

Introducing ChemKED: a new human- and machine-readable data standard for chemical kinetics experiments

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10th US National Combustion Meeting

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 [bryanwweber](https://github.com/bryanwweber)



ChemKED: Chemical Kinetic Experimental Data

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**PyKED: Python software
for working with ChemKED**

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**PyKED: Python software
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Experiments are good!

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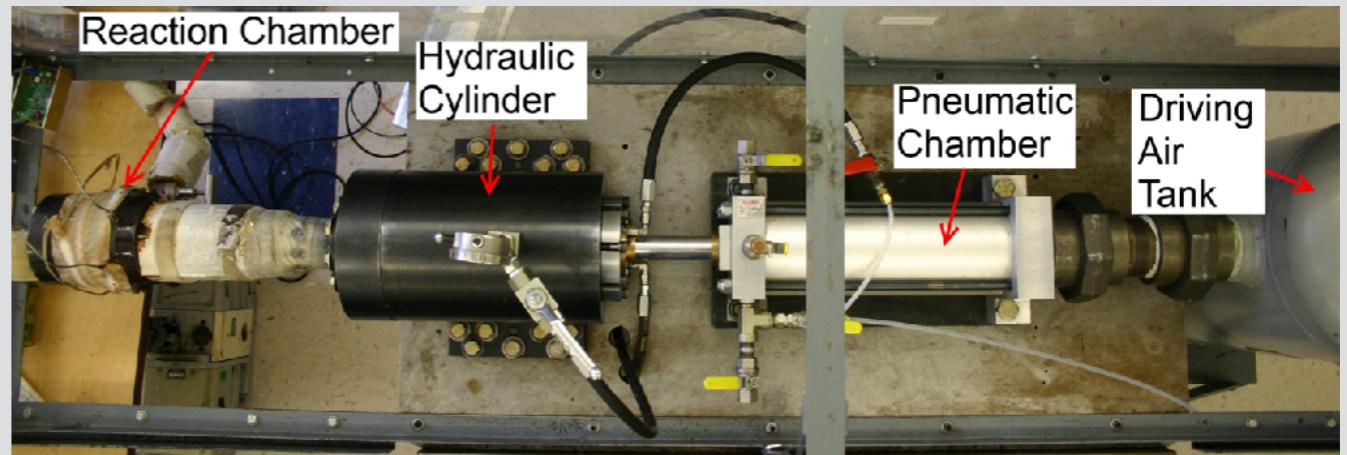


Shock tube¹

Experiments are good!



Shock tube¹

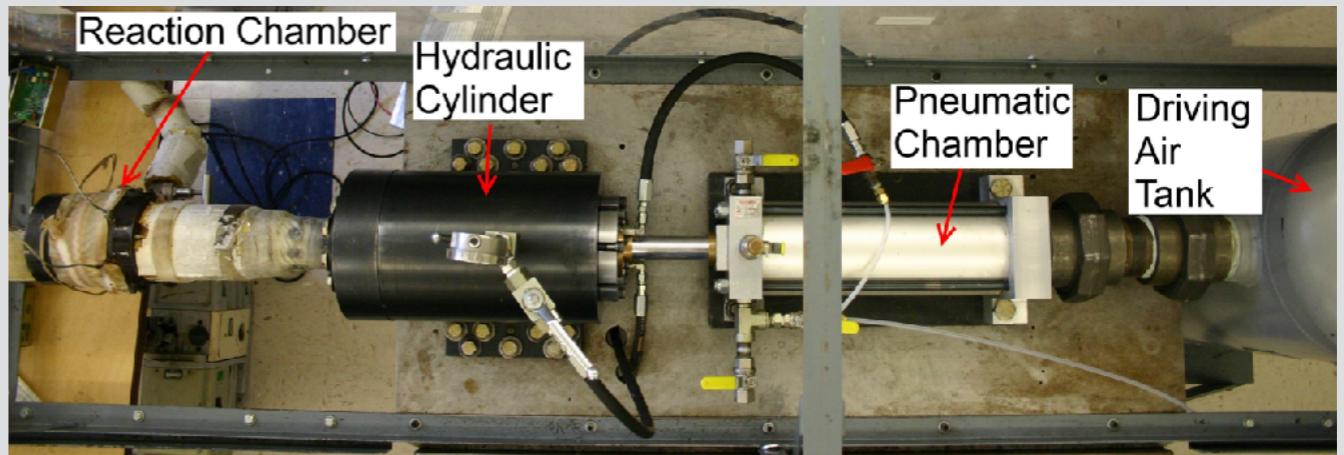


Rapid compression machine²

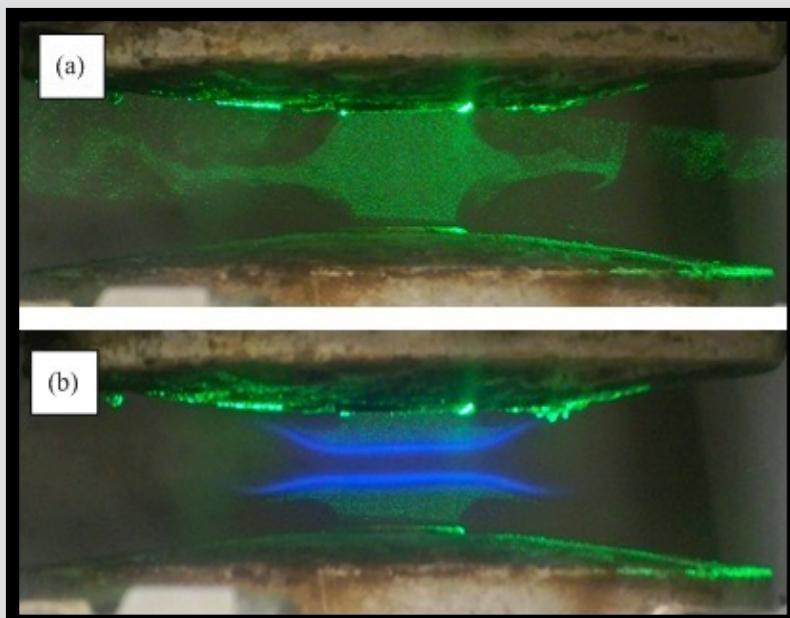
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Shock tube¹



Rapid compression machine²

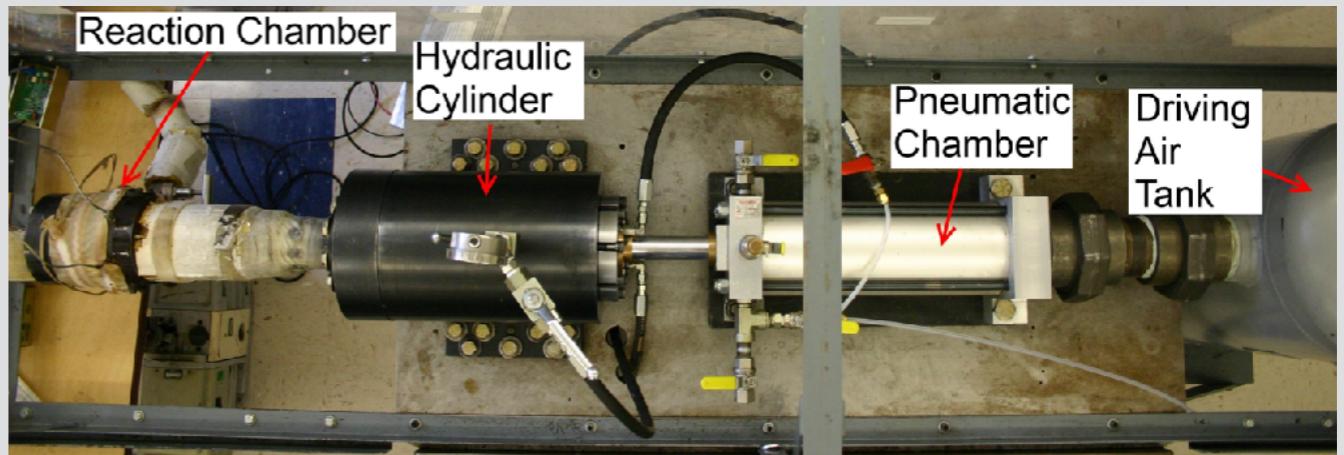


Counterflow flame³

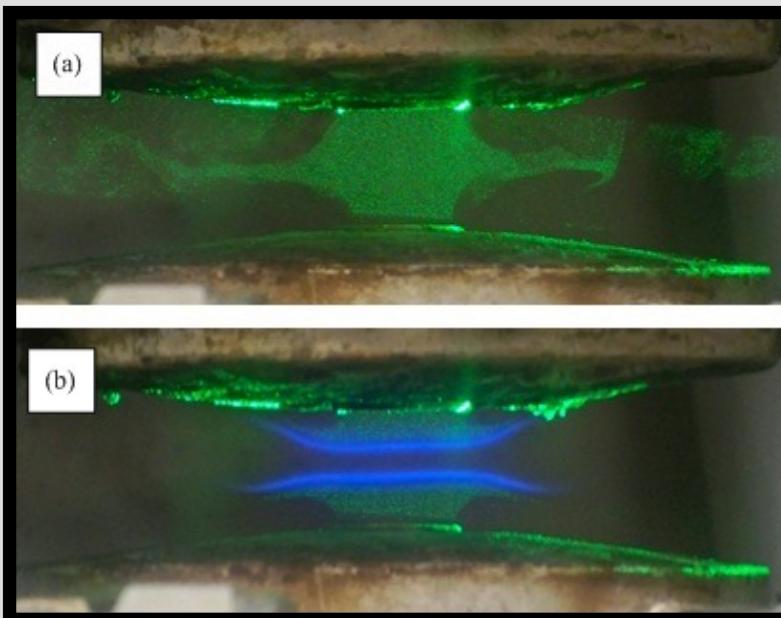
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Shock tube¹



Rapid compression machine²



Counterflow flame³

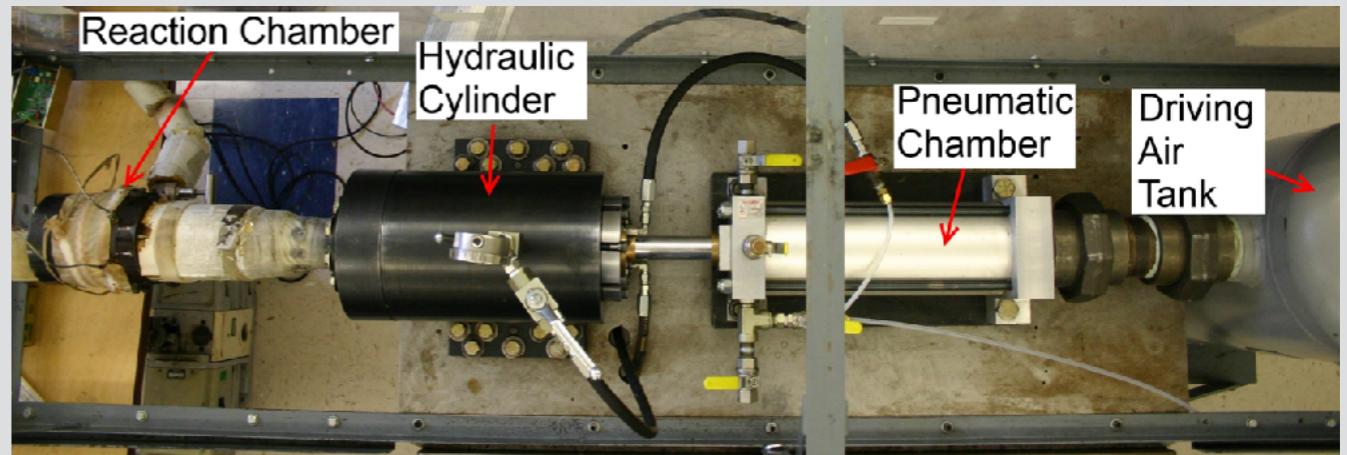


Jet-stirred reactor⁴

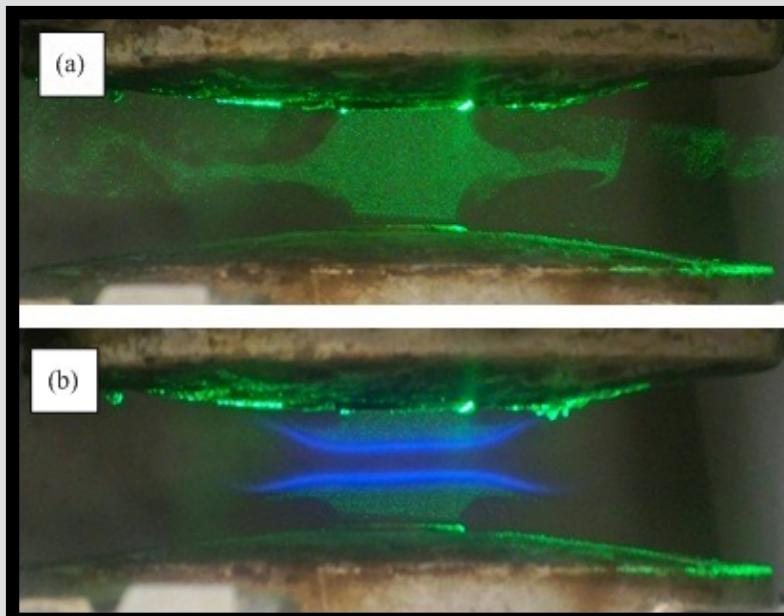
Experiments are good!



Shock tube¹



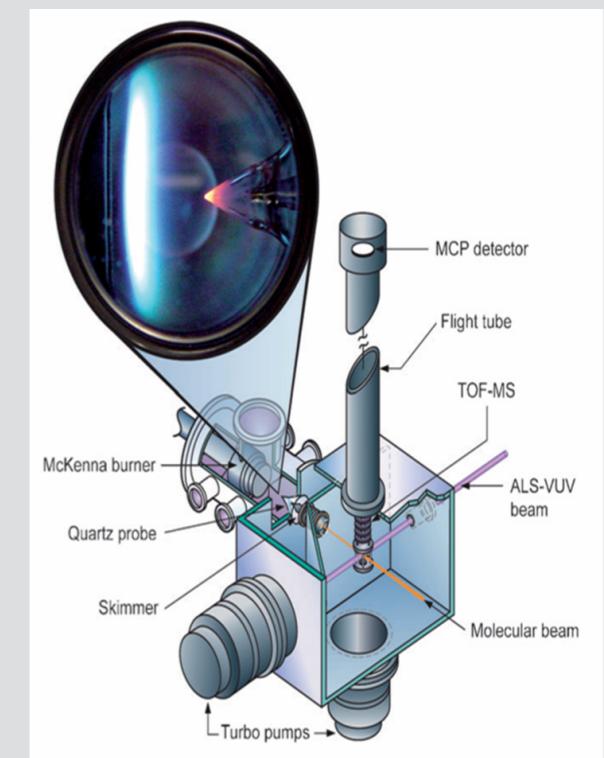
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Counterflow flame³



Jet-stirred reactor⁴

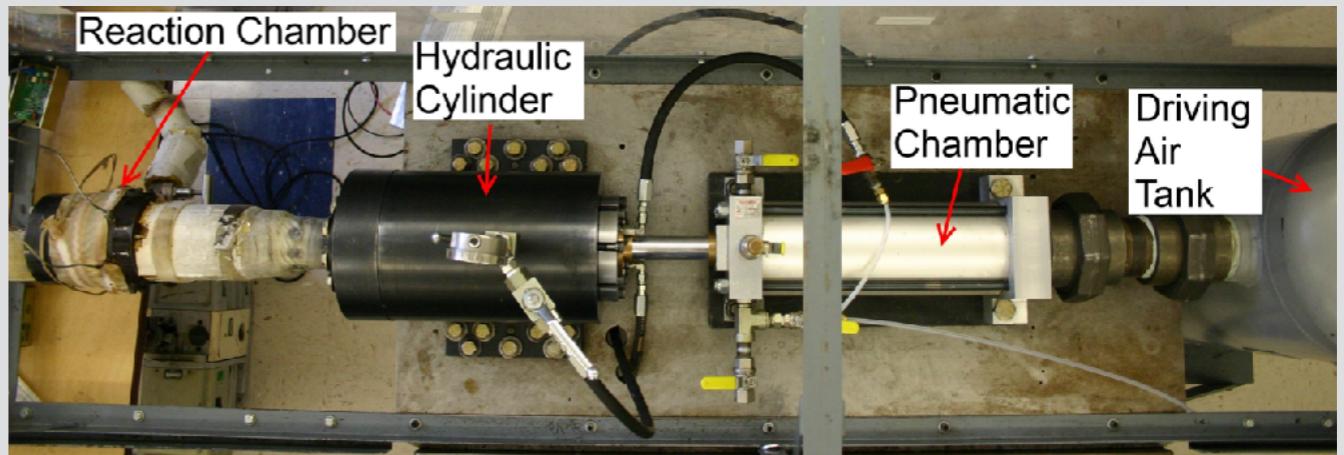


Flat flame burners⁵

Experiments are good!



Shock tube¹



Rapid compression machine²

Sharing is hard :-)

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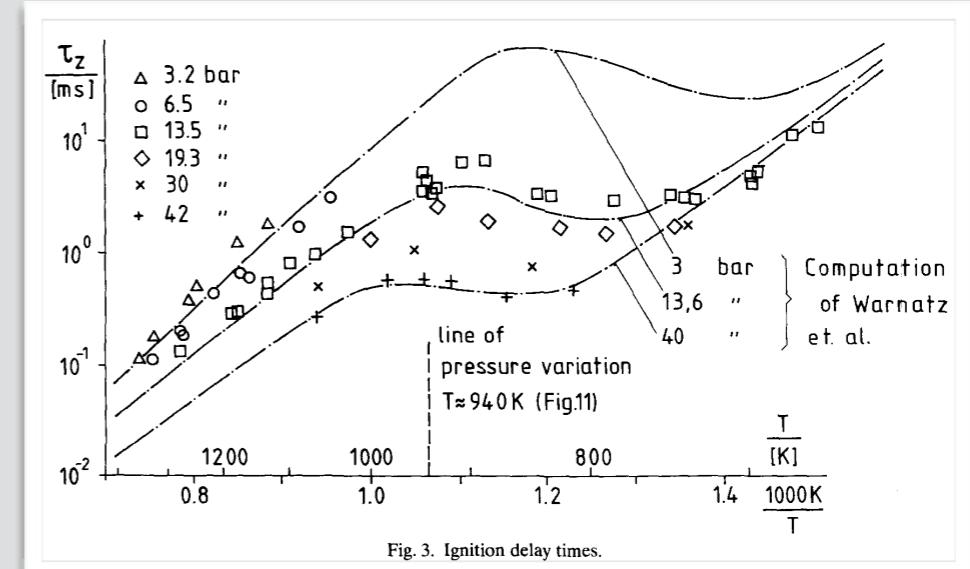
Series	Shock No.	Composition %		P_1 torr	P_5 atm	T_5 K	ρ_5 / ρ_1 mm/ μ sec	U_5 mm/ μ sec	τ μ sec
		C ₇ H ₁₆	O ₂						
A	6	1	11	116	4.66	1260	7.27	.3778	323
	10	1	11	105	5.17	1410	7.95	.3913	70
	14	1	11	103	4.52	1323	7.56	.3835	170
B	22	1	11	50	2.03	1268	7.30	.3785	647
	29	1	11	70	3.15	1341	7.64	.3851	155
	37	1	11	50	3.08	1602	8.75	.4077	25
C	41	0.5	11	100	3.81	1311	6.62	.4014	200
	45	0.5	11	101	3.51	1245	6.37	.3946	330
	57	0.5	11	100	4.81	1503	7.30	.4206	27

PDF table⁵

Sharing is hard :-(

Series	Shock No.	Composition %	P_1 torr	P_5 atm	T_5 K	ρ_5 / ρ_1 mm/ μ sec	U_5	τ μ sec
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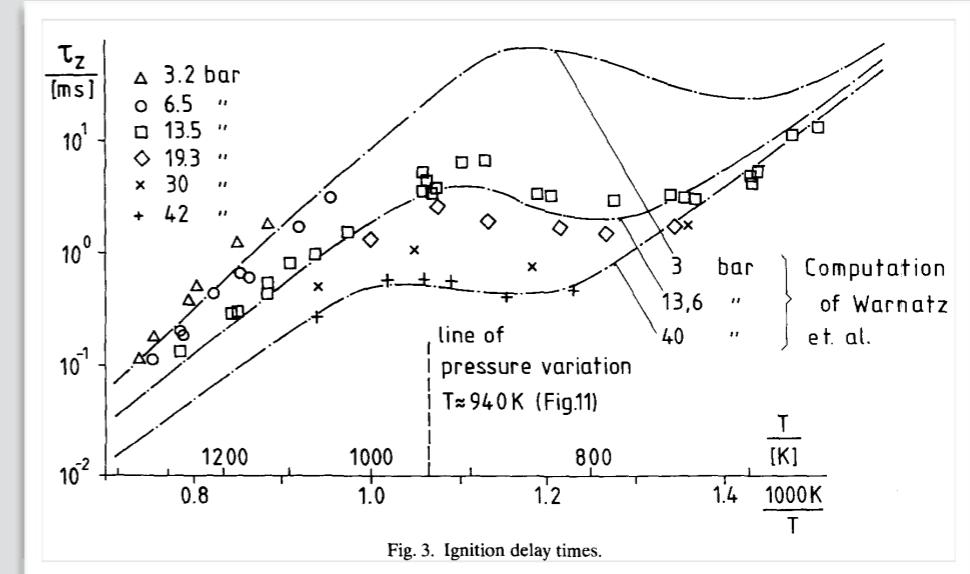


Figure⁶

Sharing is hard :-(

Series	Shock No.	Composition %	P_1 torr	P_5 atm	T_5 K	ρ_5 / ρ_1 mm/ μ sec	U_5	τ μ sec
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PDF table⁵



Figure⁶

```
# n-heptane ignition delay from Colket and Spadaccini 2001
# P (atm), T (K), Ignition Delay ( $\mu$ s)
# Mole Fraction nC7H16 O2 Ar : 0.00192 0.04224 0.95584
7.72 ,1393 ,85
7.78 ,1299 ,345
7.04 ,1235 ,631
6.38 ,1299 ,348
7.53 ,1372 ,134
6.08 ,1236 ,678
7.35 ,1340 ,148
6.63 ,1328 ,211
6.94 ,1395 ,89
```

CSV file⁷

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PDF table⁵

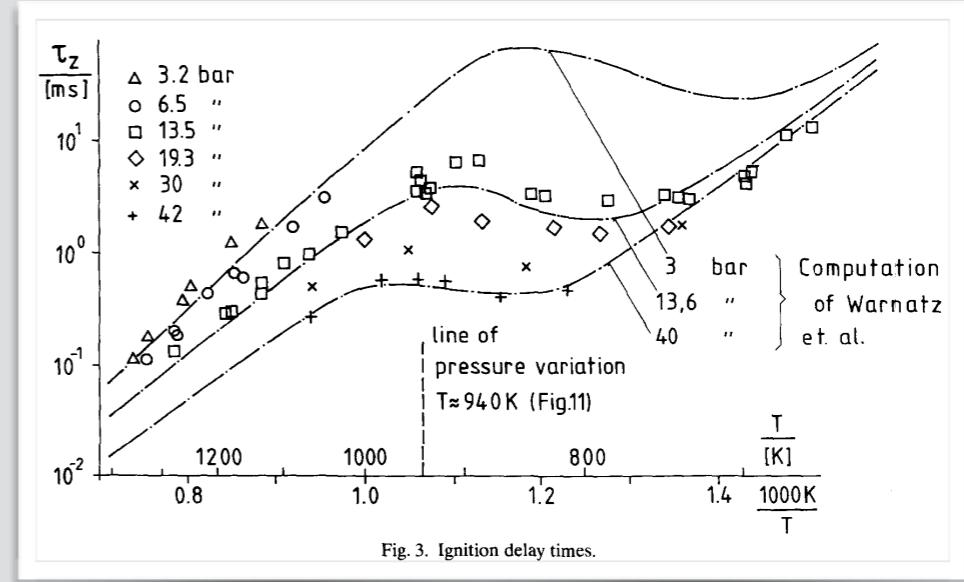


Fig. 3. Ignition delay times.

Figure⁶

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CSV file⁷

Kyle Niemeyer

August 19, 2014 at 7:38 PM

To: jeff.berghorson@mcgill.ca

request for data from 2010 alcohol shock tube paper

Hello,

I'm currently trying to evaluate the performance of various reaction mechanisms for their ability predict ethanol autoignition, and to that end the ethanol ignition delay data from your 2010 Ene

Email plea

Sharing is hard fun! :-)

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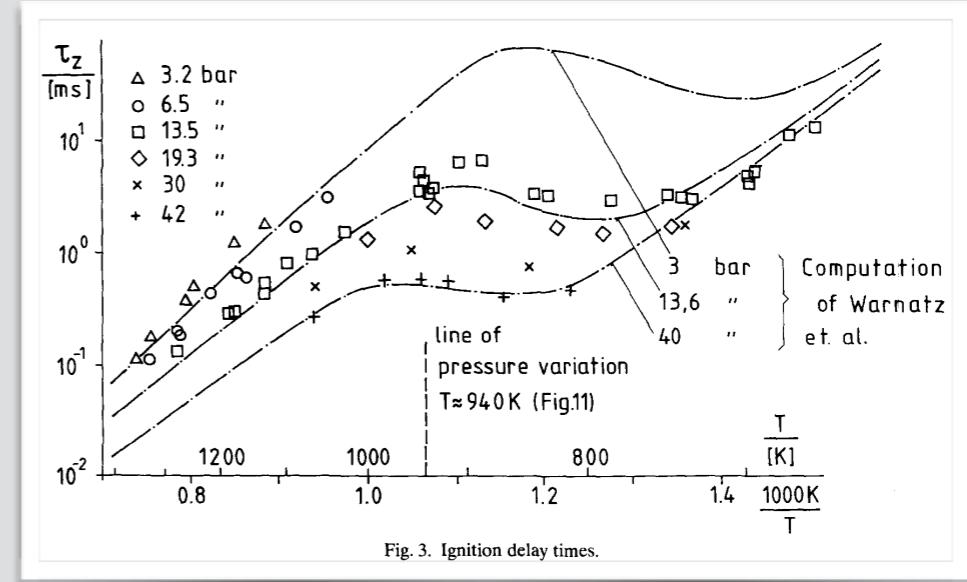


Fig. 3. Ignition delay times.

Figure⁶

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Hello,

I'm currently trying to evaluate the performance of various reaction mechanisms for their ability predict ethanol autoignition, and to that end the ethanol ignition delay data from your 2010 Ene

Email plea

We are not alone...

- PrIMe (**P**rocess **I**nformatics **M**odel): Frenklach et al. (<http://primekinetics.org>)
 - Problems: XML-based standard, missing some necessary information, & closed nature
- ReSpecTh (**R**eaction Kinetics/**S**pectroscopy/**T**hermochemistry): Varga et al. (<http://respecth.hu/>)
 - Evolution of PrIMe—now includes more data needed to reproduce experiment
 - Problems: still XML, still closed
- CloudFlame: KAUST (<https://cloudflame.kaust.edu.sa/home>)
 - CSV-based standard
 - Problems: CSV files are hard to parse automatically

Our solution

Our solution(s)

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ChemKED: Chemical Kinetics Experimental Data format

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PyKED: Python software for working with ChemKED files

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Our solution(s)

ChemKED: Chemical Kinetics Experimental Data format

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PyKED: Python software for working with ChemKED files

+

Other interfaces ...

ChemKED

```
file-author:
  name: Kyle E Niemeyer
  ORCID: 0000-0003-4425-7097
file-version: 0
chemked-version: 0.0.1
reference:
  doi: 10.1016/j.ijhydene.2007.04.008
authors:
  - name: N. Chaumeix
  - name: S. Pichon
  - name: F. Lafosse
  - name: C.-E. Paillard
journal: International Journal of Hydrogen Energy
year: 2007
volume: 32
pages: 2216-2226
detail: Fig. 12., right, open diamond
experiment-type: ignition delay
apparatus:
  kind: shock tube
  institution: CNRS-ICARE
  facility: stainless steel shock tube
common-properties:
  pressure: &pres
    - 220 kilopascal
composition: &comp
  kind: mole fraction
  species:
    - species-name: H2
      InChI: 1S/H2/h1H
      amount:
        - 0.00444
    - species-name: O2
      InChI: 1S/02/c1-2
      amount:
        - 0.00556
    - species-name: Ar
      InChI: 1S/Ar
      amount:
        - 0.99
ignition-type: &ign
  target: pressure
  type: d/dt max
datapoints:
```

ChemKED

Written in YAML –
human- AND machine-
writable!

```
file-author:  
  name: Kyle E Niemeyer  
  ORCID: 0000-0003-4425-7097  
file-version: 0  
chemked-version: 0.0.1  
reference:  
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  facility: stainless steel shock tube  
common-properties:  
  pressure: &pres  
    - 220 kilopascal  
composition: &comp  
  kind: mole fraction  
  species:  
    - species-name: H2  
      InChI: 1S/H2/h1H  
      amount:  
        - 0.00444  
    - species-name: O2  
      InChI: 1S/02/c1-2  
      amount:  
        - 0.00556  
    - species-name: Ar  
      InChI: 1S/Ar  
      amount:  
        - 0.99  
ignition-type: &ign  
  target: pressure  
  type: d/dt max  
datapoints:
```

ChemKED

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Human- AND machine-
readable!

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apparatus:  
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  facility: stainless steel shock tube  
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ignition-type: &ign  
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```

ChemKED

Written in YAML –
human- AND machine-
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Human- AND machine-
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Parsers and libraries
for nearly every
programming
language!

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      amount:  
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ignition-type: &ign  
  target: pressure  
  type: d/dt max  
datapoints:
```

Uncertainty

```
datapoints:  
  - temperature:  
    - 1164.48 kelvin  
    - uncertainty-type: absolute  
      uncertainty: 10 kelvin  
  ignition-delay:  
    - 471.54 us  
    - uncertainty-type: relative  
      uncertainty: 0.1  
  pressure:  
    - 220 kilopascal  
composition:  
  kind: mole percent  
species:  
  - species-name: H2  
    InChI: 1S/H2/h1H  
  amount:  
    - 0.444  
    - uncertainty-type: relative  
      uncertainty: 0.01  
  - species-name: O2  
    InChI: 1S/O2/c1-2  
  amount:  
    - 0.556  
    - uncertainty-type: absolute  
      uncertainty: 0.002  
  - species-name: Ar  
    InChI: 1S/Ar  
  amount:  
    - 99.0  
    - uncertainty-type: absolute  
      upper-uncertainty: 1.0  
      lower-uncertainty: 0.2  
ignition-type:  
  target: pressure  
  type: d/dt max
```

Uncertainty

- ChemKED supports specification of uncertainties for **all** quantities in a data point

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Uncertainty

- ChemKED supports specification of uncertainties for **all** quantities in a data point
 - Dimensionless: Composition (mole/mass fraction, mole percent)
 - Dimensional: temperature, pressure, ignition delay, etc.

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Uncertainty

- ChemKED supports specification of uncertainties for **all** quantities in a data point
 - Dimensionless: Composition (mole/mass fraction, mole percent)
 - Dimensional: temperature, pressure, ignition delay, etc.
- Supports relative and absolute uncertainty

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  target: pressure  
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...
```

Our schema is free & libre

```
# Common reference for authors' information
author: &author
  type: dict
  required: true
  isvalid_orcid: true
  schema:
    ORCID:
      type: string
    name:
      required: true
      type: string
#
# Common reference for value-unit schema
value-with-uncertainty: &value-with-uncertainty
  isvalid_uncertainty: true
  items:
    - type: string
    - type: dict
      schema:
        uncertainty-type:
          required: true
          type: string
          allowed:
            - absolute
            - relative
        uncertainty:
          required: true
        anyof_type:
          - string
          - float
        excludes:
          - upper-uncertainty
          - lower-uncertainty
    upper-uncertainty:
      required: true
      anyof_type:
        - string
        - float
      excludes:
        - uncertainty
      dependencies:
        - lower-uncertainty
    lower-uncertainty:
      required: true
      anyof_type:
```

Our schema is free & libre

- The ChemKED schema is also a YAML-formatted file

```
# Common reference for authors' information
author: &author
  type: dict
  required: true
  isvalid_orcid: true
  schema:
    ORCID:
      type: string
    name:
      required: true
      type: string
#
# Common reference for value-unit schema
value-with-uncertainty: &value-with-uncertainty
  isvalid_uncertainty: true
  items:
    - type: string
    - type: dict
      schema:
        uncertainty-type:
          required: true
          type: string
          allowed:
            - absolute
            - relative
        uncertainty:
          required: true
        anyof_type:
          - string
          - float
        excludes:
          - upper-uncertainty
          - lower-uncertainty
  upper-uncertainty:
    required: true
    anyof_type:
      - string
      - float
    excludes:
      - uncertainty
    dependencies:
      - lower-uncertainty
  lower-uncertainty:
    required: true
    anyof_type:
```

Our schema is free & libre

- The ChemKED schema is also a YAML-formatted file
- Ensures required data are present, have appropriate units and bounded values, etc.

```
# Common reference for authors' information
author: &author
  type: dict
  required: true
  isvalid_orcid: true
  schema:
    ORCID:
      type: string
    name:
      required: true
      type: string
#
# Common reference for value-unit schema
value-with-uncertainty: &value-with-uncertainty
  isvalid_uncertainty: true
  items:
    - type: string
    - type: dict
      schema:
        uncertainty-type:
          required: true
          type: string
          allowed:
            - absolute
            - relative
        uncertainty:
          required: true
        anyof_type:
          - string
          - float
        excludes:
          - upper-uncertainty
          - lower-uncertainty
  upper-uncertainty:
    required: true
    anyof_type:
      - string
      - float
    excludes:
      - uncertainty
    dependencies:
      - lower-uncertainty
  lower-uncertainty:
    required: true
    anyof_type:
```

Our schema is free & libre

- The ChemKED schema is also a YAML-formatted file
- Ensures required data are present, have appropriate units and bounded values, etc.
- Ensures reference information is correct if DOI is provided

```
# Common reference for authors' information
author: &author
  type: dict
  required: true
  isvalid_orcid: true
  schema:
    ORCID:
      type: string
    name:
      required: true
      type: string
#
# Common reference for value-unit schema
value-with-uncertainty: &value-with-uncertainty
  isvalid_uncertainty: true
  items:
    - type: string
    - type: dict
      schema:
        uncertainty-type:
          required: true
          type: string
          allowed:
            - absolute
            - relative
        uncertainty:
          required: true
        anyof_type:
          - string
          - float
        excludes:
          - upper-uncertainty
          - lower-uncertainty
  upper-uncertainty:
    required: true
    anyof_type:
      - string
      - float
    excludes:
      - uncertainty
    dependencies:
      - lower-uncertainty
  lower-uncertainty:
    required: true
    anyof_type:
```

PyKED

**Validation of
ChemKED files**

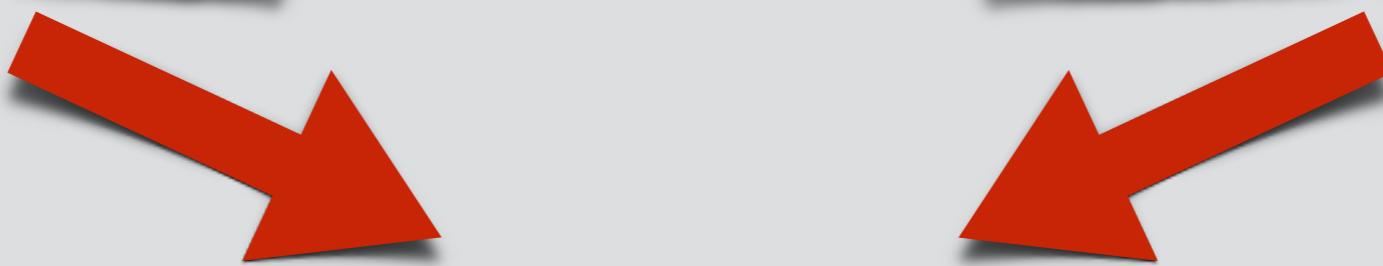


PyKED

Validation of
ChemKED files

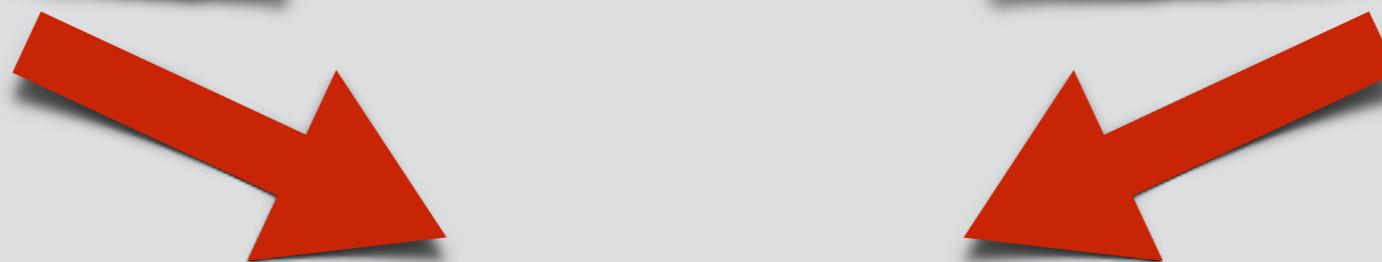
Interaction with
experimental data

PyKED



Validation of
ChemKED files

Interaction with
experimental data

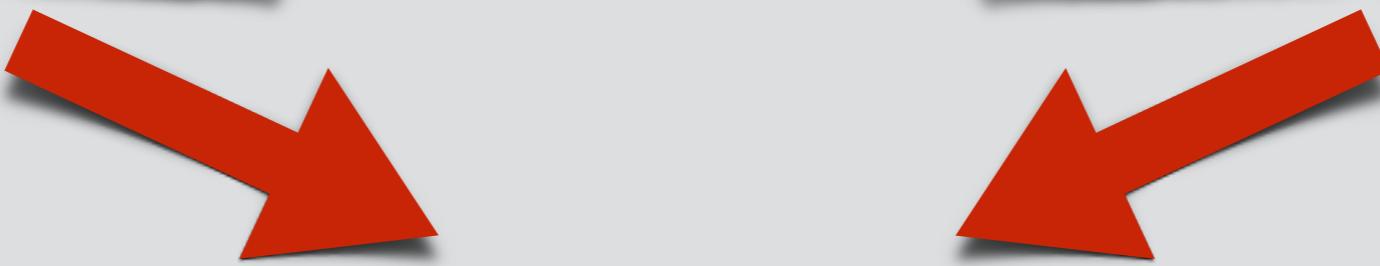


PyKED



Validation of
ChemKED files

Interaction with
experimental data



PyKED

- Version control: git & GitHub
(github.com/pr-omethe-us/PyKED)
- Python 3.5+
- Integrates Python libraries for unit handling, validation, arrays



PyKED components

- ChemKED class stores all the information from a ChemKED file

```
from pyked import ChemKED
ck = ChemKED('chemked_file.yaml')
```



```
file-author:
  name: Kyle E Niemeyer
  ORCID: 0000-0003-4425-7097
file-version: 0
chemked-version: 0.0.1
reference:
  doi: 10.1016/j.ijhydene.2007.04.008
authors:
  - name: N. Chaumeix
  - name: S. Pichon
  - name: F. Lafosse
  - name: C.-E. Paillard
journal: International Journal of Hydrogen Energy
year: 2007
volume: 32
pages: 2216-2226
detail: Fig. 12., right, open diamond
experiment-type: ignition delay
apparatus:
  kind: shock tube
  institution: CNRS-ICARE
  facility: stainless steel shock tube
common-properties:
  pressure: &pres
    - 220 kilopascal
  composition: &comp
    kind: mole fraction
  species:
    - species-name: H2
      InChI: 1S/H2/h1H
      amount:
        - 0.00444
    - species-name: O2
      InChI: 1S/02/c1-2
      amount:
        - 0.00556
    - species-name: Ar
      InChI: 1S/Ar
      amount:
        - 0.99
  ignition-type: &ign
    target: pressure
    type: d/dt max
datapoints:
  - temperature:
    - 1164.48 kelvin
    ignition-delay:
      - 471.54 us
    pressure: *pres
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.4
  - temperature:
    - 1164.97 kelvin
    ignition-delay:
      - 448.03 us
    pressure: *pres
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.4
  - temperature:
    - 1264.2 kelvin
    ignition-delay:
      - 291.57 us
    pressure: *pres
    composition: *comp
    ignition-type: *ign
    equivalence-ratio: 0.4
  - temperature:
    - 1332.57 kelvin
    ignition-delay:
      - 205.93 us
    pressure: *pres
    composition: *comp
```

PyKED components

- ChemKED class stores all the information from a ChemKED file

```
from pyked import ChemKED  
ck = ChemKED('chemked_file.yaml')  
ck.reference
```



```
reference:  
doi: 10.1016/j.ijhydene.2007.04.008  
authors:  
- name: N. Chaumeix  
- name: S. Pichon  
- name: F. Lafosse  
- name: C.-E. Paillard  
journal: International Journal of Hydrogen Energy  
year: 2007  
volume: 32  
pages: 2216–2226  
detail: Fig. 12., right, open diamond
```

PyKED components

- ChemKED class stores all the information from a ChemKED file

```
from pyked import ChemKED  
ck = ChemKED('chemked_file.yaml')  
ck.apparatus
```

apparatus:
kind: shock tube
institution: CNRS-ICARE
facility: stainless steel shock tube



PyKED components

- ChemKED class stores all the information from a ChemKED file

```
from pyked import ChemKED
ck = ChemKED('chemked_file.yaml')
ck.datapoints
```



```
datapoints:
  - temperature:
    - 1164.48 kelvin
  ignition-delay:
    - 471.54 us
  pressure: *pres
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.4
  - temperature:
    - 1164.97 kelvin
  ignition-delay:
    - 448.03 us
  pressure: *pres
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.4
  - temperature:
    - 1264.2 kelvin
  ignition-delay:
    - 291.57 us
  pressure: *pres
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.4
  - temperature:
    - 1332.57 kelvin
  ignition-delay:
    - 205.93 us
  pressure: *pres
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.4
  - temperature:
    - 1519.18 kelvin
  ignition-delay:
    - 88.11 us
  pressure: *pres
  composition: *comp
  ignition-type: *ign
  equivalence-ratio: 0.4
```

PyKED components

- DataPoint class stores the information for a single datapoint

```
dp = ck.datapoints[0]
dp.temperature
dp.ignition_delay
dp.pressure
dp.get_cantera_mole_fraction()
dp.equivalence_ratio
```

- temperature:
 - 1164.48 kelvin
- ignition-delay:
 - 471.54 us
- pressure:
 - 220 kilopascal
- composition:
 - kind: mole fraction
 - species:
 - species-name: H₂
InChI: 1S/H2/h1H
amount:
 - 0.00444
 - species-name: O₂
InChI: 1S/O2/c1-2
amount:
 - 0.00556
 - species-name: Ar
InChI: 1S/Ar
amount:
 - 0.99
 - ignition-type:
 - target: pressure
 - type: d/dt max
 - equivalence-ratio: 0.4

PyKED components

- DataPoint class stores the information for a single data point

```
dp = ck.datapoints[0]  
dp.temperature  
dp.ignition_delay  
dp.pressure  
dp.get_cantera_mole_fraction()  
dp.equivalence_ratio
```

temperature:
– 1164.48 kelvin
ignition_delay:
– 471.54 us
pressure:
– 220 kilopascal
composition:
kind: mole fraction
species:
– species-name: H₂
InChI: 1S/H₂/h1H
amount:
– 0.00444
– species-name: O₂
InChI: 1S/O₂/c1-2
amount:
– 0.00556
– species-name: Ar
InChI: 1S/Ar
amount:
– 0.99
ignition-type:
target: pressure
type: d/dt max
equivalence-ratio: 0.4

PyKED components

- DataPoint class stores the information for a single datapoint

```
dp = ck.datapoints[0]
dp.temperature
dp.ignition_delay
dp.pressure
dp.get_cantera_mole_fraction()
dp.equivalence_ratio
```

– temperature:
1164.48 kelvin
ignition-delay:
– 471.54 us
pressure:
– 220 kilopascal
composition:
kind: mole fraction
species:
– species-name: H₂
InChI: 1S/H₂/h1H
amount:
– 0.00444
– species-name: O₂
InChI: 1S/O₂/c1-2
amount:
– 0.00556
– species-name: Ar
InChI: 1S/Ar
amount:
– 0.99
ignition-type:
target: pressure
type: d/dt max
equivalence-ratio: 0.4



PyKED components

- DataPoint class stores the information for a single datapoint

```
dp = ck.datapoints[0]
dp.temperature
dp.ignition_delay
dp.pressure
dp.get_cantera_mole_fraction()
dp.equivalence_ratio
```

temperature:
– 1164.48 kelvin
ignition-delay:
– 471.54 us
pressure:
– 220 kilopascal
composition:
kind: mole fraction
species:
– species-name: H₂
InChI: 1S/H₂/h1H
amount:
– 0.00444
– species-name: O₂
InChI: 1S/O₂/c1-2
amount:
– 0.00556
– species-name: Ar
InChI: 1S/Ar
amount:
– 0.99
ignition-type:
target: pressure
type: d/dt max
equivalence-ratio: 0.4

PyKED components

- DataPoint class stores the information for a single datapoint

```
dp = ck.datapoints[0]
dp.temperature
dp.ignition_delay
dp.pressure
dp.get_cantera_mole_fraction()
dp.equivalence_ratio
```



```
- temperature:
  - 1164.48 kelvin
ignition-delay:
  - 471.54 us
pressure:
  - 220 kilopascal
composition:
  kind: mole fraction
  species:
    - species-name: H2
      InChI: 1S/H2/h1H
      amount:
        - 0.00444
    - species-name: O2
      InChI: 1S/O2/c1-2
      amount:
        - 0.00556
    - species-name: Ar
      InChI: 1S/Ar
      amount:
        - 0.99
ignition-type:
  target: pressure
  type: d/dt max
equivalence-ratio: 0.4
```

PyKED components

- DataPoint class stores the information for a single datapoint

```
dp = ck.datapoints[0]
dp.temperature
dp.ignition_delay
dp.pressure
dp.get_cantera_mole_fraction()
dp.equivalence_ratio
```

– temperature:
– 1164.48 kelvin
ignition-delay:
– 471.54 us
pressure:
– 220 kilopascal
composition:
kind: mole fraction
species:
– species-name: H₂
InChI: 1S/H₂/h1H
amount:
– 0.00444
– species-name: O₂
InChI: 1S/O₂/c1-2
amount:
– 0.00556
– species-name: Ar
InChI: 1S/Ar
amount:
– 0.99
ignition-type:
target: pressure
type: d/dt max
equivalence-ratio: 0.4

Example: RCM

```
file-author:  
    name: Kyle E Niemeyer  
    ORCID: 0000-0003-4425-7097  
file-version: 0  
chemked-version: 0.0.1  
reference:  
    doi: 10.1002/kin.20180  
authors:  
    - name: Gaurav Mittal  
    - name: Chih-Jen Sung  
      ORCID: 0000-0003-2046-8076  
    - name: Richard A Yetter  
journal: International Journal of Chemical Kinetics  
year: 2006  
volume: 38  
pages: 516–529  
detail: Fig. 6, open circle  
experiment-type: ignition delay  
apparatus:  
    kind: rapid compression machine  
institution: Case Western Reserve University  
facility: CWRU RCM
```

```
datapoints:
  - temperature:
    - 297.4 kelvin
  ignition-delay:
    - 1.0 ms
  pressure:
    - 958.0 torr
  composition:
    kind: mole fraction
    species:
      - species-name: H2
        InChI: 1S/H2/h1H
        amount:
          - 0.12500
      - species-name: O2
        InChI: 1S/O2/c1-2
        amount:
          - 0.06250
      - species-name: N2
        InChI: 1S/N2/c1-2
        amount:
          - 0.18125
      - species-name: Ar
        InChI: 1S/Ar
        amount:
          - 0.63125
  ignition-type:
    target: pressure
    type: d/dt max
  compression-time:
    - 38.0 ms
  volume-history:
    time:
      units: s
      column: 0
    volume:
      units: cm3
      column: 1
    values:
      - [0.00E+000, 5.47669375000E+002]
      - [1.00E-003, 5.46608789894E+002]
      - [2.00E-003, 5.43427034574E+002]
      - [3.00E-003, 5.38124109043E+002]
      - [4.00E-003, 5.30700013298E+002]
      - [5.00E-003, 5.21154747340E+002]
```

Example: RCM modeling

```
import cantera as ct
from pyked import ChemKED

# Load the ChemKED file and retrieve the first element of the
# datapoints list, which is an instance of the DataPoint class
ck = ChemKED('testfile_rcm.yaml')
dp = ck.datapoints[0]

T_0 = dp.temperature.to('K').magnitude
P_0 = dp.pressure.to('Pa').magnitude
X_0 = dp.get_cantera_mole_fraction()

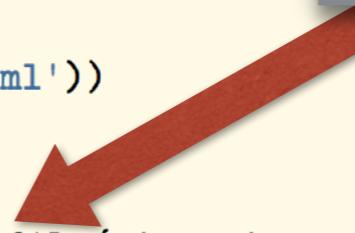
# Load the mechanism and set the initial state of the mixture
gas = ct.Solution('h2-co-mechanism.cti')
gas.TPX = T_0, P_0, X_0

# Create the reactor and the outside environment
reac = ct.IdealGasReactor(gas)
env = ct.Reservoir(ct.Solution('air.xml'))
time = dp.volume_history.time
volume = dp.volume_history.volume
ct.Wall(reac, env, velocity=VolumeProfile(time=time, volume=volume))

netw = ct.ReactorNet([reac])

# Integrate for 50 ms
while netw.time < 0.05:
    netw.step()
```

User Defined Function



Installation

```
conda install -c prometheus pyked
```

or

```
pip install pyked[dataframes]
```

Plans for ChemKED/PyKED



https://cdn.shopify.com/s/files/1/0746/4589/products/Help_Wanted_Sign_1024x1024.jpg?v=1482422422

Plans for ChemKED/PyKED

- Add examples and schema reference to documentation



https://cdn.shopify.com/s/files/1/0746/4589/products/Help_Wanted_Sign_1024x1024.jpg?v=1482422422

Plans for ChemKED/PyKED

- Add examples and schema reference to documentation
- Support other fundamental experimental methods: laminar flames, jet-stirred reactors, ...



https://cdn.shopify.com/s/files/1/0746/4589/products/Help_Wanted_Sign_1024x1024.jpg?v=1482422422

Plans for ChemKED/PyKED

- Add examples and schema reference to documentation
- Support other fundamental experimental methods: laminar flames, jet-stirred reactors, ...
- Converters to/from other common formats: CSV, NumPy, Excel, etc.



https://cdn.shopify.com/s/files/1/0746/4589/products/Help_Wanted_Sign_1024x1024.jpg?v=1482422422

Prometheus

- Goal: community database for experimental data, models, and calculations
- **Initial team:**
 - Kyle Niemeyer (Oregon State)
 - Bryan Weber (Univ. Connecticut)
 - Richard West (Northeastern)
 - Nicole Labbe (CU Boulder)



<https://pr.omethe.us/>
<https://github.com/pr-omethe-us>

Thank you! Questions?

- Add examples and schema reference to documentation
- Support other fundamental experimental methods: laminar flames, jet-stirred reactors, ...
- Converters to/from other common formats: CSV, NumPy, Excel, etc.



PyKED

<https://github.com/pr-omethe-us/PyKED>

DOI 10.5281/zenodo.546143

build passing

build pending

codecov 100%

Dependency CI passing

code of conduct contributor covenant

license BSD

Anaconda Cloud 0.1.4

XML VS YAML

```

<?xml version="1.0" encoding="utf-8"?>
<experiment>
  <fileAuthor>Laboratory for Chemical Kinetics, ELTE, Budapest, Hungary</fileAuthor>
  <fileVersion>
    <major>1</major>
    <minor>0</minor>
  </fileVersion>
  <ReSpecThVersion>
    <major>1</major>
    <minor>0</minor>
  </ReSpecThVersion>
  <experimentType>Ignition delay measurement</experimentType>
  <bibliographyLink preferredKey="Chaumeix, N., Pichon, S., Lafosse, F., Paillard, C.-E., International Journal of Hydrogen Energy, 2007, 32, 2216-2226, Fig. 12., right, open diamond"></bibliographyLink>
  <apparatus>
    <kind>shock tube</kind>
  </apparatus>
  <commonProperties>
    <property description="" label="P" name="pressure" units="atm">
      <value>2.05</value>
    </property>
    <property name="initial composition">
      <component>
        <speciesLink preferredKey="H2"/>
        <amount units="mole fraction">0.00667</amount>
      </component>
      <component>
        <speciesLink preferredKey="O2"/>
        <amount units="mole fraction">0.00333</amount>
      </component>
      <component>
        <speciesLink preferredKey="Ar"/>
        <amount units="mole fraction">0.99</amount>
      </component>
    </property>
  </commonProperties>
  <dataGroup id="dg1" label="">
    <dataGroupLink dataGroupID="" dataPointID="" />
    <property description="" id="x1" label="T" plotaxis="x" plotscale="inv" name="temperature" units="K"/>
    <property description="" id="x2" label="tau" plotaxis="y" plotscale="log" name="ignition delay" units="us"/>
    <dataPoint>
      <x1>1181.06</x1>
      <x2>560.39</x2>
    </dataPoint>
    <dataPoint>
      <x1>1011.00</x1>
      <x2>1000.00</x2>
    </dataPoint>
  </dataGroup>
</experiment>

```

```

file-author:
  name: Kyle E Niemeyer
  ORCID: 0000-0003-4425-7097
file-version: 0
chemked-version: 0.0.1
reference:
  doi: 10.1016/j.ijhydene.2007.04.008
  authors:
    - name: N. Chaumeix
    - name: S. Pichon
    - name: F. Lafosse
    - name: C.-E. Paillard
  journal: International Journal of Hydrogen Energy
  year: 2007
  volume: 32
  pages: 2216–2226
  detail: Fig. 12., right, open diamond
experiment-type: ignition delay
apparatus:
  kind: shock tube
  institution: CNRS-ICARE
  facility: stainless steel shock tube
common-properties:
  pressure: &pres
    - 220 kilopascal
  composition: &comp
    kind: mole fraction
    species:
      - species-name: H2
        InChI: 1S/H2/h1H
        amount:
          - 0.00444
      - species-name: O2
        InChI: 1S/O2/c1-2
        amount:
          - 0.00556
      - species-name: Ar
        InChI: 1S/Ar
        amount:
          - 0.99
  ignition-type: &ign
    target: pressure
    type: d/dt max

```

References

1. http://hanson.stanford.edu/index.php?loc=facilities_kst
2. <http://combdiaglab.enr.uconn.edu/facilities/rapid-compression-machine/new-rapid-compression-machine>
3. <http://combdiaglab.enr.uconn.edu/facilities/atmospheric-pressure-counterflow-setup-for-flame-studies>
4. Olivier Herbinet, Dayma Guillaume. Jet-Stirred Reactors. F Battin-Leclerc, J M Simmie, E Blurock, eds. *Cleaner Combustion: Developing Detailed Chemical Kinetic Models*, Springer, pp. 183–210, 2013, Green Energy and Technology, 978-1-4471-5306-1. <10.1007/978-1-4471-5307-8>. <[hal-00880195](https://hal.archives-ouvertes.fr/hal-00880195)>
5. <http://www.chemicaldynamics.lbl.gov/flames.html>

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