, F. M. Rupley, and J. A. Miller, Chemkin-II: A Fortran chemical kinetics package for the analysis of gas phase chemical kinetics. Technical Report SAND89-8009, Sandia National Laboratories, 1989.

[4] S. Sarathy, C. Westbrook, M. Mehl, W. Pitz, C. Togbe, P. Dagaut, H. Wang, M. Oehlschlaeger, U. Niemann, K. Seshadri, P. Veloo, C. Ji, F. Egolfopoulos, and T. Lu, Comprehensive chemical kinetic modeling of the oxidation of 2-methylalkanes from C_7 to C_{20}, Combust. Flame 158 (2011) 2338–2357. DOI: `10.1016/j.combustflame.2011.05.007`.

[5] M. A. Oehlschlaeger, J. Steinberg, C. K. Westbrook, and W. J. Pitz, The autoignition of iso-cetane at high to moderate temperatures and elevated pressures: Shock tube experiments and kinetic modeling, Combust. Flame 156 (2009) 2165–2172. DOI: `10.1016/j.combustflame.2009.05.007`.

[6] D. Chen, K. Wang, and H. Wang, Violation of collision limit in recently published reaction models, Combust. Flame 186 (2017) 208–210. DOI: `10.1016/j.combustflame.2017.08.005`.

[7] K. K. Yalamanchi, E.-A. Tingas, H. G. Im, and S. M. Sarathy, Screening gas-phase chemical kinetic models: Collision limit compliance and ultrafast timescales, Int. J. Chem. Kinet. 52 (2020) 599–610. DOI: `10.1002/kin.21373`.

[8] N. J. Killingsworth, M. J. McNenly, R. A. Whitesides, and S. W. Wagnon, Cloud based tool for analysis of chemical kinetic mechanisms, Combust. Flame 221 (2020) 170–179. DOI: `10.1016/j.combustflame.2020.06.010`.

[9] D. G. Goodwin, R. L. Speth, H. K. Moffat, and B. W. Weber, *Cantera: An Object-oriented Software Toolkit for Chemical Kinetics, Thermodynamics, and Transport Processes*, `https://www.cantera.org`, Version 2.4.0, 2018, DOI: `10.5281/zenodo.1174508`.

[10] D. S. Foundation, *Django*, `https://djangoproject.com.`, Version 1.5, 2013.

[11] M. D. Bohon, T. F. Guiberti, S. Mani Sarathy, and W. L. Roberts, Variations in non-thermal NO formation pathways in alcohol flames, Proc. Combust. Inst. 36 (2017) 3995–4002. DOI: `10.1016/j.proci.2016.05.024`.

[12] Z. Cheng, Q. Niu, Z. Wang, H. Jin, G. Chen, M. Yao, and L. Wei, Experimental and kinetic modeling studies of low-pressure premixed laminar 2-methylfuran flames, Proc. Combust. Inst. 36 (2017) 1295–1302. DOI: `10.1016/j.proci.2016.07.032`.

[13] M. J. Al Rashidi, S. Thion, C. Togbé, G. Dayma, M. Mehl, P. Dagaut, W. J. Pitz, J. Zádor, and S. M. Sarathy, Elucidating reactivity regimes in cyclopentane oxidation: Jet stirred reactor experiments, computational chemistry, and kinetic modeling, Proc. Combust. Inst. 36 (2017) 469–477. DOI: `10.1016/j.proci.2016.05.036`.

[14] N. J. Labbe, R. Sivaramakrishnan, C. F. Goldsmith, Y. Georgievskii, J. A. Miller, and S. J. Klippenstein, Ramifications of including non-equilibrium effects for HCO in flame chemistry, Proc. Combust. Inst. 36 (2017) 525–532. DOI: `10.1016/j.proci.2016.06.038`.

[15] M. Pelucchi, E. Ranzi, A. Frassoldati, and T. Faravelli, Alkyl radicals rule the low temperature oxidation of long chain aldehydes, Proc. Combust. Inst. 36 (2017) 393–401. DOI: `10.1016/j.proci.2016.05.051`.

[16] L.-S. Tran, J. Pieper, H.-H. Carstensen, H. Zhao, I. Graf, Y. Ju, F. Qi, and K. Kohse-Höinghaus, Experimental and kinetic modeling study of diethyl ether flames, Proc. Combust. Inst. 36 (2017) 1165–1173. DOI: `10.1016/j.proci.2016.06.087`.

[17] N. Atef, G. Kukkadapu, S. Y. Mohamed, M. A. Rashidi, C. Banyon, M. Mehl, K. A. Heufer, E. F. Nasir, A. Alfazazi, A. K. Das, C. K. Westbrook, W. J. Pitz, T. Lu, A. Farooq, C.-J. Sung, H. J. Curran, and S. M. Sarathy, A comprehensive iso-octane combustion model with improved thermochemistry and chemical kinetics, Combust. Flame 178 (2017) 111–134. DOI: `10.1016/j.combustflame.2016.12.029`.

[18] H. Jin, G. Wang, Y. Wang, X. Zhang, Y. Li, Z. Zhou, J. Yang, and F. Qi, Experimental and kinetic modeling study of laminar coflow diffusion methane flames doped with iso-butanol, Proc. Combust. Inst. 36 (2017) 1259–1267. DOI: `10.1016/j.proci.2016.06.111`.

[19] P. Marshall and P. Glarborg, Ab initio and kinetic modeling studies of formic acid oxidation, Proc. Combust. Inst. 35 (2015) 153–160. DOI: `10.1016/j.proci.2014.05.091`.

[20] A. Nawdiyal, N. Hansen, T. Zeuch, L. Seidel, and F. Mauß, Experimental and modelling study of speciation and benzene formation pathways in premixed 1-hexene flames, Proc. Combust. Inst. 35 (2015) 325–332. DOI: `10.1016/j.proci.2014.06.047`.

[21] W. Wang, Z. Li, M. A. Oehlschlaeger, D. Healy, H. J. Curran, S. M. Sarathy, M. Mehl, W. J. Pitz, and C. K. Westbrook, An experimental and modeling study of the autoignition of 3-methylheptane, Proc. Combust. Inst. 34 (2013) 335–343. DOI: `10.1016/j.proci.2012.06.001`.

[22] X. Zhang, B. Yang, W. Yuan, Z. Cheng, L. Zhang, Y. Li, and F. Qi, Pyrolysis of 2-methyl-1-butanol at low and atmospheric pressures: Mass spectrometry and modeling studies, Proc. Combust. Inst. 35 (2015) 409–417. DOI: `10.1016/j.proci.2014.06.080`.

[23] S. M. Sarathy, S. Vranckx, K. Yasunaga, M. Mehl, P. Oßwald, W. K. Metcalfe, C. K. Westbrook, W. J. Pitz, K. Kohse-Höinghaus, R. X. Fernandes, and H. J. Curran, A comprehensive chemical kinetic combustion model for the four butanol isomers, Combust. Flame 159 (2012) 2028–2055. DOI: `10.1016/j.combustflame.2011.12.017`.

[24] M. Schenk, L. Leon, K. Moshammer, P. Oßwald, T. Zeuch, L. Seidel, F. Mauss, and K. Kohse-Höinghaus, Detailed mass spectrometric and modeling study of isomeric butene flames, Combust. Flame 160 (2013) 487–503. DOI: `10.1016/j.combustflame.2012.10.023`.

[25] D. M. Karwat, S. W. Wagnon, M. S. Wooldridge, and C. K. Westbrook, Low-temperature speciation and chemical kinetic studies of n-heptane, Combust. Flame 160 (2013) 2693–2706. DOI: `10.1016/j.combustflame.2013.06.029`.

[26] A. A. Konnov, Implementation of the NCN pathway of prompt-NO formation in the detailed reaction mechanism, Combust. Flame 156 (2009) 2093–2105. DOI: `10.1016/j.combustflame.2009.03.016`.

[27] N. J. Brown, L. A. Bastien, and P. N. Price, Transport properties for combustion modeling, Progress in Energy and Combustion Science 37 (2011) 565–582. DOI: `10.1016/j.pecs.2010.12.001`.

[28] P. D. Neufeld, A. R. Janzen, and R. A. Aziz, Empirical Equations to Calculate 16 of the Transport Collision Integrals $\Omega^{(l,s)*}$ for the Lennard-Jones (12-6) Potential, J. Chem. Phys. 57 (1972) 1100–1102. DOI: `10.1063/1.1678363`.

[29] N. Lamoureux, H. E. Merhubi, L. Pillier, S. de Persis, and P. Desgroux, Modeling of NO formation in low pressure premixed flames, Combust. Flame 163 (2016) 557–575. DOI: `10.1016/j.combustflame.2015.11.007`.