Comparing the autoignition performance of chemical kinetic models for toluene using data extracted from the literature

By
Morgan Mayer

A THESIS

submitted to

Oregon State University

Honors College

in partial fulfillment of
the requirements for the
degree of

Honors Baccalaureate of Science in Chemical Engineering
(Honors Associate)

Presented May 13, 2019
Commencement June 2019

AN ABSTRACT OF THE THESIS OF

Morgan Mayer for the degree of Honors Baccalaureate of Science in Chemical Engineering presented on May 13, 2019. Title: Comparing the autoignition performance of chemical kinetic models for toluene using data extracted from the literature

Abstract approved:

Kyle Niemeyer

Real transportation fuels contain a wide range of hydrocarbon species, and this complexity poses challenges for modeling. Surrogates with a simpler blend of hydrocarbon reference fuels can approximate the physical and chemical characteristics of real fuels and enable practical simulation of the reacting flows that occur in engines and combustors. Surrogates for gasoline, diesel, and jet fuels commonly include toluene as a representative for aromatic components. The literature contains several chemical kinetic models for toluene oxidation, but an inclusive and comprehensive comparison of these has not been performed. This study objectively compares the performance of toluene oxidation models and identifies the best-performing models. A performance metric was generated for each model accounting for differences in experimental and simulated ignition delay. I performed a sensitivity analysis of the high-performing CaltechMech model to further reveal reactions that independently, significantly affect the model's performance. Experimental data were collected from

the literature for measurements of toluene autoignition in shock tube experiments. I converted the data into the ChemKED standard data format and used the PyTeCK software for the validation of the kinetic models. All experimental data encoded in ChemKED for this study are openly available via the Prometheus online database.

Key Words: chemical kinetic model validation, ChemKED, autoignition, toluene

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Toni Doolen, Dean, Oregon State University Honors College

I understand that my project will become part of the permanent collection of Oregon State University Honors College. My signature below authorizes release of my project to any reader upon request.

Morgan Mayer, Author

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Contents

1 Introduction

Roughly 80% of the world's energy comes from combustion of nonrenewable hydrocarbon fuels. Although work is being done to replace combustion with cleaner energy sources, the world will still rely on hydrocarbon fuels for the next several decades. Chemical kinetic studies help influence engine design to support more efficient combustion and energy use from transportation fuels. Transportation fuels include gasoline, jet fuel, and diesel.

Ignition delay is a characteristic property of a fuel that influences its energy efficiency in an engine. Generally, short ignition delays are preferred for diesel engines which inject fuel into compressed air to cause ignition. Ignition delay is the time between fuel injection and combustion in diesel engines. For compression-ignition engines that use diesel, the ignition quality of the fuel is important for controlling the time of ignition. Fuel should be relatively easy to autoignite in a compression-ignition engine. Autoignition is the event in which a fuel-oxidizer mixture ignites at a certain temperature and pressure that supplies enough activation energy to initialize oxidation. For spark-ignition engines, longer ignition delays are preferred because ignition should be initiated by a spark instead of through autoignition; this phenomena is called knock, or uncontrolled spontaneous combustion ahead of the flame [1]. Gasoline, which is used in spark-ignition engines, is characterized by an octane rating—a combination of the research and motor octane numbers—which indicates the antiknock properties, or resistance to knock.

Ignition delay is primarily determined through shock tube or rapid compression machine experiments. Shock tube experiments involve rupturing a membrane in a tube that separates high-pressure inert gas and the low-pressure fuel-oxygen mixture. A shock wave rapidly compresses the mixture, increasing the temperature and pressure, which then leads to autoignition after a certain period of time: the ignition delay. In rapid compression machine experiments, a piston compresses a fuel-oxidizer mixture, quickly raising the temperature and pressure and resulting in ignition after a time period: the ignition delay. Chemical kinetics of the fuel and oxidizer ultimately determine the ignition behavior in these fundamental combustion experiments. Modeling the chemical kinetics becomes increasingly more complicated with more components in the mixture. Gasoline, jet fuel, and diesel can have thousands of intermediate species and reactions, which makes ignition delay extremely difficult to computationally model. In addition, the composition of these fuels may vary from batch to batch. For these reasons, surrogate models with a few representative components are used to predict the global properties of transportation fuels such as the ignition delay.

Transportation fuels contain many different classes of hydrocarbons such as alkanes, cycloalkanes, and aromatics. Gasoline surrogate models commonly include the primary reference fuels (PRFs)—n-heptane and isooctane— to represent alkanes without additional components. Using PRFs allows surrogates to have similar autoignition resistance as the fuels they represent by adjusting the n-heptane and isooctane ratio,

which determines the octane rating values: research octane number (RON) and motor octane number (MON) [1, 2]. *n*-Heptane has a defined octane number of zero and isooctane has a defined octane number of 100. Additionally, it is important to account for aromatic compounds, because practical fuels can contain up to 50% aromatic hydrocarbons [1]. The addition of toluene can represent the aromatic hydrocarbons in these surrogates. Autoignition resistance, reflected in the octane rating, can be closely matched with that of a PRF mixture only at specified operating conditions. The real fuel sensitivity (RON − MON) cannot be replicated with the two PRF components alone since PRFs have zero octane sensitivity by definition. Other components must be added to reflect the real fuel sensitivity since RON and MON do not account for reaction kinetics. Toluene reference fuels (TRFs) have a sensitivity similar to gasoline for the same RON, so the surrogate will have a comparable octane rating for a larger range of operating conditions [2, 3]. Toluene is the most common aromatic component in practical fuels, with mole compositions as high as 35%, so toluene can serve as the aromatic representative in a surrogate fuel mixture [4]. Therefore, including both alkane and aromatic representatives in surrogate fuels offers more accuracy than the PRFs alone for computationally modeling computational engines and other combustion devices.

One major challenge in creating chemical kinetic models is determining elementary reaction rates. Intermediate reaction rates are difficult to standardize due to the complex nature of combustion reactions and current data-collection technologies.

Reaction rates are presently based on experimental data, reaction rate estimations, quantum chemical theory calculations, and/or transition state theory estimations [5–7]. Rates determined from these various methods can vary by significant factors. Models are typically manually validated against experimental data from several oxidation experiments, then followed by a "brute force" sensitivity analysis to identify candidates for model updates [7–9]. Model development methods have improved in the combustion community and are moving towards detailing the kinetics of more-complex hydrocarbon mixtures.

Although several models have been published for the same fuels, few performance studies quantify and validate multiple models against a large share of published data describing ignition delay. Exceptions include Olm et al. [10, 11], who comprehensively evaluated many hydrogen and syngas (i.e., synthesis gas, comprised mostly of hydrogen and carbon monoxide) models with data from various fundamental combustion experiments. The hydrogen study compared 19 models with 770 data points, while the syngas study compared 16 models with 732 data points [10, 11]. Niemeyer [12] described a preliminary study quantifying the performance of nine PRF and TRF models by applying the same methods to n-heptane models using shock tube and rapid compression machine data from 14 autoignition studies. Sirumalla et al. [13] employed similar tools for identifying the impact of discrepancies in thermochemical and rate parameters in one kinetic model for the butanol isomers. Many earlier studies do not compare several models together in this way or compile and use a

larger portion of published experimental data. For example, the chemical kinetics literature contains several detailed models for toluene oxidation in ranges of engine-relevant conditions [4, 7, 9, 14–16]; however, no study has comprehensively validated or compared the performance of these kinetic models. This observation motivates the current study.

This study aims to quantitatively evaluate a selection of published toluene kinetic models from the chemical kinetics literature. This evaluation method validates the performance of proposed models against available experimental data, using the standard ChemKED data format. A local sensitivity analysis was performed for engine-relevant conditions to reveal reactions that greatly influence ignition delay prediction. In addition, a sensitivity analysis of model performance was done to reveal intermediate reactions that significantly affect overall model performance. This study represents a next step in describing surrogate component autoignition behavior.

2 Methods

2.1 PyTeCK

I used the Python-based model validation tool PyTeCK [17] to automatically simulate experiments based on kinetic models and experimental conditions, and quantify the overall model performance using an error metric. PyTeCK performs Cantera-

based [18] simulations using the conditions of each experimental data set. Cantera is an open-source software library for solving problems with chemical kinetics, thermodynamics, and transport processes. It uses chemical kinetic theory in combination with reactor or flame models and solves ordinary differential equations to model specific systems with user-given inputs. PyTeCK uses the YAML-based standard data format ChemKED, which describes the experimental conditions and measurements. After performing simulations and analyzing their results, PyTeCK uses the performance metric of Olm et al. [10, 11] to evaluate the performance of the chemical kinetic models. The agreement between experimental and simulated ignition delay values is given by the average error E over N data sets:

$$E = \frac{1}{N} \sum_{i=1}^{N} E_i \ , \tag{1}$$

where E_i is the average error for the i$^{\text{th}}$ dataset:

$$E_i = \frac{1}{N_i} \sum_{j=1}^{N_i} \left(\frac{\log \tau_{ij}^{\text{exp}} - \log \tau_{ij}^{\text{sim}}}{\sigma\big(\log \tau_{ij}^{\text{exp}}\big)} \right)^2 , \tag{2}$$

N_i is the number of data points in set i, τ_{ij}^{exp} and τ_{ij}^{sim} are the experimental and simulated ignition delay times for the j^{th} data point in set i, and σ is the standard deviation. The log function represents the natural logarithm. Scatter in experimental results is proportional to the ignition delay, so the logarithm of ignition delay is used in the calculation, as suggested by Olm et al. [10, 11].

The approach to calculating standard deviation of a data set, $\sigma\left(\log \tau_{ij}^{\text{exp}}\right)$, follows that of Olm et al [10, 11]. PyTeCK fits a spline to the experimental ignition delay values with respect to the changing variable (usually temperature) using the `SciPy` function `interpolation.UnivariateSpline`. A minimum standard deviation of $\sigma = 0.10$ is used. Relative and absolute uncertainties for temperature, pressure, and ignition delay were included in the ChemKED files if they were provided in the study, though these are not currently used in the calculation of standard deviation or to track overall uncertainty. PyTeCK uses three primary modules to generate the model error: `parse_files`, `simulation`, and `eval_model`. `parse_files` has functions that read the ChemKED data using `PyYAML`. `simulation` contains a class that initializes shock tube and rapid compression machine governing equations, runs simulations, and processes the results to obtain ignition delay using the `detect_peaks` module version 1.0.5 by Duarte [19]. `eval_model` uses the other two modules to set up and run the simulations that run in parallel using the `multiprocessing` module. More details about PyTeCK can be found in the article by Niemeyer [17], and the software is available openly [20].

2.2 ChemKED standard

ChemKED (**Chem**ical **K**inetics **E**xperimental **D**ata), developed by Weber and Niemeyer [21], is a human- and machine-readible, YAML-based file format for describing fundamental combustion measurements with sufficient information to simulate experi-

mental data points. A ChemKED file contains information about the file author, study authors, experimental apparatus, and experimental data points in a key-value format. Each shock tube data point includes an initial temperature, initial pressure, fuel mixture composition, equivalence ratio, ignition type, and ignition delay. Often, the composition and ignition type is the same for several datapoints, so these and other properties may be specified in a `common-properties` section, which can be referenced within individual datapoints for simplicity and convenience. Units for each quantity are also specified for each quantity. Relative and absolute uncertainties can also be specified in initial conditions within datapoints, but these values are not currently taken into account in the model performance calculation. All ChemKED files created and used in this study can be found on the Prometheus database on Github [22]. Below is a ChemKED file from a shock tube study from Davidson et al. [8].

```
---
file-authors:
  - name: Morgan Mayer
    ORCID: 0000-0001-7137-5721
file-version: 0
chemked-version: 0.4.1
reference:
  doi: 10.1016/j.proci.2004.08.004
  authors:
    - name: D.F. Davidson
    - name: B.M. Gauthier
    - name: R.K. Hanson
  journal: Proceedings of the Combustion Institute
  year: 2005
  volume: 30
  pages: 1175-1182
  detail: Davidson_2005_toluene_phi0.5_15atm
experiment-type: ignition delay
apparatus:
  kind: shock tube
```

```
  institution: Stanford University
  facility: stainless steel shock tube
common-properties:
  composition: &comp
    kind: mole fraction
    species:
      - species-name: toluene
        InChI: 1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3
        amount:
          - 0.01154
      - species-name: O2
        InChI: 1S/O2/c1-2
        amount:
          - 0.20766
      - species-name: N2
        InChI: 1S/N2/c1-2
        amount:
          - 0.78080
  ignition-type: &ign
    target: OH*
    type: d/dt max extrapolated
datapoints:
  - temperature:
      - 1112.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.018
    ignition-delay:
      - 1250.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 15.3 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.5
  - temperature:
      - 1125.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.018
    ignition-delay:
      - 1454.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 13.1 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.5
  - temperature:
      - 1206.0 kelvin
      - uncertainty-type: relative
```

```
      uncertainty: 0.018
  ignition-delay:
    - 598.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 14.1 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.5
- temperature:
    - 1269.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.018
  ignition-delay:
    - 279.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 14.4 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.5
...
```

3 Models

Table 1 includes the detailed chemical kinetic models for toluene used in this study. Eleven models [4, 7, 9, 14–16, 23–31] are evaluated and compared against experimental data. These models are a selection of common models that were openly published or obtained from the author. Models were converted to a Cantera [18] format from the original Chemkin model file. Models were selected for this study based on availability of the experimental data from the literature or from author correspondence.

The detailed chemical kinetic model from Sivaramakrishnan et al. [4] in 2005 predicts the oxidation of toluene in the temperatures between 1200–1500 K over a pres-

Table 1: Summary of the detailed chemical kinetic models used for this study. "Coverage" describes the range of fuels included in the model. "Ar/He" describes if the model includes interactions with the inert gases argon or helium in the model in addition to nitrogen. The Dalian-2013 model was supplemented with argon data from the Princeton-2015 model.

Model	Coverage	# Species	# Reactions	Ar/He	Ref.
Sivaramakrishnan-2005	Toluene	98	538	✓/–	[4]
USCMechII-2007	C_0–C_4 + toluene	111	784	✓/✓	[23]
CNRS-2009	TRF + NO_x	536	3000	✓/✓	[14]
Sakai-2009	TRF	783	2883	✓/✓	[15]
Princeton-2011	Toluene	329	1888	✓/✓	[9]
LLNL-2012	TRF + 1-hexene	1550	8000	✓/✓	[16]
Andrae-2013	TRF	138	641	✓/–	[7]
Dalian-2013	TRF	57	191	✓/–	[24]
Tsinghua-2014	TRF + ethanol	91	411	✓/–	[25]
CRECK-2014	TRF + ethanol	317	12353	✓/✓	[26]
CaltechMech-2015	C_0–C_4 + TRF	174	1156	✓/–	[27]

sure range 25–610 bar. The model was made based on experimental data obtained in the high pressure shock tube experiments at the University of Illinois at Chicago [32]. Sivaramakrishnan et al. [4] used a toluene oxidation model developed by Dagaut et al [33] that was originally created with experimental shock tube data from toluene jet-stirred reactor experiments at 1 atm in a temperature range of 1000–1375 K.

The USCMechII-2007 by Wang et al. [23] was specifically updated for H_2, CO, and C_1–C_4 chemistry in 2007. They also updated several rate parameters for C_1 and C_4 chemistry. The model was validated against several H_2, CO, and C_1–C_4 experimental combustion studies.

Anderlohr et al. [14] proposed the CNRS-2009 detailed chemical kinetic model for PRF and toluene oxidation, which combines the PRF autoignition model from Buda

et al. [34] and the toluene oxidation model from Bounaceur et al. [35]. Additionally, reactions with NO_x are included. The model includes the interactions of NO_x on hydrocarbon oxidation, and was validated against HCCI and perfectly stirred reactor experiments for neat fuels and fuel blends [14].

The model published by Sakai et al. [15] in 2009 includes low temperature toluene kinetics at engine conditions. The starting model was by Pitz et al. [36], and rate coefficients for low temperature toluene and benzyl reactions were modified based on theoretical estimations. The model was validated against existing shock tube and flow tube data. The toluene submechanism was merged into the PRF model by Ogura et al. [37], and cross reactions between PRFs and toluene were added.

Metcalfe et al. [9] built upon their previous unpublished works to make a PRF and toluene oxidation model, which here is termed the Princeton-2011 model. The Princeton-2011 model [9] has been validated over a wide range of experimental conditions, including flow reactor, shock tube, jet-stirred reactor, and flame experiments. Rate constants were updated after new quantum chemical rate constant studies [6, 38]. The work on their toluene submechanism is based on the work of Bounaceur et al. [35].

For the LLNL-2012 model, Mehl et al. [16, 39] updated a previous LLNL mechanism to predict ignition times for PRFs, 1-hexene, toluene, and their mixtures in a rapid compression machine and jet stirred reactor. The cyclopentadiene mechanism was revised for the toluene mechanism, and was validated against the work of Butler

et al. [40].

Andrae [7] updated the reaction parameters for neat toluene and its mixtures in the previous semidetailed model for gasoline surrogate fuels including TRFs [41]. Updates to the previous toluene submechanism [41] were based on quantum kinetic calculations by Murakami et al. [38] and individual rates from the literature. The simulations from the updated and the less detailed model shows better agreement than the previous detailed model.

The Dalian-2013 model was developed by Liu et al. [24] by combining a previous skeletal PRF model with a reduced model for toluene. Ignition chemistry was described using a semi-decoupling method that reduces large molecule mechanisms while leaving the small hydrocarbon mechanisms in its previous form. Liu et al. [24] modified toluene pathways from the models of Andrae et al. [41], Mehl et al. [42], and Sakai et al. [15] based on shock-tube ignition delays and jet-stirred reactor species profiles. For this model comparison, the Dalian-2013 model was supplemented with argon data from the Princeton-2015 model.

Zhong and Zheng [25] developed the five-component Tsinghua-2014 model by combining their earlier three-component model with reduced models to predict ignition behavior of the PRFs, ethanol, toluene, and diisobutadiene. The toluene submechanism in the current five-component model was revised from Andrae et al. [41]. Low-temperature oxidation pathways came from Tanaka et al. [43].

The CRECK-2014 model version 1412 [26, 44, 45] combines ethanol pathways with a prior model for hydrocarbon oxidation [44]. The model includes chemistry for PRFs, alcohols, and ethers. The CaltechMech-2015 model [27–31] currently contains 174 species and 1156 reactions in version 2.3. It takes into account all major pathways of PAH formation.

4 Experimental data

Ignition delay data was used from a selection of published shock tube studies. The data was taken directly from publications or from direct communication with the authors. Each data set was arranged in the YAML-based ChemKED format. A total of 175 datapoints were used which were incorporated into 21 datasets, or ChemKED files.

Table 2: Summary of the experimental conditions for toluene oxidation, where $\chi_{O_2}(\%)$ is the mole percent of oxygen gas as reactant.

Study	P (atm)	T (K)	ϕ	$\chi_{O_2}(\%)$	No. points
Burcat et al. [46]	1.95–8.85	1339–1797	0.331–1.0	4.5–13.5	54
Davidson et al. [8]	14–59	855–1269	0.5, 1.0	20.5	25
Vasudevan et al. [47]	1.5–5.0	1400–2000	0.5–1.875	0.2–4.5	24
Shen et al. [5]	10–61	1021–1400	0.25, 0.5, 1.0	20.5	58
Hartmann et al. [48]	39.5	700–1200	0.5, 1.0	20.5	14

5 Results and discussion

5.1 Simulations

Cantera [18] performed all simulations, driven by PyTeCK [17, 20]. The experimental conditions for each shock-tube simulation include the reflected shock temperature and pressure, in addition to the initial reactant compositions. Shock tube simulations in this study were modeled using the assumption of adiabatic constant-volume conditions based on the reflected shock temperature and pressure, and initial reactant composition [17]. Cases with longer ignition delay times above 1 ms can exhibit polytropic pressure increases prior to ignition, but this is not accounted for here since none of the sampled studies provided the necessary pressure-history information or a pressure-rise rate [49, 50]. Neglecting this could result in greater predicted ignition delay values [51]. The experimental conditions for rapid compression machine experiments include initial temperature, initial pressure, initial reactant composition, and a volume history (to model compression as well as post-compression heat loss through isentropic volume expansion).

5.2 Model performance

This section compares the performance of the eleven kinetic models listed in Table 1 using the experimental data described in Table 2. I standardized a total of 175 data points spread across 21 datasets. Davidson et al. [8] and Shen et al. [5] defined

ignition delay as the extrapolated maximum derivative of OH^* radical concentration. Hartmann et al. [48] defined ignition delay as the maximum derivative of CH^* radical concentration. Vasudevan et al. [47] specified ignition delay as the time of half the maximum OH concentration.

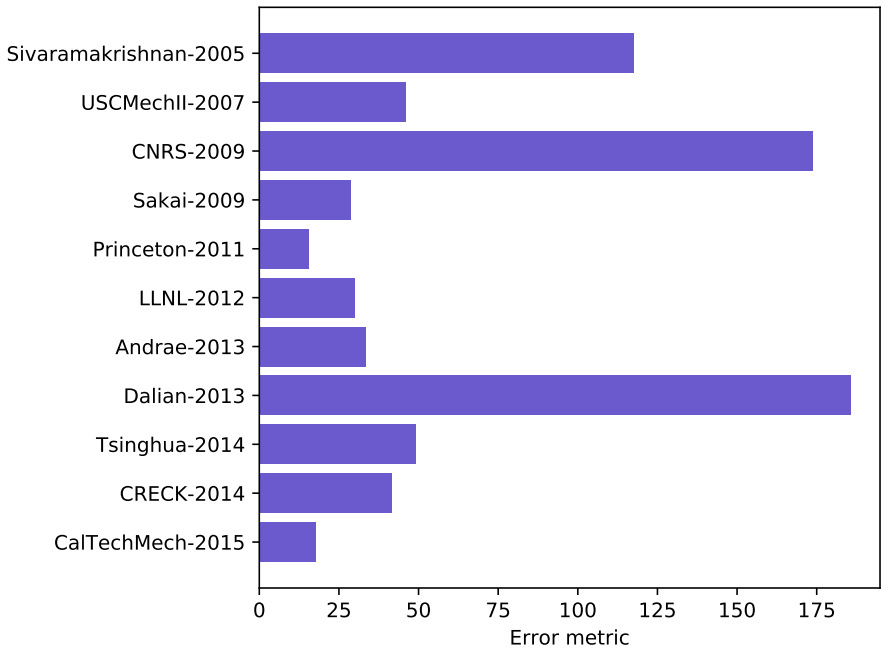

Figure 1: Mean error function for the chemical kinetic models in toluene oxidation simulations of ignition delay times, with error bars indicating the standard deviation among the datasets. Errors were sampled using 175 data points grouped into 21 datasets. Lower values indicate better agreement between a model and the experimental data.

Figure 1 describes the performance of the models in predicting ignition delay in toluene oxidation based on experimental data. From the models included in this study, the Princeton-2011 model best-predicts ignition delay based on the experimental data included in this study, with the lowest error function value of 15.5, closely followed by the CaltechMech model which had an error metric of 17.8. The Dalian-2013 model

performed the worst of the model set with an error function value of 185.6. The CNRS-2009 model performed similarly with an error function value of 173.8.

5.3 Ignition delay sensitivity analysis

A local sensitivity analysis of the model reactions on ignition delay was performed for the CalTechMech model. This model was chosen because it had a relatively low error metric and handled pressure dependencies simply (compared with the Princeton-2011 model, which requires manually changing reactions for different pressure ranges and bath gases). The CalTechMech model contains three types of reactions: standard Arrhenius reactions, third-body reactions, and fall-off reactions. For fall-off reactions, the pre-exponential factors of both the high- and low-pressure limits (e.g., k_f and k_{f0}) were doubled for that respective perturbed model. For each reaction in the CalTechMech model, a new model was created with that reaction's preexponential factor doubled. Likewise, additional perturbed models with the preexponential factor halved were also created in this way. Sensitivity was calculated using the simulated ignition delay values generated via PyTeCK from these perturbed models. Local sensitivity of the reaction was calculated with Equation 3:

$$S_i = 100\,\% \times \frac{\ln\left(\tau(2k_i)/\tau(0.5k_i)\right)}{\ln(2/0.5)}\,, \tag{3}$$

where $\tau(2k)$ is the simulated ignition delay from the model with the rate of reaction i doubled, and $\tau(0.5k)$ is the simulated ignition delay from the model with the rate

of reaction i is halved. Figure 2 shows local sensitivity results for a low pressure and high temperature condition. The simulated ignition delay at these conditions are most sensitive to the $H + O_2$ reaction, which is the notably one of the most important chain branching reactions in combustion because its components greatly influence many subsequent reactions. Figure 3 shows the local sensitivity results for an engine-relevant case: low temperature and high pressure. There are more reactions that have a sensitivity greater than % for the engine-relevant conditions because generally there are more complicated reaction mechanisms at lower temperatures.

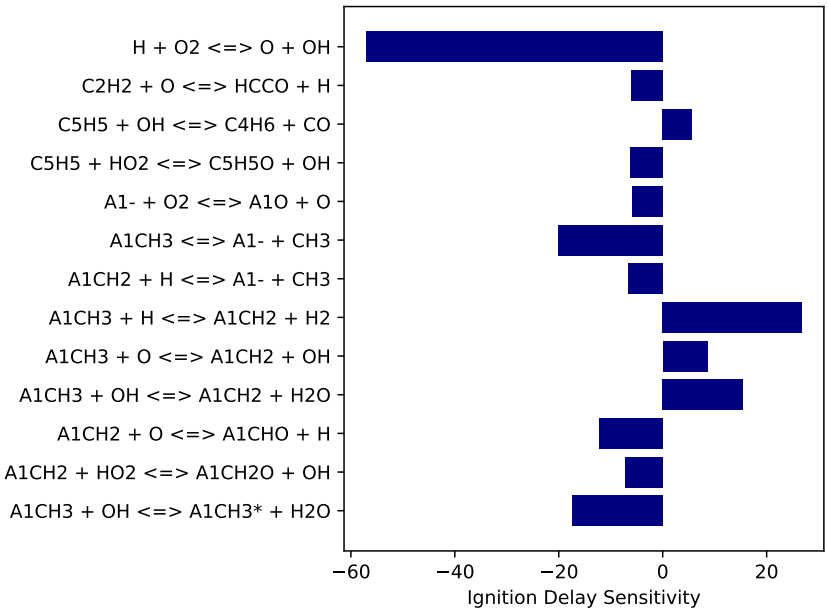

Figure 2: Ignition delay sensitivity of reactions in CalTechMech model at engine-relevant conditions: 1748 K, 3.7 bar, $\phi = 1.0$, $\chi_{O_2} = 0.1345$. Reactions with a sensitivity greater than 5% shown.

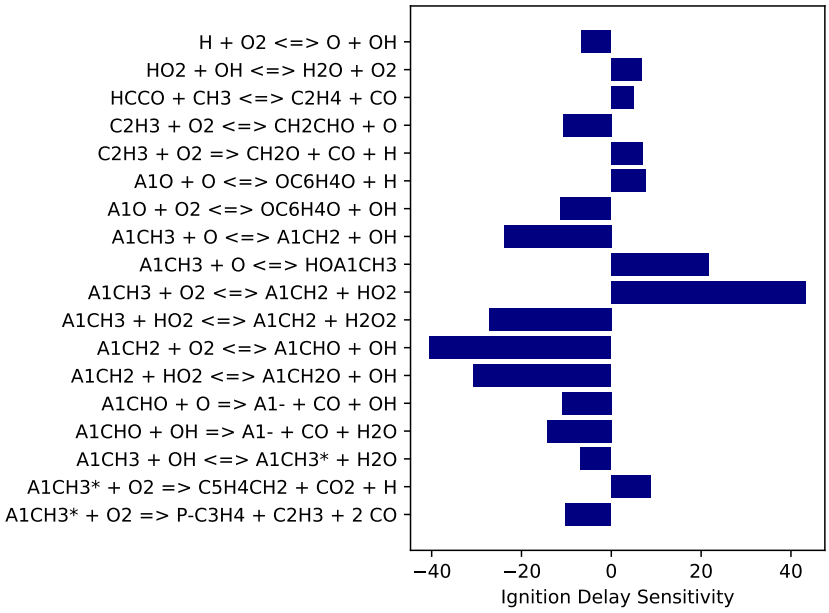

Figure 3: Ignition delay sensitivity of reactions in CalTechMech model at 942 K, 40.4 bar, $\phi = 0.5$, $\chi_{O_2} = 0.208$. Reactions with a sensitivity greater than 5% shown.

5.4 Performance sensitivity analysis

A performance sensitivity analysis was done for the CalTechMech model which compares the overall model performance metric with that for the model with an individual rate constant doubled. Individual rate constants were independently doubled in a perturbed CalTechMech model. All 1156 generated model variants were validated using PyTeCK against experimental data. To rank the sensitivity of a model to its performance in predicting experimental ignition delay, a new metric is defined: the "performance sensitivity", which represents the percentage change in model error (with respect to experimental data) due to doubling the rate of reaction i, calculated

using

$$P_i = 100\,\% \;\times\; \left[E\left(2k_i\right) - E\left(k_i\right)\right] / E(k_i)\;, \tag{4}$$

where E is the average error associated with a model based on PyTeCK simulations.

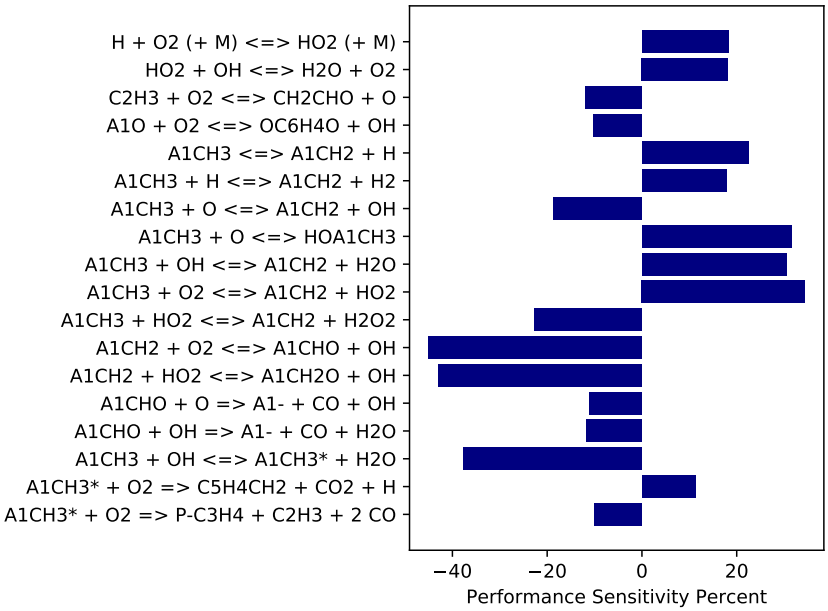

Figure 4: Performance sensitivity percent for the CaltechMech-2015 [27–31] model reactions. Model performance error was validated with 175 data points grouped into 21 datasets. Models were perturbed for the sensitivity analysis by doubling the reaction rate.

Figure 4 shows the performance sensitivities of the most-sensitive reactions (i.e., above 10%). However, many of the high-sensitivity reactions are fuel-specific ("A1CH3" represents toluene in the CalTechMech model), so the analysis identifies reactions that may require further attention to improve toluene model performance.

6 Conclusions

This study compared the performance of kinetic models in predicting autoignition delay for toluene using a set of ignition measurements from shock tube experiments. A performance sensitivity analysis was also done for a high-performing model to reveal key reactions that affect model performance compared with experimental data. The Princeton-2011 model performs best, with CaltechMech close behind, and the Dalian-2013 model performs worst for the experimental data considered. Eight of the eleven models considered perform similarly, with error metrics in the range of 15 to 50, while the Dalian-2013 model exhibits an overall error metric almost five times larger than the average of the other models. Influential reactions to model performance were revealed for the high-performing model CaltechMech-2015. In addition to quantifying the ability of the models to predict ignition delay, a useful data set from shock tube experiments were collected and standardized for such mixtures. The ChemKED files used for validation are included in the the Appendix, Section 7. These data files and the supporting software are shared openly via the Prometheus project (https://github.com/pr-omethe-us) to support continuing model evaluation and improvement. The next steps for this project include collecting more available models for toluene oxidation, and standardizing a more diverse set of autoignition data.

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7 Appendix

7.1 Burcat ChemKED files

The following ChemKED files were created based on the experimental data provided by Burcat et al. [46].

`Burcat_1986_mixA.yaml`

```
---
file-authors:
  - name: Morgan Mayer
    ORCID: 0000-0001-7137-5721
file-version: 0
chemked-version: 0.4.1
reference:
  authors:
    - name: Alexander Burcat
    - name: Christopher Snyder
    - name: Theodore Brabbs
  journal: NASA Technical Memorandum
  year: 1986
  detail: Burcat_mixA, https://ntrs.nasa.gov/search.jsp?R=19860015959
experiment-type: ignition delay
apparatus:
  kind: shock tube
  institution: NASA Lewis Research Center; Cleveland, OH
  facility: stainless steel shock tube
common-properties:
  composition: &comp
    kind: mole fraction
    species:
      - species-name: toluene
        InChI: 1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3
        amount:
          - 0.01495
      - species-name: O2
        InChI: 1S/O2/c1-2
        amount:
          - 0.1345
      - species-name: Ar
        InChI: 1S/Ar
        amount:
          - 0.85055
  ignition-type: &ign
    target: pressure
```

```
    type: d/dt max
datapoints:
  - temperature:
      - 1429.0 kelvin
    ignition-delay:
      - 356.0 us
      - uncertainty-type: absolute
        uncertainty: 0.1 us
    pressure:
      - 2.54 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 1368.0 kelvin
    ignition-delay:
      - 975.0 us
      - uncertainty-type: absolute
        uncertainty: 0.1 us
    pressure:
      - 2.36 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 1358.0 kelvin
    ignition-delay:
      - 1030.0 us
      - uncertainty-type: absolute
        uncertainty: 0.1 us
    pressure:
      - 2.33 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 1447.0 kelvin
    ignition-delay:
      - 328.0 us
      - uncertainty-type: absolute
        uncertainty: 0.1 us
    pressure:
      - 2.6 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 1489.0 kelvin
    ignition-delay:
      - 185.0 us
      - uncertainty-type: absolute
```

```
      uncertainty: 0.1 us
  pressure:
    - 2.73 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1540.0 kelvin
  ignition-delay:
    - 100.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 2.89 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1574.0 kelvin
  ignition-delay:
    - 62.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 3.0 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1629.0 kelvin
  ignition-delay:
    - 42.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 3.18 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1552.0 kelvin
  ignition-delay:
    - 80.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 2.94 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
```

```
      - 1651.0 kelvin
    ignition-delay:
      - 29.0 us
      - uncertainty-type: absolute
        uncertainty: 0.1 us
    pressure:
      - 3.26 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 1758.0 kelvin
    ignition-delay:
      - 8.0 us
      - uncertainty-type: absolute
        uncertainty: 0.1 us
    pressure:
      - 3.61 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 1394.0 kelvin
    ignition-delay:
      - 596.0 us
      - uncertainty-type: absolute
        uncertainty: 0.1 us
    pressure:
      - 2.44 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
...
```

Burcat_1986_mixB.yaml

```
---
file-authors:
  - name: Morgan Mayer
    ORCID: 0000-0001-7137-5721
file-version: 0
chemked-version: 0.4.1
reference:
  authors:
    - name: Alexander Burcat
    - name: Christopher Snyder
    - name: Theodore Brabbs
  journal: NASA Technical Memorandum
  year: 1986
```

```
  detail: Burcat_mixB, https://ntrs.nasa.gov/search.jsp?R=19860015959
experiment-type: ignition delay
apparatus:
  kind: shock tube
  institution: NASA Lewis Research Center; Cleveland, OH
  facility: stainless steel shock tube
common-properties:
  composition: &comp
    kind: mole fraction
    species:
      - species-name: toluene
        InChI: 1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3
        amount:
          - 0.00497
      - species-name: O2
        InChI: 1S/O2/c1-2
        amount:
          - 0.1351
      - species-name: Ar
        InChI: 1S/Ar
        amount:
          - 0.85993
  ignition-type: &ign
    target: pressure
    type: d/dt max
datapoints:
  - temperature:
      - 1509.0 kelvin
    ignition-delay:
      - 73.0 us
      - uncertainty-type: absolute
        uncertainty: 0.1 us
    pressure:
      - 2.37 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.331
  - temperature:
      - 1448.0 kelvin
    ignition-delay:
      - 124.0 us
      - uncertainty-type: absolute
        uncertainty: 0.1 us
    pressure:
      - 2.32 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.331
  - temperature:
      - 1437.0 kelvin
    ignition-delay:
```

```
    - 186.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 2.18 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.331
- temperature:
    - 1363.0 kelvin
  ignition-delay:
    - 556.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 1.99 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.331
- temperature:
    - 1339.0 kelvin
  ignition-delay:
    - 847.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 1.93 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.331
- temperature:
    - 1424.0 kelvin
  ignition-delay:
    - 221.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 2.15 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.331
- temperature:
    - 1358.0 kelvin
  ignition-delay:
    - 657.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 1.98 atm
  composition: *comp
  ignition-type: *ign
```

```
  equivalence-ratio: 0.331
- temperature:
    - 1501.0 kelvin
  ignition-delay:
    - 95.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 2.34 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.331
- temperature:
    - 1642.0 kelvin
  ignition-delay:
    - 20.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 2.74 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.331
- temperature:
    - 1615.0 kelvin
  ignition-delay:
    - 27.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 2.64 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.331
- temperature:
    - 1582.0 kelvin
  ignition-delay:
    - 40.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 2.55 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.331
- temperature:
    - 1572.0 kelvin
  ignition-delay:
    - 42.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
```

```
    pressure:
      - 2.53 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.331
  - temperature:
      - 1443.0 kelvin
    ignition-delay:
      - 183.0 us
      - uncertainty-type: absolute
        uncertainty: 0.1 us
    pressure:
      - 2.2 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.331
  - temperature:
      - 1412.0 kelvin
    ignition-delay:
      - 287.0 us
      - uncertainty-type: absolute
        uncertainty: 0.1 us
    pressure:
      - 2.12 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.331
  - temperature:
      - 1391.0 kelvin
    ignition-delay:
      - 388.0 us
      - uncertainty-type: absolute
        uncertainty: 0.1 us
    pressure:
      - 2.06 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.331
...
```

Burcat_1986_mixC.yaml

```
---
file-authors:
  - name: Morgan Mayer
    ORCID: 0000-0001-7137-5721
file-version: 0
chemked-version: 0.4.1
reference:
```

```yaml
  authors:
    - name: Alexander Burcat
    - name: Christopher Snyder
    - name: Theodore Brabbs
  journal: NASA Technical Memorandum
  year: 1986
  detail: Burcat_mixC, https://ntrs.nasa.gov/search.jsp?R=19860015959
experiment-type: ignition delay
apparatus:
  kind: shock tube
  institution: NASA Lewis Research Center; Cleveland, OH
  facility: stainless steel shock tube
common-properties:
  composition: &comp
    kind: mole fraction
    species:
      - species-name: toluene
        InChI: 1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3
        amount:
          - 0.00497
      - species-name: O2
        InChI: 1S/O2/c1-2
        amount:
          - 0.0448
      - species-name: Ar
        InChI: 1S/Ar
        amount:
          - 0.95023
  ignition-type: &ign
    target: pressure
    type: d/dt max
datapoints:
  - temperature:
      - 1423.0 kelvin
    ignition-delay:
      - 563.0 us
      - uncertainty-type: absolute
        uncertainty: 0.1 us
    pressure:
      - 5.82 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 1387.0 kelvin
    ignition-delay:
      - 741.0 us
      - uncertainty-type: absolute
        uncertainty: 0.1 us
    pressure:
      - 5.58 atm
```

```
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1439.0 kelvin
  ignition-delay:
    - 490.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 5.93 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1481.0 kelvin
  ignition-delay:
    - 330.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 6.22 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1521.0 kelvin
  ignition-delay:
    - 237.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 6.51 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1545.0 kelvin
  ignition-delay:
    - 175.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 6.65 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1597.0 kelvin
  ignition-delay:
    - 96.0 us
```

```
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 7.01 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1660.0 kelvin
  ignition-delay:
    - 42.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 7.45 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1663.0 kelvin
  ignition-delay:
    - 39.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 7.5 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1700.0 kelvin
  ignition-delay:
    - 26.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 7.74 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1765.0 kelvin
  ignition-delay:
    - 16.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 8.2 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
```

```
  - temperature:
      - 1630.0 kelvin
    ignition-delay:
      - 1629.0 us
      - uncertainty-type: absolute
        uncertainty: 0.1 us
    pressure:
      - 7.24 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 1602.0 kelvin
    ignition-delay:
      - 63.0 us
      - uncertainty-type: absolute
        uncertainty: 0.1 us
    pressure:
      - 7.04 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 1524.0 kelvin
    ignition-delay:
      - 208.0 us
      - uncertainty-type: absolute
        uncertainty: 0.1 us
    pressure:
      - 6.51 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
...
```

Burcat_1986_mixD.yaml

```
---
file-authors:
  - name: Morgan Mayer
    ORCID: 0000-0001-7137-5721
file-version: 0
chemked-version: 0.4.1
reference:
  authors:
    - name: Alexander Burcat
    - name: Christopher Snyder
    - name: Theodore Brabbs
  journal: NASA Technical Memorandum
```

```
  year: 1986
  detail: Burcat1986_mixD, https://ntrs.nasa.gov/search.jsp?R=19860015959
experiment-type: ignition delay
apparatus:
  kind: shock tube
  institution: NASA Lewis Research Center; Cleveland, OH
  facility: stainless steel shock tube
common-properties:
  composition: &comp
    kind: mole fraction
    species:
      - species-name: toluene
        InChI: 1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3
        amount:
          - 0.00497
      - species-name: O2
        InChI: 1S/O2/c1-2
        amount:
          - 0.0448
      - species-name: Ar
        InChI: 1S/Ar
        amount:
          - 0.95023
  ignition-type: &ign
    target: pressure
    type: d/dt max
datapoints:
  - temperature:
      - 1797.0 kelvin
    ignition-delay:
      - 19.0 us
      - uncertainty-type: absolute
        uncertainty: 0.1 us
    pressure:
      - 2.81 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 1566.0 kelvin
    ignition-delay:
      - 207.0 us
      - uncertainty-type: absolute
        uncertainty: 0.1 us
    pressure:
      - 2.27 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 1501.0 kelvin
```

```
  ignition-delay:
    - 452.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 2.12 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1441.0 kelvin
  ignition-delay:
    - 1104.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 1.98 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1446.0 kelvin
  ignition-delay:
    - 990.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 1.99 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1509.0 kelvin
  ignition-delay:
    - 452.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 2.14 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1618.0 kelvin
  ignition-delay:
    - 101.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 2.39 atm
  composition: *comp
```

```
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1646.0 kelvin
  ignition-delay:
    - 85.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 2.45 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1669.0 kelvin
  ignition-delay:
    - 63.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 2.51 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1736.0 kelvin
  ignition-delay:
    - 33.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 2.66 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1524.0 kelvin
  ignition-delay:
    - 335.0 us
    - uncertainty-type: absolute
      uncertainty: 0.1 us
  pressure:
    - 2.17 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1430.0 kelvin
  ignition-delay:
    - 1311.0 us
    - uncertainty-type: absolute
```

```
      uncertainty: 0.1 us
    pressure:
      - 1.96 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 1509.0 kelvin
    ignition-delay:
      - 370.0 us
      - uncertainty-type: absolute
        uncertainty: 0.1 us
    pressure:
      - 2.14 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
...
```

7.2 Davidson ChemKED files

The following ChemKED files were created based on the experimental data provided by Davidson et al. [8].

`Davidson_2005_toluene_phi0.5_15atm.yaml`

```yaml
---
file-authors:
  - name: Morgan Mayer
    ORCID: 0000-0001-7137-5721
file-version: 0
chemked-version: 0.4.1
reference:
  doi: 10.1016/j.proci.2004.08.004
  authors:
    - name: D.F. Davidson
    - name: B.M. Gauthier
    - name: R.K. Hanson
  journal: Proceedings of the Combustion Institute
  year: 2005
  volume: 30
  pages: 1175-1182
  detail: Davidson_2005_toluene_phi0.5_15atm
experiment-type: ignition delay
apparatus:
  kind: shock tube
  institution: Stanford University
  facility: stainless steel shock tube
common-properties:
  composition: &comp
    kind: mole fraction
    species:
      - species-name: toluene
        InChI: 1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3
        amount:
          - 0.01154
      - species-name: O2
        InChI: 1S/O2/c1-2
        amount:
          - 0.20766
      - species-name: N2
        InChI: 1S/N2/c1-2
        amount:
          - 0.78080
  ignition-type: &ign
    target: OH*
    type: d/dt max extrapolated
```

```
datapoints:
  - temperature:
      - 1112.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.018
    ignition-delay:
      - 1250.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 15.3 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.5
  - temperature:
      - 1125.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.018
    ignition-delay:
      - 1454.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 13.1 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.5
  - temperature:
      - 1206.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.018
    ignition-delay:
      - 598.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 14.1 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.5
  - temperature:
      - 1269.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.018
    ignition-delay:
      - 279.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 14.4 atm
    composition: *comp
```

```
    ignition-type: *ign
    equivalence-ratio: 0.5
...
```

Davidson_2005_toluene_phi0.5_50atm.yaml

```
---
file-authors:
  - name: Morgan Mayer
    ORCID: 0000-0001-7137-5721
file-version: 0
chemked-version: 0.4.1
reference:
  doi: 10.1016/j.proci.2004.08.004
  authors:
    - name: D.F. Davidson
    - name: B.M. Gauthier
    - name: R.K. Hanson
  journal: Proceedings of the Combustion Institute
  year: 2005
  volume: 30
  pages: 1175-1182
  detail: Davidson_2005_toluene_phi0.5_50atm
experiment-type: ignition delay
apparatus:
  kind: shock tube
  institution: Stanford University
  facility: stainless steel shock tube
common-properties:
  composition: &comp
    kind: mole fraction
    species:
      - species-name: toluene
        InChI: 1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3
        amount:
          - 0.01154
      - species-name: O2
        InChI: 1S/O2/c1-2
        amount:
          - 0.20766
      - species-name: N2
        InChI: 1S/N2/c1-2
        amount:
          - 0.78080
  ignition-type: &ign
    target: OH*
    type: d/dt max extrapolated
datapoints:
  - temperature:
```

```
    - 1091.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.018
  ignition-delay:
    - 1186.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 50.5 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.5
- temperature:
    - 1135.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.018
  ignition-delay:
    - 669.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 46.5 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.5
- temperature:
    - 1149.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.018
  ignition-delay:
    - 579.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 44.4 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.5
- temperature:
    - 1211.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.018
  ignition-delay:
    - 250.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 44.4 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.5
```

...

Davidson_2005_toluene_phi1.0_15-20atm.yaml

```yaml
---
file-authors:
  - name: Morgan Mayer
    ORCID: 0000-0001-7137-5721
file-version: 0
chemked-version: 0.4.1
reference:
  doi: 10.1016/j.proci.2004.08.004
  authors:
    - name: D.F. Davidson
    - name: B.M. Gauthier
    - name: R.K. Hanson
  journal: Proceedings of the Combustion Institute
  year: 2005
  volume: 30
  pages: 1175-1182
  detail: Davidson_2005_toluene_phi1.0_15-20atm
experiment-type: ignition delay
apparatus:
  kind: shock tube
  institution: Stanford University
  facility: stainless steel shock tube
common-properties:
  composition: &comp
    kind: mole fraction
    species:
      - species-name: toluene
        InChI: 1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3
        amount:
          - 0.02281
      - species-name: O2
        InChI: 1S/O2/c1-2
        amount:
          - 0.20529
      - species-name: N2
        InChI: 1S/N2/c1-2
        amount:
          - 0.77190
  ignition-type: &ign
    target: OH*
    type: d/dt max extrapolated
datapoints:
  - temperature:
      - 971.0 kelvin
      - uncertainty-type: relative
```

```
      uncertainty: 0.018
  ignition-delay:
    - 1314.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 17.2 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 995.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.018
  ignition-delay:
    - 1100.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 16.5 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1053.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.018
  ignition-delay:
    - 1288.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 17.1 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1067.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.018
  ignition-delay:
    - 1646.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 16.1 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1076.0 kelvin
```

```
      - uncertainty-type: relative
        uncertainty: 0.018
    ignition-delay:
      - 1174.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 16.5 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 1097.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.018
    ignition-delay:
      - 1223.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 16.6 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 1138.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.018
    ignition-delay:
      - 716.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 22.2 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 1173.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.018
    ignition-delay:
      - 767.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 14.9 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
...
```

Davidson_2005_toluene_phi1.0_50atm.yaml

```yaml
---
file-authors:
  - name: Morgan Mayer
    ORCID: 0000-0001-7137-5721
file-version: 0
chemked-version: 0.4.1
reference:
  doi: 10.1016/j.proci.2004.08.004
  authors:
    - name: D.F. Davidson
    - name: B.M. Gauthier
    - name: R.K. Hanson
  journal: Proceedings of the Combustion Institute
  year: 2005
  volume: 30
  pages: 1175-1182
  detail: Davidson_2005_toluene_phi1.0_50atm
experiment-type: ignition delay
apparatus:
  kind: shock tube
  institution: Stanford University
  facility: stainless steel shock tube
common-properties:
  composition: &comp
    kind: mole fraction
    species:
      - species-name: toluene
        InChI: 1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3
        amount:
          - 0.02281
      - species-name: O2
        InChI: 1S/O2/c1-2
        amount:
          - 0.20529
      - species-name: N2
        InChI: 1S/N2/c1-2
        amount:
          - 0.77190
  ignition-type: &ign
    target: OH*
    type: d/dt max extrapolated
datapoints:
  - temperature:
      - 977.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.018
    ignition-delay:
      - 1173.0 us
      - uncertainty-type: relative
```

```
      uncertainty: 0.15
  pressure:
    - 54.3 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 990.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.018
  ignition-delay:
    - 952.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 50.5 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1005.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.018
  ignition-delay:
    - 870.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 50.4 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1068.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.018
  ignition-delay:
    - 605.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 48.0 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1111.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.018
  ignition-delay:
    - 397.0 us
```

```
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 46.7 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1166.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.018
  ignition-delay:
    - 276.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 44.6 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1179.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.018
  ignition-delay:
    - 273.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 41.5 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1183.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.018
  ignition-delay:
    - 191.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 46.2 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1242.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.018
  ignition-delay:
```

```
      - 121.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 42.4 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
...
```

7.3 Hartmann ChemKED files

The following ChemKED files were created based on the experimental data provided by Hartmann et al. [48].

`Hartmann_2009_phi0.5.yaml`

```
---
file-authors:
  - name: Morgan Mayer
    ORCID: 0000-0001-7137-5721
file-version: 0
chemked-version: 0.4.1
reference:
  doi: 10.1016/j.combustflame.2010.08.005
  authors:
    - name: M. Hartmann
    - name: I. Gushterova
    - name: M. Fikri
    - name: C. Schulz
    - name: R. Schießl
    - name: U. Maas
  journal: Combustion and Flame
  year: 2011
  volume: 158
  pages: 172-178
  detail: Hartmann-40bar-phi0.5
experiment-type: ignition delay
apparatus:
  kind: shock tube
  institution: Institute for Combustion and Gasdynamics, University of Duisburg-Essen
  facility: stainless steel shock tube
common-properties:
  composition: &comp
    kind: mole fraction
    species:
      - species-name: toluene
        InChI: 1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3
        amount:
          - 0.01154
      - species-name: O2
        InChI: 1S/O2/c1-2
        amount:
          - 0.20766
      - species-name: N2
        InChI: 1S/N2/c1-2
        amount:
          - 0.78080
```

```
  ignition-type: &ign
    target: CH*
    type: d/dt max
datapoints:
  - temperature:
      - 942.0 kelvin
    ignition-delay:
      - 8815.0 us
    pressure:
      - 40.4 bar
      - uncertainty-type: absolute
        uncertainty: 2 bar
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.5
  - temperature:
      - 967.0 kelvin
    ignition-delay:
      - 5144.0 us
    pressure:
      - 39.0 bar
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.5
  - temperature:
      - 1029.0 kelvin
    ignition-delay:
      - 1998.0 us
    pressure:
      - 40.5 bar
      - uncertainty-type: absolute
        uncertainty: 2 bar
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.5
  - temperature:
      - 1069.0 kelvin
    ignition-delay:
      - 1300.0 us
    pressure:
      - 39.9 bar
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.5
  - temperature:
      - 1115.0 kelvin
    ignition-delay:
      - 783.0 us
    pressure:
      - 39.6 bar
      - uncertainty-type: absolute
```

```
        uncertainty: 2 bar
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.5
  - temperature:
      - 1140.0 kelvin
    ignition-delay:
      - 545.0 us
    pressure:
      - 36.5 bar
      - uncertainty-type: absolute
        uncertainty: 2 bar
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.5
...
```

Hartmann_2009_phi1.0.yaml

```
---
file-authors:
  - name: Morgan Mayer
    ORCID: 0000-0001-7137-5721
file-version: 0
chemked-version: 0.4.1
reference:
  doi: 10.1016/j.combustflame.2010.08.005
  authors:
    - name: M. Hartmann
    - name: I. Gushterova
    - name: M. Fikri
    - name: C. Schulz
    - name: R. Schießl
    - name: U. Maas
  journal: Combustion and Flame
  year: 2011
  volume: 158
  pages: 172-178
  detail: Hartmann-40bar-phi1.0
experiment-type: ignition delay
apparatus:
  kind: shock tube
  institution: Institute for Combustion and Gasdynamics, University of Duisburg-Essen
  facility: stainless steel shock tube
common-properties:
  composition: &comp
    kind: mole fraction
    species:
      - species-name: toluene
```

```
        InChI: 1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3
        amount:
          - 0.02281
      - species-name: O2
        InChI: 1S/O2/c1-2
        amount:
          - 0.20529
      - species-name: N2
        InChI: 1S/N2/c1-2
        amount:
          - 0.77190
  ignition-type: &ign
    target: CH*
    type: d/dt max
datapoints:
  - temperature:
      - 859.0 kelvin
    ignition-delay:
      - 4911.0 us
    pressure:
      - 42.3 bar
      - uncertainty-type: absolute
        uncertainty: 2 bar
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 882.0 kelvin
    ignition-delay:
      - 3214.0 us
    pressure:
      - 41.6 bar
      - uncertainty-type: absolute
        uncertainty: 2 bar
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 911.0 kelvin
    ignition-delay:
      - 3375.0 us
    pressure:
      - 41.7 bar
      - uncertainty-type: absolute
        uncertainty: 2 bar
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 954.0 kelvin
    ignition-delay:
```

```
    - 2276.0 us
  pressure:
    - 43.4 bar
    - uncertainty-type: absolute
      uncertainty: 2 bar
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 996.0 kelvin
  ignition-delay:
    - 1529.0 us
  pressure:
    - 44.0 bar
    - uncertainty-type: absolute
      uncertainty: 2 bar
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1034.0 kelvin
  ignition-delay:
    - 1256.0 us
  pressure:
    - 42.9 bar
    - uncertainty-type: absolute
      uncertainty: 2 bar
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1100.0 kelvin
  ignition-delay:
    - 639.0 us
  pressure:
    - 40.2 bar
    - uncertainty-type: absolute
      uncertainty: 2 bar
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1149.0 kelvin
  ignition-delay:
    - 342.0 us
  pressure:
    - 39.0 bar
    - uncertainty-type: absolute
      uncertainty: 2 bar
  composition: *comp
  ignition-type: *ign
```

```
    equivalence-ratio: 1.0
...
```

7.4 Shen ChemKED files

The following ChemKED files are based on the experimental data provided by Shen et al. [5].

`Shen_2009_phi0.5_12atm.yaml`

```yaml
---
file-authors:
  - name: Morgan Mayer
    ORCID: 0000-0001-7137-5721
file-version: 0
chemked-version: 0.4.1
reference:
  doi: 10.1016/j.proci.2008.05.004
  authors:
    - name: Hsi-Ping S. Shen
    - name: Jeremy Vanderover
    - name: Matthew A. Oehlschlaeger
  journal: Proceedings of the Combustion Institute
  year: 2009
  volume: 32
  pages: 165-172
  detail: Shen_toluene_phi0.5_12atm
experiment-type: ignition delay
apparatus:
  kind: shock tube
  institution: Department of Mechanical, Aerospace, and Nuclear Engineering, Rensselaer
    Polytechnic Institute
  facility: stainless steel shock tube
common-properties:
  composition: &comp
    kind: mole fraction
    species:
      - species-name: toluene
        InChI: 1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3
        amount:
          - 0.0115
      - species-name: O2
        InChI: 1S/O2/c1-2
        amount:
          - 0.2077
      - species-name: N2
        InChI: 1S/N2/c1-2
        amount:
          - 0.7808
  ignition-type: &ign
    target: OH*
```

```
    type: d/dt max extrapolated
datapoints:
  - temperature:
      - 1110.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 1244.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 13.3 atm
      - uncertainty-type: relative
        uncertainty: 0.015
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.5
  - temperature:
      - 1153.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 920.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 12.3 atm
      - uncertainty-type: relative
        uncertainty: 0.015
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.5
  - temperature:
      - 1186.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 480.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 14.7 atm
      - uncertainty-type: relative
        uncertainty: 0.015
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.5
  - temperature:
      - 1188.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.01
```

```
  ignition-delay:
    - 533.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 13.5 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.5
- temperature:
    - 1200.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 508.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 14.0 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.5
- temperature:
    - 1220.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 409.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 13.4 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.5
- temperature:
    - 1226.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 400.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 13.3 atm
```

```
      - uncertainty-type: relative
        uncertainty: 0.015
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.5
  - temperature:
      - 1299.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 205.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 12.5 atm
      - uncertainty-type: relative
        uncertainty: 0.015
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.5
  - temperature:
      - 1320.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 159.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 12.1 atm
      - uncertainty-type: relative
        uncertainty: 0.015
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.5
...
```

Shen_2009_phi0.5_50atm.yaml

```
---
file-authors:
  - name: Morgan Mayer
    ORCID: 0000-0001-7137-5721
file-version: 0
chemked-version: 0.4.1
reference:
  doi: 10.1016/j.proci.2008.05.004
  authors:
    - name: Hsi-Ping S. Shen
```

```
    - name: Jeremy Vanderover
    - name: Matthew A. Oehlschlaeger
  journal: Proceedings of the Combustion Institute
  year: 2009
  volume: 32
  pages: 165-172
  detail: Shen_toluene_phi0.5_50atm
experiment-type: ignition delay
apparatus:
  kind: shock tube
  institution: Department of Mechanical, Aerospace, and Nuclear Engineering, Rensselaer
    Polytechnic Institute
  facility: stainless steel shock tube
common-properties:
  composition: &comp
    kind: mole fraction
    species:
      - species-name: toluene
        InChI: 1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3
        amount:
          - 0.0115
      - species-name: O2
        InChI: 1S/O2/c1-2
        amount:
          - 0.2077
      - species-name: N2
        InChI: 1S/N2/c1-2
        amount:
          - 0.7808
  ignition-type: &ign
    target: OH*
    type: d/dt max extrapolated
datapoints:
  - temperature:
      - 1119.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 793.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 40.2 atm
      - uncertainty-type: relative
        uncertainty: 0.015
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.5
  - temperature:
      - 1128.0 kelvin
      - uncertainty-type: relative
```

```
      uncertainty: 0.01
  ignition-delay:
    - 619.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 46.7 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.5
- temperature:
    - 1170.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 343.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 45.6 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.5
- temperature:
    - 1171.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 353.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 45.2 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.5
- temperature:
    - 1179.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 339.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
```

```
    - 47.1 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.5
- temperature:
    - 1251.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 149.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 50.9 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.5
- temperature:
    - 1268.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 126.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 45.1 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.5
- temperature:
    - 1277.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 127.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 45.7 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.5
```

```
  - temperature:
      - 1301.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 96.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 43.5 atm
      - uncertainty-type: relative
        uncertainty: 0.015
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.5
...
```

Shen_2009_phi0.25_12atm.yaml

```
---
file-authors:
  - name: Morgan Mayer
    ORCID: 0000-0001-7137-5721
file-version: 0
chemked-version: 0.4.1
reference:
  doi: 10.1016/j.proci.2008.05.004
  authors:
    - name: Hsi-Ping S. Shen
    - name: Jeremy Vanderover
    - name: Matthew A. Oehlschlaeger
  journal: Proceedings of the Combustion Institute
  year: 2009
  volume: 32
  pages: 165-172
  detail: Shen_toluene_phi0.25_12atm
experiment-type: ignition delay
apparatus:
  kind: shock tube
  institution: Department of Mechanical, Aerospace, and Nuclear Engineering, Rensselaer
    Polytechnic Institute
  facility: stainless steel shock tube
common-properties:
  composition: &comp
    kind: mole fraction
    species:
      - species-name: toluene
        InChI: 1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3
        amount:
```

```
          - 0.0058
      - species-name: O2
        InChI: 1S/O2/c1-2
        amount:
          - 0.2089
      - species-name: N2
        InChI: 1S/N2/c1-2
        amount:
          - 0.7853
  ignition-type: &ign
    target: OH*
    type: d/dt max extrapolated
datapoints:
  - temperature:
      - 1152.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 966.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 11.6 atm
      - uncertainty-type: relative
        uncertainty: 0.015
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.25
  - temperature:
      - 1169.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 600.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 12.4 atm
      - uncertainty-type: relative
        uncertainty: 0.015
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.25
  - temperature:
      - 1171.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 687.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
```

```
  pressure:
    - 12.4 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.25
- temperature:
    - 1191.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 639.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 13.5 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.25
- temperature:
    - 1220.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 465.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 13.4 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.25
- temperature:
    - 1230.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 398.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 13.5 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
```

```
  equivalence-ratio: 0.25
- temperature:
    - 1231.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 475.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 11.5 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.25
- temperature:
    - 1263.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 342.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 11.9 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.25
- temperature:
    - 1268.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 298.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 11.1 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.25
- temperature:
    - 1291.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
```

```
      - 233.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 10.8 atm
      - uncertainty-type: relative
        uncertainty: 0.015
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.25
  - temperature:
      - 1385.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 151.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 10.3 atm
      - uncertainty-type: relative
        uncertainty: 0.015
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.25
  - temperature:
      - 1400.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 94.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 12.1 atm
      - uncertainty-type: relative
        uncertainty: 0.015
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.25
...
```

Shen_2009_phi0.25_50atm.yaml

```
---
file-authors:
  - name: Morgan Mayer
    ORCID: 0000-0001-7137-5721
file-version: 0
```

```
chemked-version: 0.4.1
reference:
  doi: 10.1016/j.proci.2008.05.004
  authors:
    - name: Hsi-Ping S. Shen
    - name: Jeremy Vanderover
    - name: Matthew A. Oehlschlaeger
  journal: Proceedings of the Combustion Institute
  year: 2009
  volume: 32
  pages: 165-172
  detail: Shen_toluene_phi0.25_50atm
experiment-type: ignition delay
apparatus:
  kind: shock tube
  institution: Department of Mechanical, Aerospace, and Nuclear Engineering, Rensselaer
    Polytechnic Institute
  facility: stainless steel shock tube
common-properties:
  composition: &comp
    kind: mole fraction
    species:
      - species-name: toluene
        InChI: 1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3
        amount:
          - 0.005802
      - species-name: O2
        InChI: 1S/O2/c1-2
        amount:
          - 0.2089
      - species-name: N2
        InChI: 1S/N2/c1-2
        amount:
          - 0.7853
  ignition-type: &ign
    target: OH*
    type: d/dt max extrapolated
datapoints:
  - temperature:
      - 1085.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 1280.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 43.7 atm
      - uncertainty-type: relative
        uncertainty: 0.015
    composition: *comp
```

```
  ignition-type: *ign
  equivalence-ratio: 0.25
- temperature:
    - 1092.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 1181.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 46.9 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.25
- temperature:
    - 1152.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 767.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 43.6 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.25
- temperature:
    - 1153.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 662.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 46.7 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.25
- temperature:
    - 1165.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
```

```
  ignition-delay:
    - 604.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 45.7 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.25
- temperature:
    - 1171.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 559.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 42.8 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.25
- temperature:
    - 1190.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 399.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 41.5 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.25
- temperature:
    - 1241.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 280.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 43.8 atm
```

```
      - uncertainty-type: relative
        uncertainty: 0.015
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.25
  - temperature:
      - 1261.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 224.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 41.7 atm
      - uncertainty-type: relative
        uncertainty: 0.015
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.25
  - temperature:
      - 1302.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 171.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 40.7 atm
      - uncertainty-type: relative
        uncertainty: 0.015
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.25
...
```

Shen_2009_phi1.0_12atm.yaml

```
---
file-authors:
  - name: Morgan Mayer
    ORCID: 0000-0001-7137-5721
file-version: 0
chemked-version: 0.4.1
reference:
  doi: 10.1016/j.proci.2008.05.004
  authors:
    - name: Hsi-Ping S. Shen
```

```
    - name: Jeremy Vanderover
    - name: Matthew A. Oehlschlaeger
  journal: Proceedings of the Combustion Institute
  year: 2009
  volume: 32
  pages: 165-172
  detail: Shen_toluene_phi1.0_12atm
experiment-type: ignition delay
apparatus:
  kind: shock tube
  institution: Department of Mechanical, Aerospace, and Nuclear Engineering, Rensselaer
    Polytechnic Institute
  facility: stainless steel shock tube
common-properties:
  composition: &comp
    kind: mole fraction
    species:
      - species-name: toluene
        InChI: 1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3
        amount:
          - 0.02281
      - species-name: O2
        InChI: 1S/O2/c1-2
        amount:
          - 0.2053
      - species-name: N2
        InChI: 1S/N2/c1-2
        amount:
          - 0.7719
  ignition-type: &ign
    target: OH*
    type: d/dt max extrapolated
datapoints:
  - temperature:
      - 1129.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 1380.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 13.4 atm
      - uncertainty-type: relative
        uncertainty: 0.015
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 1164.0 kelvin
      - uncertainty-type: relative
```

```
      uncertainty: 0.01
  ignition-delay:
    - 934.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 13.5 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1197.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 798.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 12.4 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1235.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 483.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 11.3 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1239.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 471.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
```

```
      - 14.5 atm
      - uncertainty-type: relative
        uncertainty: 0.015
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 1290.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 281.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 11.2 atm
      - uncertainty-type: relative
        uncertainty: 0.015
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 1371.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 137.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 13.2 atm
      - uncertainty-type: relative
        uncertainty: 0.015
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
...
```

Shen_2009_phi1.0_50atm.yaml

```
---
file-authors:
  - name: Morgan Mayer
    ORCID: 0000-0001-7137-5721
file-version: 0
chemked-version: 0.4.1
reference:
  doi: 10.1016/j.proci.2008.05.004
  authors:
```

```
    - name: Hsi-Ping S. Shen
    - name: Jeremy Vanderover
    - name: Matthew A. Oehlschlaeger
  journal: Proceedings of the Combustion Institute
  year: 2009
  volume: 32
  pages: 165-172
  detail: Shen_toluene_phi1.0_50atm
experiment-type: ignition delay
apparatus:
  kind: shock tube
  institution: Department of Mechanical, Aerospace, and Nuclear Engineering, Rensselaer
    Polytechnic Institute
  facility: stainless steel shock tube
common-properties:
  composition: &comp
    kind: mole fraction
    species:
      - species-name: toluene
        InChI: 1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3
        amount:
          - 0.02281
      - species-name: O2
        InChI: 1S/O2/c1-2
        amount:
          - 0.2053
      - species-name: N2
        InChI: 1S/N2/c1-2
        amount:
          - 0.7719
  ignition-type: &ign
    target: OH*
    type: d/dt max extrapolated
datapoints:
  - temperature:
      - 1021.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 1255.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 53.8 atm
      - uncertainty-type: relative
        uncertainty: 0.015
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 1041.0 kelvin
```

```
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 1203.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 47.6 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1082.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 757.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 46.9 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1085.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 546.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 51.0 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1116.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 492.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
```

```
  pressure:
    - 49.5 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1117.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 459.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 46.2 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1135.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 346.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 50.9 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1218.0 kelvin
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 117.0 us
    - uncertainty-type: relative
      uncertainty: 0.15
  pressure:
    - 51.4 atm
    - uncertainty-type: relative
      uncertainty: 0.015
  composition: *comp
  ignition-type: *ign
```

```
    equivalence-ratio: 1.0
  - temperature:
      - 1232.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 97.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 57.5 atm
      - uncertainty-type: relative
        uncertainty: 0.015
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 1256.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 61.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 61.5 atm
      - uncertainty-type: relative
        uncertainty: 0.015
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 1305.0 kelvin
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 44.0 us
      - uncertainty-type: relative
        uncertainty: 0.15
    pressure:
      - 60.7 atm
      - uncertainty-type: relative
        uncertainty: 0.015
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
...
```

7.5 Vasudevan ChemKED files

The following ChemKED files were created based on the experimental data provided by Vasudevan et al. [47].

`Vasudevan_2005_phi_0.5.yaml`

```
---
file-authors:
  - name: Morgan Mayer
    ORCID: 0000-0001-7137-5721
file-version: 0
chemked-version: 0.4.1
reference:
  doi: 10.1016/j.proci.2004.07.039
  authors:
    - name: V. Vasudevan
    - name: D. F. Davidson
    - name: R. K. Hanson
  journal: Proceedings of the Combustion Institute
  year: 2005
  volume: 30
  pages: 1155-1163
  detail: Vasudevan_phi_0.5
experiment-type: ignition delay
apparatus:
  kind: shock tube
  institution: High Temperature Gas dynamics Laboratory, Mechanical Engineering Department,
    Stanford University
  facility: stainless steel shock tube
common-properties:
  composition: &comp
    kind: mole fraction
    species:
      - species-name: toluene
        InChI: 1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3
        amount:
          - 0.001
      - species-name: O2
        InChI: 1S/O2/c1-2
        amount:
          - 0.018
      - species-name: Ar
        InChI: 1S/Ar
        amount:
          - 0.981
  ignition-type: &ign
    target: OH
```

```
    type: 1/2 max
datapoints:
  - temperature:
      - 1458.0 K
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 1123.0 us
      - uncertainty-type: relative
        uncertainty: 0.1
    pressure:
      - 1.99 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.5
  - temperature:
      - 1504.0 K
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 725.0 us
      - uncertainty-type: relative
        uncertainty: 0.1
    pressure:
      - 1.98 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.5
  - temperature:
      - 1540.0 K
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 501.0 us
      - uncertainty-type: relative
        uncertainty: 0.1
    pressure:
      - 1.96 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.5
  - temperature:
      - 1550.0 K
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 386.0 us
      - uncertainty-type: relative
        uncertainty: 0.1
    pressure:
      - 1.94 atm
```

```
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.5
  - temperature:
      - 1666.0 K
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 153.0 us
      - uncertainty-type: relative
        uncertainty: 0.1
    pressure:
      - 1.92 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.5
...
```

Vasudevan_2005_phi_1.0_250ppm.yaml

```
---
file-authors:
  - name: Morgan Mayer
    ORCID: 0000-0001-7137-5721
file-version: 0
chemked-version: 0.4.1
reference:
  doi: 10.1016/j.proci.2004.07.039
  authors:
    - name: V. Vasudevan
    - name: D. F. Davidson
    - name: R. K. Hanson
  journal: Proceedings of the Combustion Institute
  year: 2005
  volume: 30
  pages: 1155-1163
  detail: Vasudevan_phi_1.0_250ppm
experiment-type: ignition delay
apparatus:
  kind: shock tube
  institution: High Temperature Gas dynamics Laboratory, Mechanical Engineering Department,
    Stanford University
  facility: stainless steel shock tube
common-properties:
  composition: &comp
    kind: mole fraction
    species:
      - species-name: toluene
        InChI: 1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3
```

```
        amount:
          - 0.00025
      - species-name: O2
        InChI: 1S/O2/c1-2
        amount:
          - 0.00225
      - species-name: Ar
        InChI: 1S/Ar
        amount:
          - 0.9975
  ignition-type: &ign
    target: OH
    type: 1/2 max
datapoints:
  - temperature:
      - 1607.0 K
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 949.0 us
      - uncertainty-type: relative
        uncertainty: 0.1
    pressure:
      - 2.03 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 1648.0 K
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 608.0 us
      - uncertainty-type: relative
        uncertainty: 0.1
    pressure:
      - 2.03 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 1700.0 K
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 369.0 us
      - uncertainty-type: relative
        uncertainty: 0.1
    pressure:
      - 1.89 atm
    composition: *comp
```

```
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 1783.0 K
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 136.0 us
      - uncertainty-type: relative
        uncertainty: 0.1
    pressure:
      - 1.84 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
...
```

Vasudevan_2005_phi_1.0_1000ppm.yaml

```
---
file-authors:
  - name: Morgan Mayer
    ORCID: 0000-0001-7137-5721
file-version: 0
chemked-version: 0.4.1
reference:
  doi: 10.1016/j.proci.2004.07.039
  authors:
    - name: V. Vasudevan
    - name: D. F. Davidson
    - name: R. K. Hanson
  journal: Proceedings of the Combustion Institute
  year: 2005
  volume: 30
  pages: 1155-1163
  detail: Vasudevan_phi_1.0_1000ppm
experiment-type: ignition delay
apparatus:
  kind: shock tube
  institution: High Temperature Gas dynamics Laboratory, Mechanical Engineering Department,
    Stanford University
  facility: stainless steel shock tube
common-properties:
  composition: &comp
    kind: mole fraction
    species:
      - species-name: toluene
        InChI: 1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3
        amount:
```

```
          - 0.001
      - species-name: O2
        InChI: 1S/O2/c1-2
        amount:
          - 0.009
      - species-name: Ar
        InChI: 1S/Ar
        amount:
          - 0.99
  ignition-type: &ign
    target: OH
    type: 1/2 max
datapoints:
  - temperature:
      - 1564.0 K
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 1068.0 us
      - uncertainty-type: relative
        uncertainty: 0.1
    pressure:
      - 1.95 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 1586.0 K
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 702.0 us
      - uncertainty-type: relative
        uncertainty: 0.1
    pressure:
      - 1.9 atm
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 1.0
  - temperature:
      - 1614.0 K
      - uncertainty-type: relative
        uncertainty: 0.01
    ignition-delay:
      - 389.0 us
      - uncertainty-type: relative
        uncertainty: 0.1
    pressure:
      - 1.8 atm
    composition: *comp
    ignition-type: *ign
```

```
  equivalence-ratio: 1.0
- temperature:
    - 1689.0 K
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 209.0 us
    - uncertainty-type: relative
      uncertainty: 0.1
  pressure:
    - 1.79 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1527.0 K
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 798.0 us
    - uncertainty-type: relative
      uncertainty: 0.1
  pressure:
    - 4.54 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1541.0 K
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 651.0 us
    - uncertainty-type: relative
      uncertainty: 0.1
  pressure:
    - 4.43 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1697.0 K
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 150.0 us
    - uncertainty-type: relative
      uncertainty: 0.1
  pressure:
    - 4.26 atm
  composition: *comp
```

```
    ignition-type: *ign
    equivalence-ratio: 1.0
...
```

Vasudevan_2005_phi_1.0_5000ppm.yaml

```
---
file-authors:
  - name: Morgan Mayer
    ORCID: 0000-0001-7137-5721
file-version: 0
chemked-version: 0.4.1
reference:
  doi: 10.1016/j.proci.2004.07.039
  authors:
    - name: V. Vasudevan
    - name: D. F. Davidson
    - name: R. K. Hanson
  journal: Proceedings of the Combustion Institute
  year: 2005
  volume: 30
  pages: 1155-1163
  detail: Vasudevan_phi_1.0_5000ppm
experiment-type: ignition delay
apparatus:
  kind: shock tube
  institution: High Temperature Gas dynamics Laboratory, Mechanical Engineering Department,
    Stanford University
  facility: stainless steel shock tube
common-properties:
  composition: &comp
    kind: mole fraction
    species:
      - species-name: toluene
        InChI: 1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3
        amount:
          - 0.005
      - species-name: O2
        InChI: 1S/O2/c1-2
        amount:
          - 0.045
      - species-name: Ar
        InChI: 1S/Ar
        amount:
          - 0.95
  ignition-type: &ign
    target: OH
    type: 1/2 max
datapoints:
```

```
- temperature:
    - 1434.0 K
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 1070.0 us
    - uncertainty-type: relative
      uncertainty: 0.1
  pressure:
    - 2.03 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1454.0 K
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 750.0 us
    - uncertainty-type: relative
      uncertainty: 0.1
  pressure:
    - 1.66 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1618.0 K
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 130.0 us
    - uncertainty-type: relative
      uncertainty: 0.1
  pressure:
    - 1.88 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.0
- temperature:
    - 1635.0 K
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 107.0 us
    - uncertainty-type: relative
      uncertainty: 0.1
  pressure:
    - 1.83 atm
  composition: *comp
  ignition-type: *ign
```

```
    equivalence-ratio: 1.0
...
```

Vasudevan_2005_phi_1.5.yaml

```
---
file-authors:
  - name: Morgan Mayer
    ORCID: 0000-0001-7137-5721
file-version: 0
chemked-version: 0.4.1
reference:
  doi: 10.1016/j.proci.2004.07.039
  authors:
    - name: V. Vasudevan
    - name: D. F. Davidson
    - name: R. K. Hanson
  journal: Proceedings of the Combustion Institute
  year: 2005
  volume: 30
  pages: 1155-1163
  detail: Vasudevan_phi_1.5
experiment-type: ignition delay
apparatus:
  kind: shock tube
  institution: High Temperature Gas dynamics Laboratory, Mechanical Engineering Department,
    Stanford University
  facility: stainless steel shock tube
common-properties:
  composition: &comp
    kind: mole fraction
    species:
      - species-name: toluene
        InChI: 1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3
        amount:
          - 0.001
      - species-name: O2
        InChI: 1S/O2/c1-2
        amount:
          - 0.006
      - species-name: Ar
        InChI: 1S/Ar
        amount:
          - 0.993
  ignition-type: &ign
    target: OH
    type: 1/2 max
datapoints:
  - temperature:
```

```
    - 1616.0 K
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 1090.0 us
    - uncertainty-type: relative
      uncertainty: 0.1
  pressure:
    - 1.82 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.5
- temperature:
    - 1627.0 K
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 922.0 us
    - uncertainty-type: relative
      uncertainty: 0.1
  pressure:
    - 1.92 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.5
- temperature:
    - 1714.0 K
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 384.0 us
    - uncertainty-type: relative
      uncertainty: 0.1
  pressure:
    - 1.77 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.5
- temperature:
    - 1847.0 K
    - uncertainty-type: relative
      uncertainty: 0.01
  ignition-delay:
    - 143.0 us
    - uncertainty-type: relative
      uncertainty: 0.1
  pressure:
    - 1.75 atm
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 1.5
```