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

Bryan W Weber
University of Connecticut

Kyle E Niemeyer
Oregon State University

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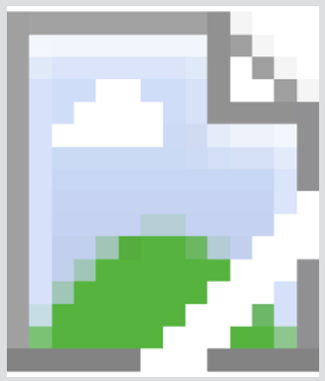
Kyle.Niemeyer@oregonstate.edu
@kyleniemeyer
https://git.io/nrg

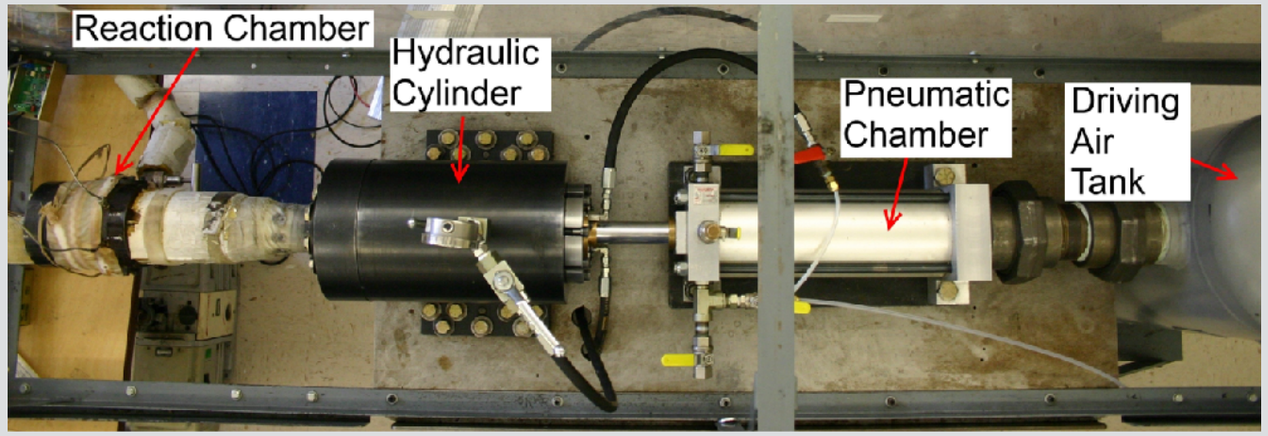
ChemKED: **Chem**ical **K**inetic **E**xperimental **D**ata

PyKED: **Py**thon software for working with ChemKED

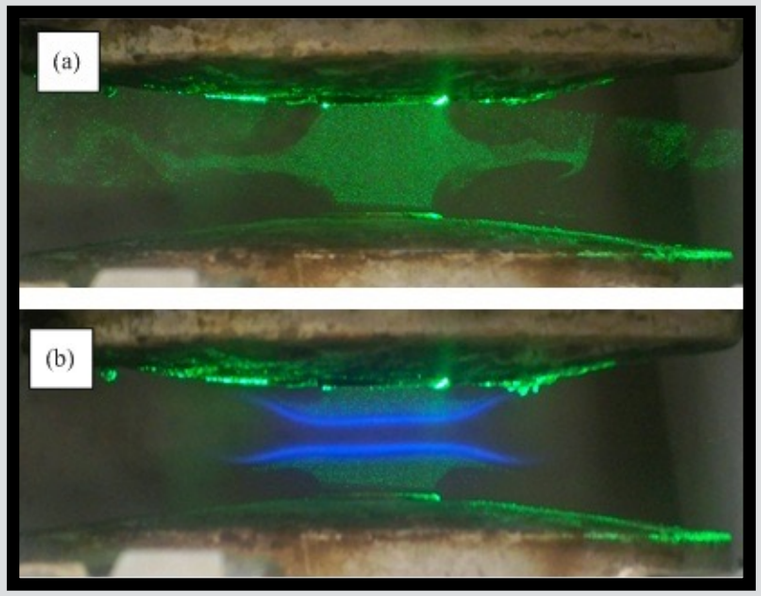


Validation, schmalidation.

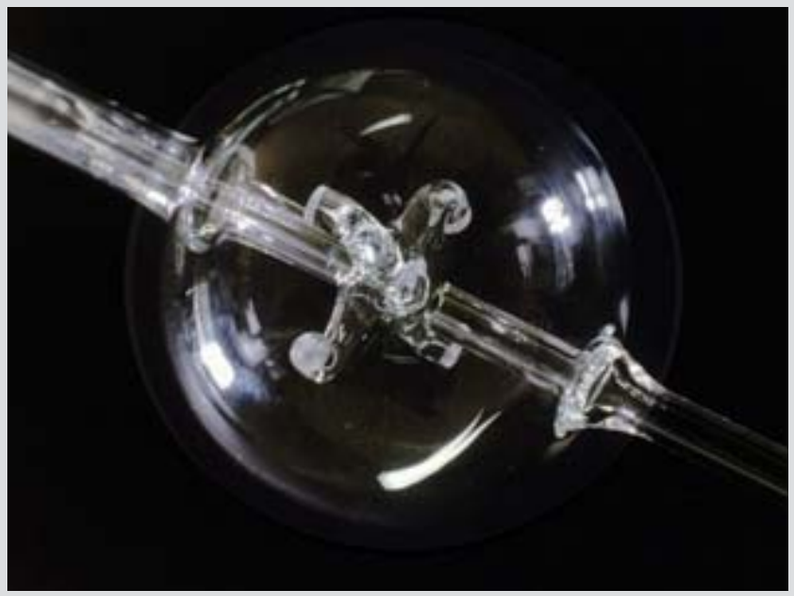
Shock tube[1]



Rapid compression machine[2]

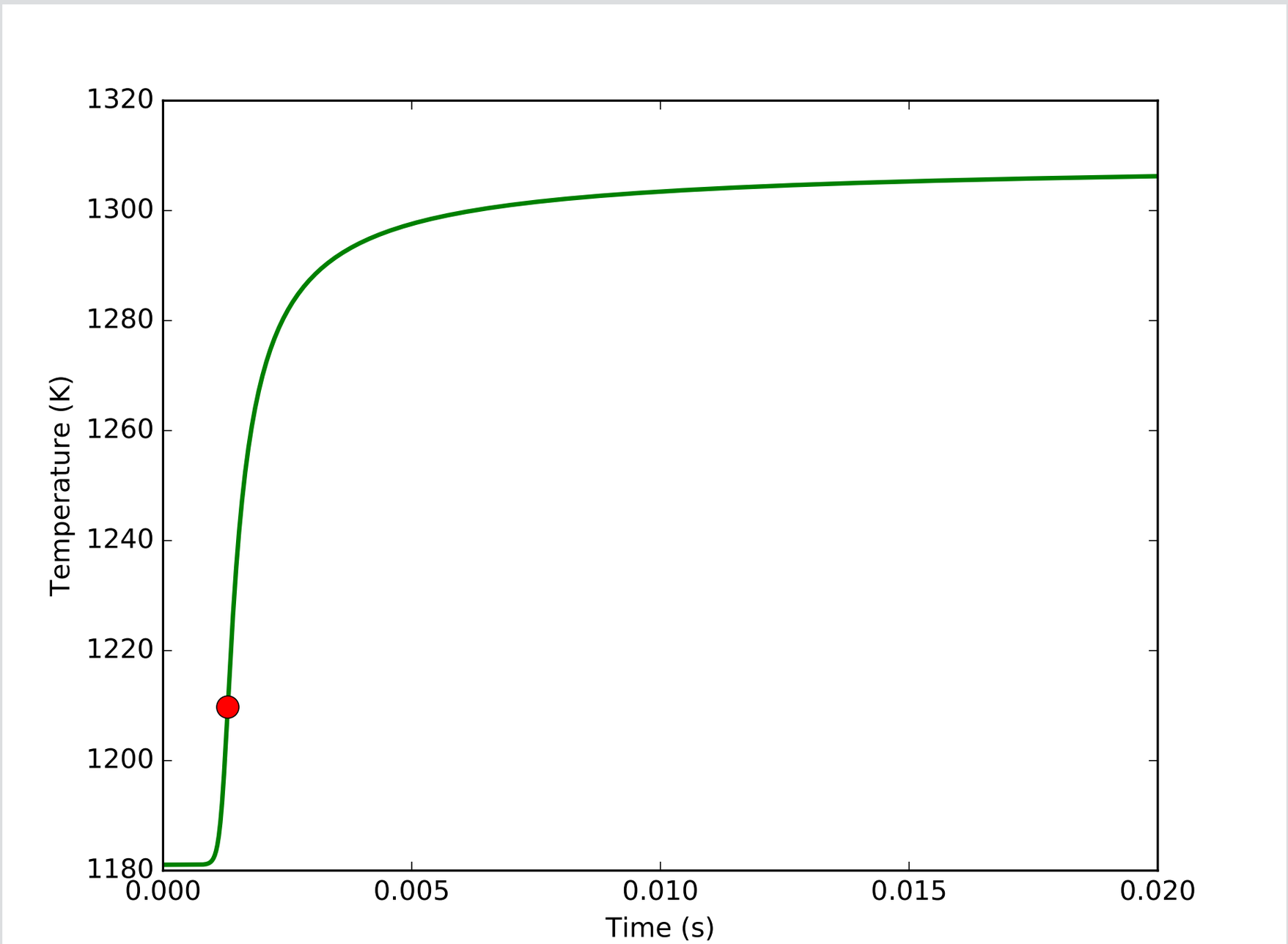


Counterflow flame[3]



Jet-stirred reactor[4]

Autoignition



The problem: experimental data

Series	Shock No.	Composition % C_7H_{16}	Composition % O_2	P_1 torr	P_5 atm	T_5 K	ρ_5/ρ_1	U_5 mm/µsec	τ µsec
	6	1	11	116	4.66	1260	7.27	.3778	323
A	10	1	11	105	5.17	1410	7.95	.3913	70
	14	1	11	103	4.52	1323	7.56	.3835	170
	22	1	11	50	2.03	1268	7.30	.3785	647
B	29	1	11	70	3.15	1341	7.64	.3851	155
	37	1	11	50	3.08	1602	8.75	.4077	25
	41	0.5	11	100	3.81	1311	6.62	.4014	200
C	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 table[5]

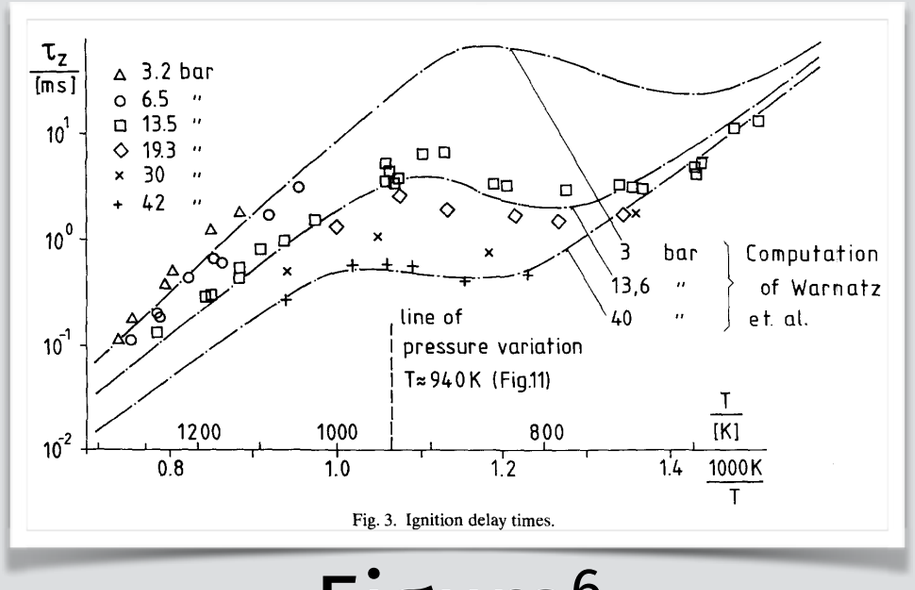


Fig. 3. Ignition delay times.

Figure[6]

```
# n-heptane ignition delay from Colket and Spadaccini 2001
# P (atm), T (K), Ignition Delay (µs)
# 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 file[7]

Kyle Niemeyer August 19, 2014 at 7:38 PM

To: jeff.bergthorson@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

Related work

- PrIMe (**Pr**ocess **I**nformatics **M**odel): Frenklach et al. (http://primekinetics.org)
  - XML-based standard
  - Problems: XML, reliance on internal identifiers, missing some necessary information, & closed nature
- ReSpecTh: Varga et al. (http://respecth.hu/)
  - Evolution of PrIMe—now includes more data needed to reproduce experiment
  - Problems: still XML, still closed

Our solution(s)

ChemKED: Chemical **K**inetics **E**xperimental **D**ata format

+

PyKED: Python software for working with Chem**KED** files

ChemKED

Written in YAML

Human- AND machine-readable!

Parsers and libraries for nearly every programming language!

```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/O2/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 components

```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
```

ChemKED components (2)

```yaml
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
```

ChemKED components (3)

```yaml
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
```

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

```yaml
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
...
```

PyKED

- Version control: git & GitHub (github.com/pr-omethe-us/PyKED)
- Validation of files: cerberus (python-cerberus.org)
  - DOI validation: Crossref lookup via habanero (habanero.rtfd.org)
  - ORCID lookup via orcid (github.com/ORCID/python-orcid)
  - Interpreting & converting units (including uncertainties!): Pint (pint.readthedocs.org) & uncertainties (pythonhosted.org/uncertainties/)
- Code unit testing: pytest (docs.pytest.org), with codecov-measured test coverage
- Continuous integration: Travis-CI (travis-ci.org)

Validation

- PyKED validates ChemKED YAML files using our validation schema
- Ensures required data are present, appropriate units, bounded values, etc.
- Ensures reference information is valid and correct if DOI is provided

```yaml
# 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:
```

Example: RCM

```yaml
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
```

```yaml
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

```python
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()
```

Plans for ChemKED/PyKED

- Add examples to documentation
- Support other fundamental experimental methods: laminar flames and 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)

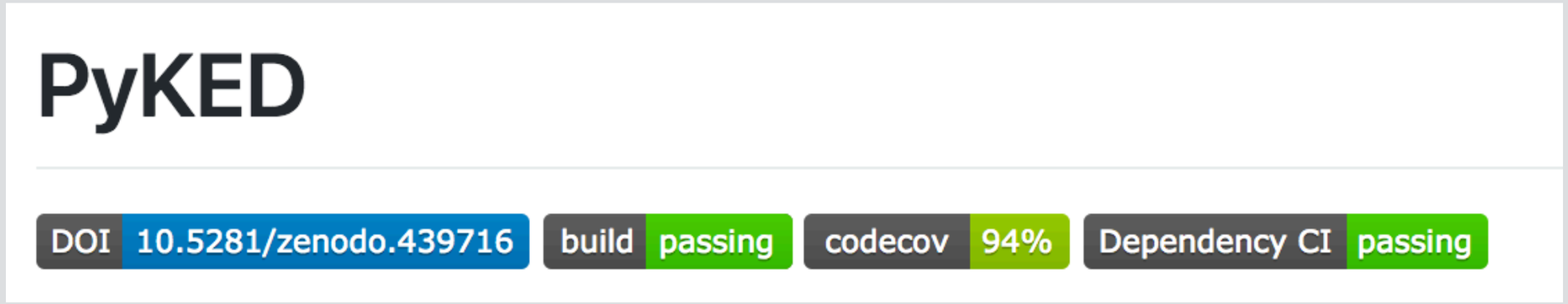
https://pr.omethe.us/

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

Thank you! Questions?

?

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



XML vs YAML

```xml
<?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
    <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>
```

```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/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.engr.uconn.edu/facilities/rapid-compression-machine/new-rapid-compression-machine
3. http://combdiaglab.engr.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>