Development of Automated Calibration Tools for Determining Fire Model Input Parameters

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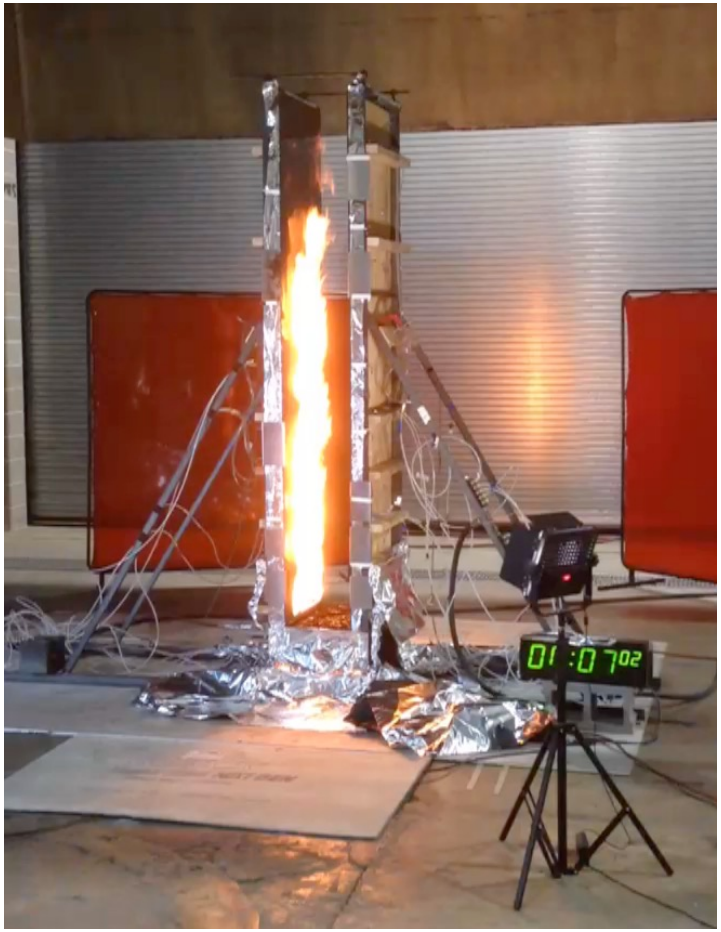
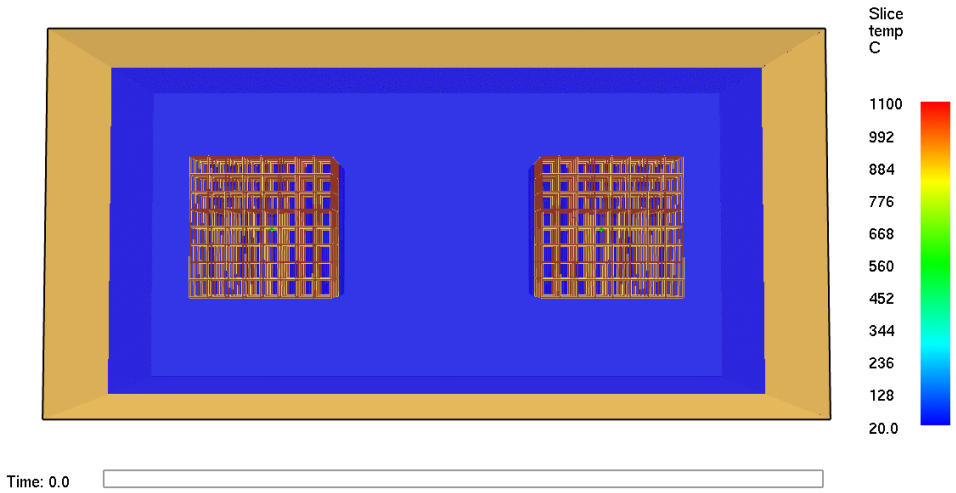
Predicting Fire Growth

- To engineer safer:
  - Buildings
  - Products
  - Materials
- Accurate predictions require **condensed phase pyrolysis models**



Condensed Phase Challenges



- Physics
  - Multiphase
  - Mechanical deformation
- Numerics
  - Gas phase coupling
  - Multiscale
  - Moving boundary
- **Materials**
  - Many parameters
  - Many materials

How Many Parameters?

$$\frac{\partial \rho_i}{\partial t} = \dot{m}_i''', \quad i = 1, \ldots N$$

$$\rho c \frac{\partial T}{\partial T} = \nabla \cdot (k \nabla T) + \dot{q}'''$$

$$\dot{m}_i''' = -A_i \rho_i \exp\left(-\frac{E_i}{RT}\right), \quad i = 1, \ldots, N$$

$$\rho c = \sum_{i=1}^{N} \rho_i c_i$$

$$k = f\left(\rho_1, \ldots, \rho_N, k_1, \ldots, k_N\right)$$

$$\dot{q}''' = -\sum_{i=1}^{N} \Delta h_i \dot{m}_i'''$$

$$\rho_i\left(t = 0\right) = \rho_{0,i}, \quad i = 1, \ldots, N$$

Neglecting
- Radiation
- Mass transport
- Charring
- Temperature dependence

At least ~$6N$ material property parameters need to be quantified

How many materials?

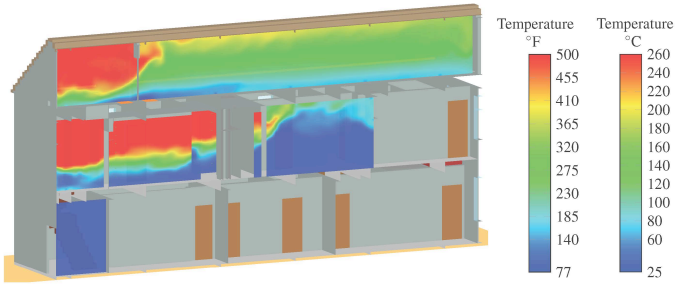
- NFIRS categorizes **38 distinct "types"** of solid materials "First Ignited"
- These "types" are extremely broad categories such as "Plastic", "Rubber", and "Plywood"
- For example, Lyon and Janssens (2005) contains data on **50 common plastics**
- Additional diversity due to processing variability, additives, blends, ageing, etc.

On the order of 10^3 distinct materials relevant to fire growth predictions

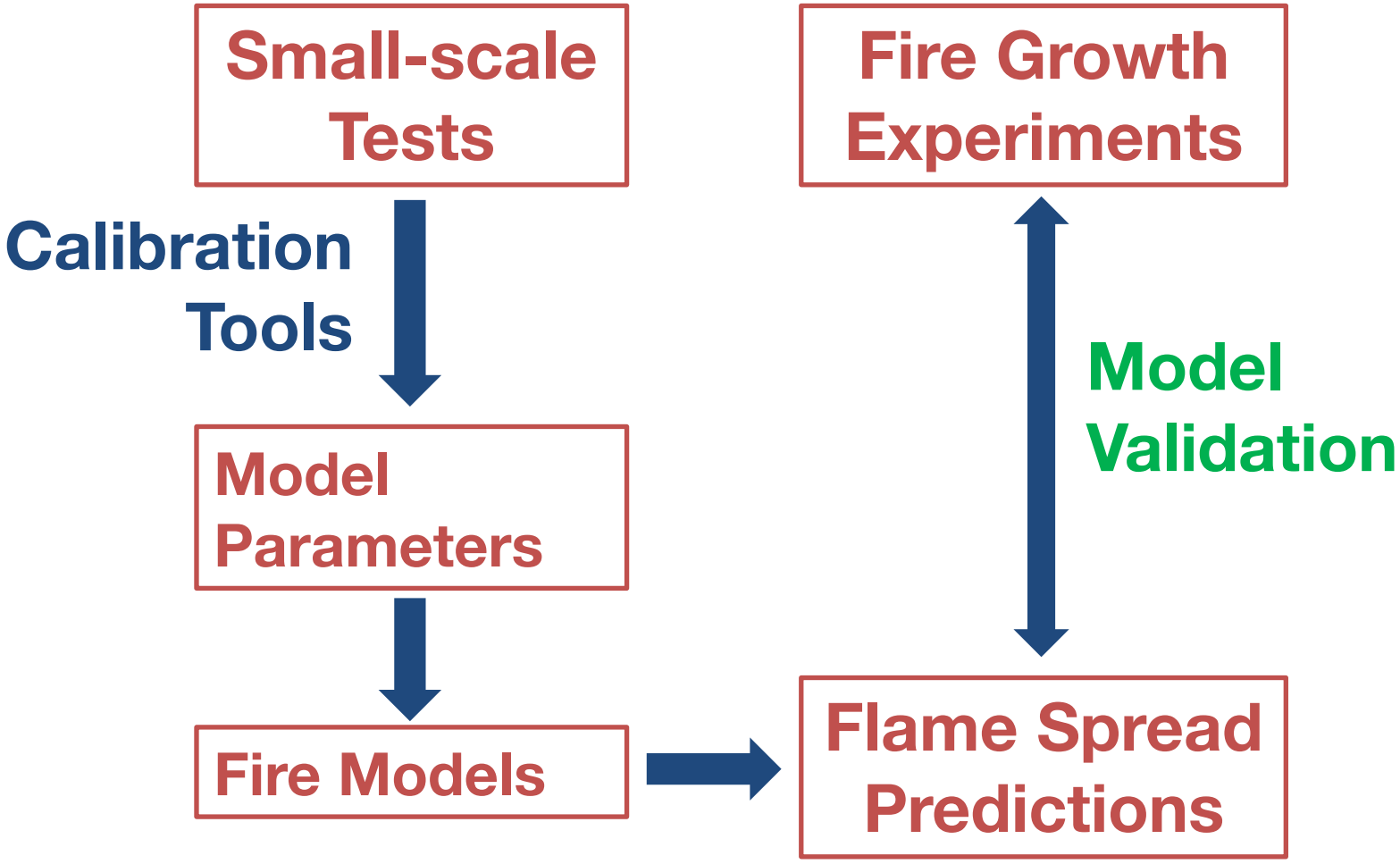
$(10^1$ Parameters) × $(10^3$ Materials)
= **10^4 Properties for reliable fire growth predictions**

A **Material Property Database** is needed

Material Property Database



- See previous presentation…
- Adopting “Hierarchical” approach
- Critical components
  1. Standard formatting
  2. Standard metadata
  3. **Calibration tools**



Quality of **calibration tools** is ultimately determined in **model validation**—*do the parameters predict fire growth?*

Global Approach

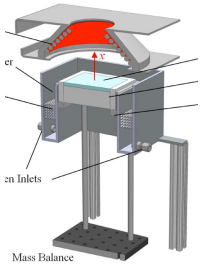
$$A_i, E_i, c_i, k_i, \Delta h_i, \rho_{0,i}$$

Fire Model

Hierarchical Approach

$$A_i, E_i, \rho_{0,i}$$

$$c_i, \Delta h_i$$



$$k_i$$

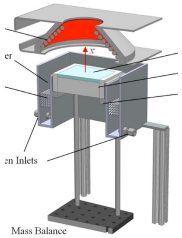
Micro Combustion Calorimeter

$\Delta h_{c,i}$

Thermogravimetric Analysis

$A_i, E_i, \rho_{0,i}$

Controlled Atmosphere Pyrolysis



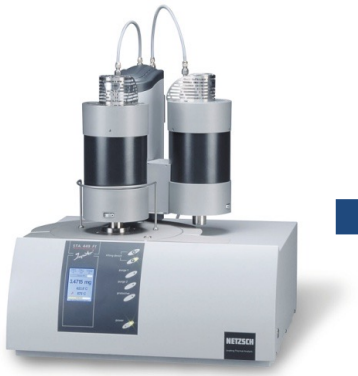
k_i

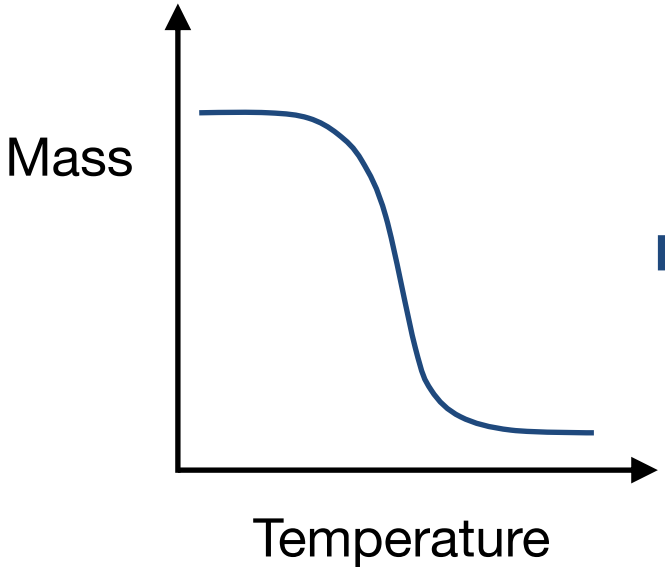
Differential Scanning Calorimetry

$c_i, \Delta h_i$

Analysis of TGA Data

How should we estimate pyrolysis kinetic parameters from raw TGA data?



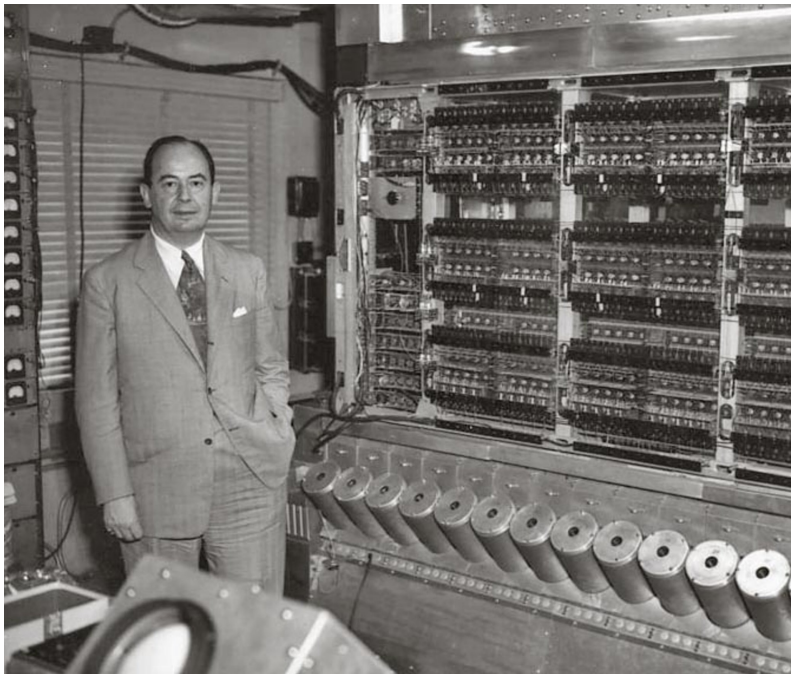


$A_i, E_i, \rho_{0,i}$

Method Requirements

1. Parameters predict data → **Accurate**
2. Many different materials → **Efficient**
3. Many different behaviors→ **Robust**
4. Parameters do not vary → **Consistent**

How to be Consistent



"With four parameters I can fit an elephant, and with five I can make him wiggle his trunk."

~John von Neumann

1. **No free parameters**
2. **No random numbers**

For given data, the method should always produce the same parameters

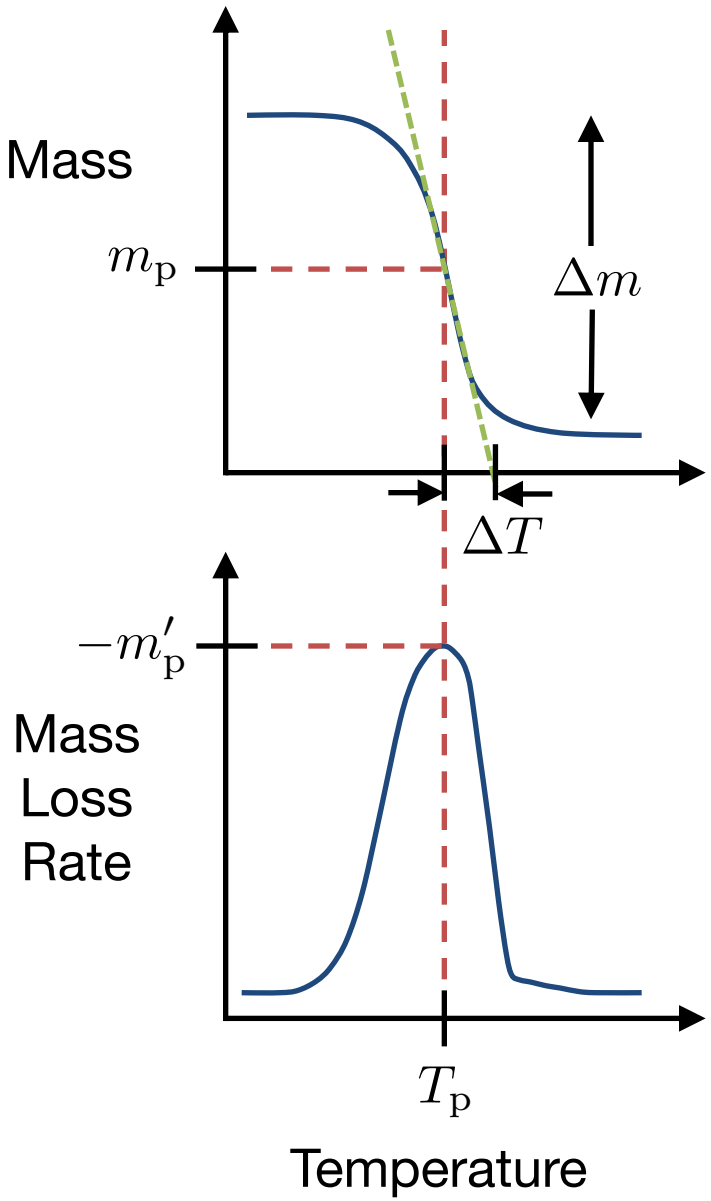
Pyrolysis Model: Independent First-Order Reactions

$$\text{Reactant} \xrightarrow{k} \nu\text{Char} + (1-\nu)\,\text{Gas}$$

$$k = \left(\frac{A}{\beta}\right)\exp\left(-\frac{E}{RT}\right)$$

$$m' \equiv \frac{\mathrm{d}m}{\mathrm{d}T} = -(1-\nu)\,km, \quad m(T_0) = m_0$$

Appropriateness to be determined by ability to predict fire growth.



Characteristic temperature and mass changes:

$$\Delta T \equiv \frac{m_\mathrm{p}}{-m'_\mathrm{p}}$$

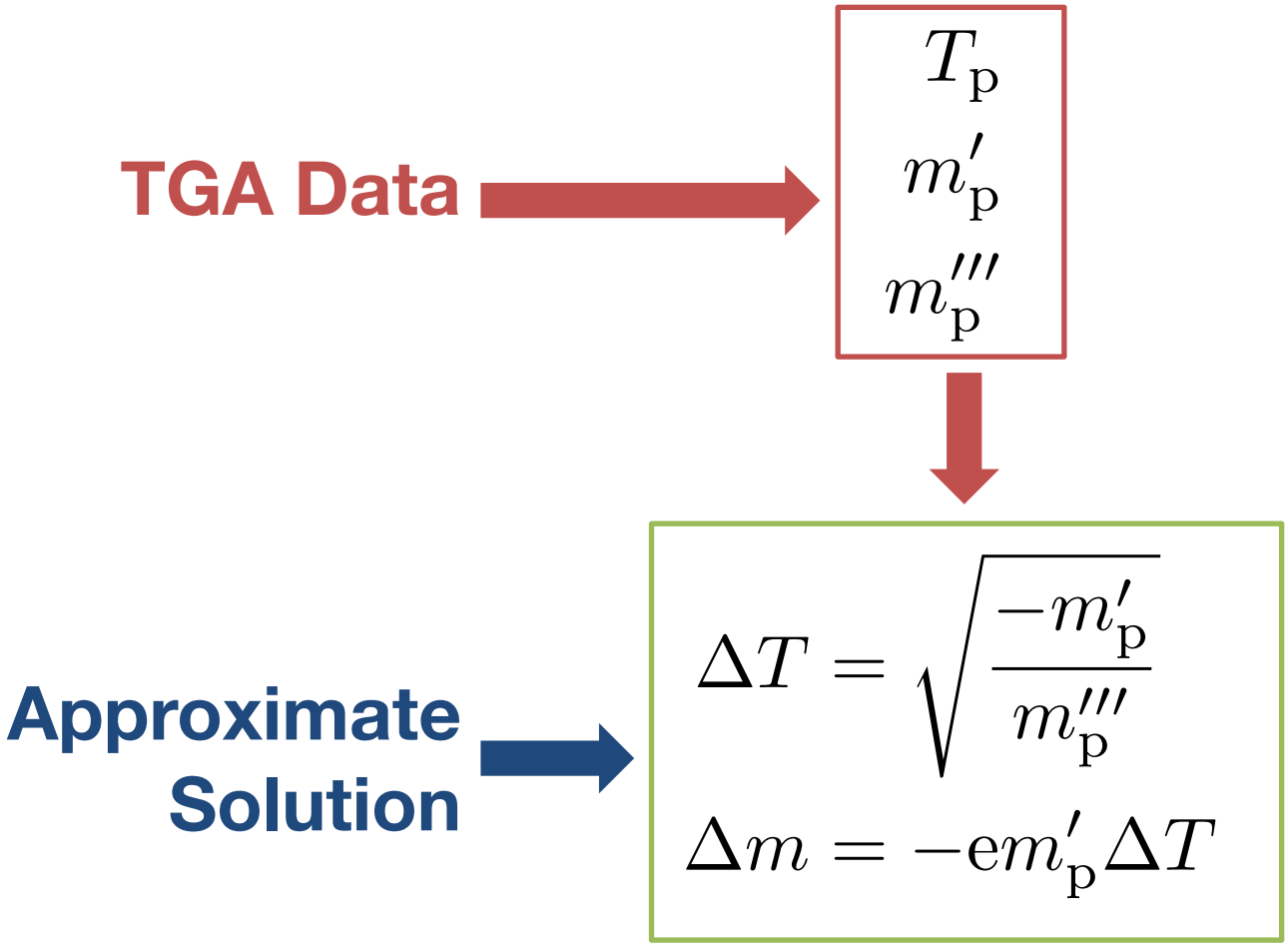
$$\Delta m \equiv m_0 \left(1 - \nu\right)$$

Analysis of peak condition yields:

$$E = \frac{RT_\mathrm{p}^2}{\Delta T}$$

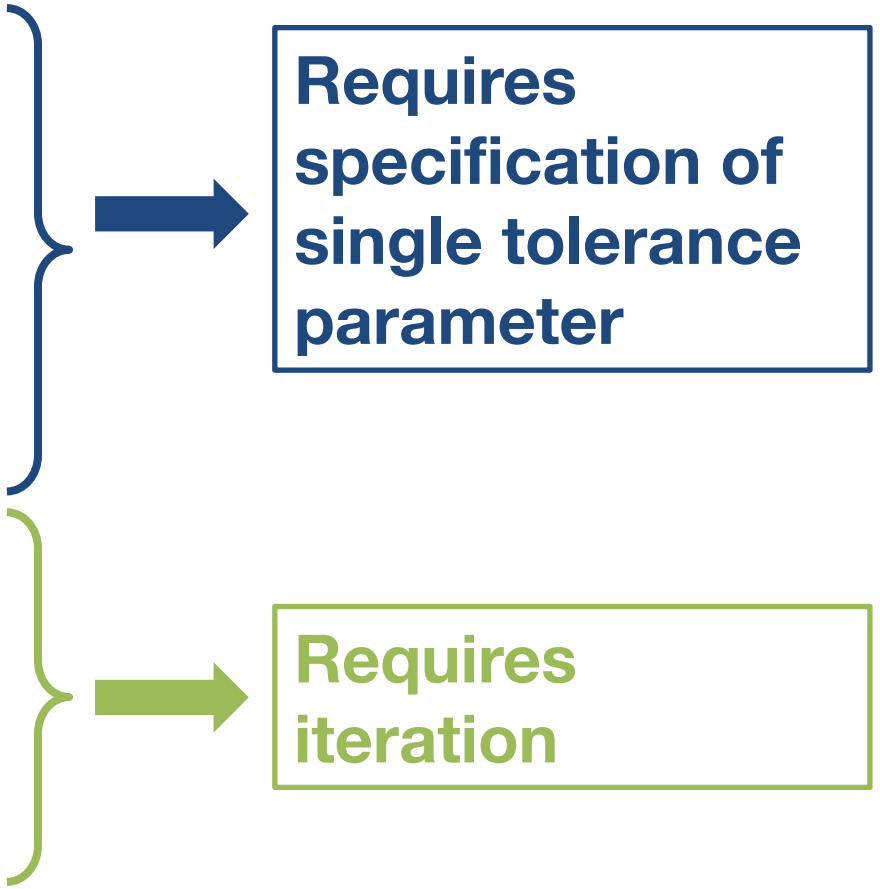
$$A = \frac{\beta}{\Delta T} \exp\left(\frac{T_\mathrm{p}}{\Delta T}\right)$$

Estimating Parameters



Some Details

1. Smoothed data derivatives are found using Savitzky-Golay filter
2. “Small” mass loss rate peaks are neglected
3. Algorithm corrects for overlapping reactions
4. Mass changes corrected to conserve mass



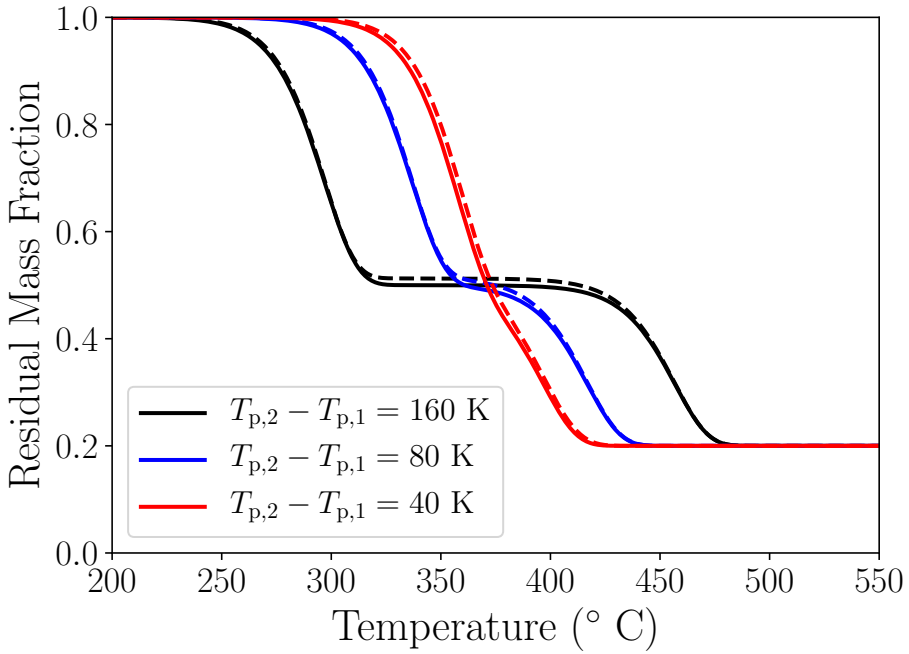
TGA Fit Verification

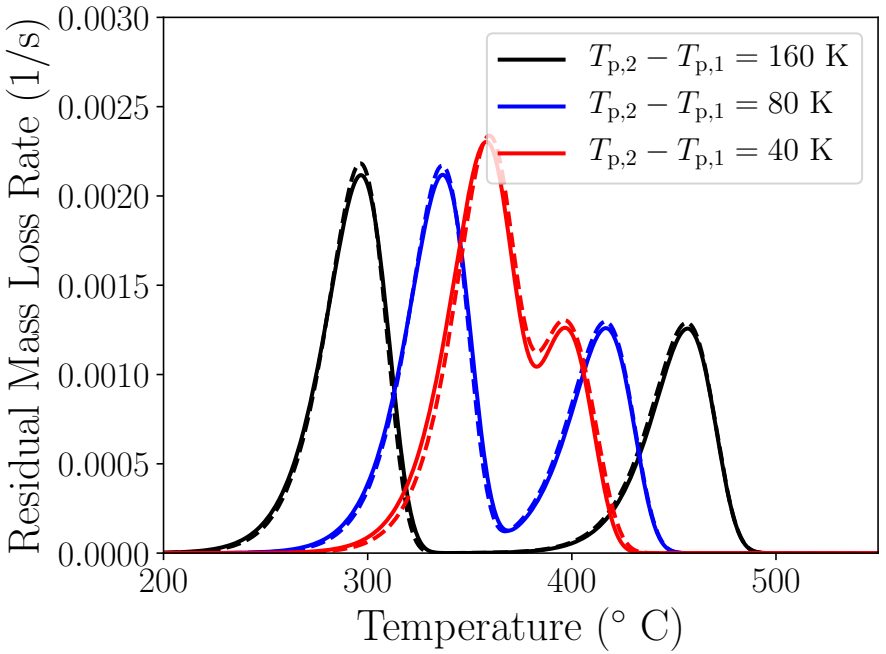
1. Assume **kinetic parameters**
2. Generate TGA data
3. Use algorithm to find assumed parameters

Purpose:

1. Check implementation
2. Test validity of approximate solution

Two Reactions Verification





Closer fit for more separated reactions

Validation

Purpose:

1. Test algorithm with real TGA data

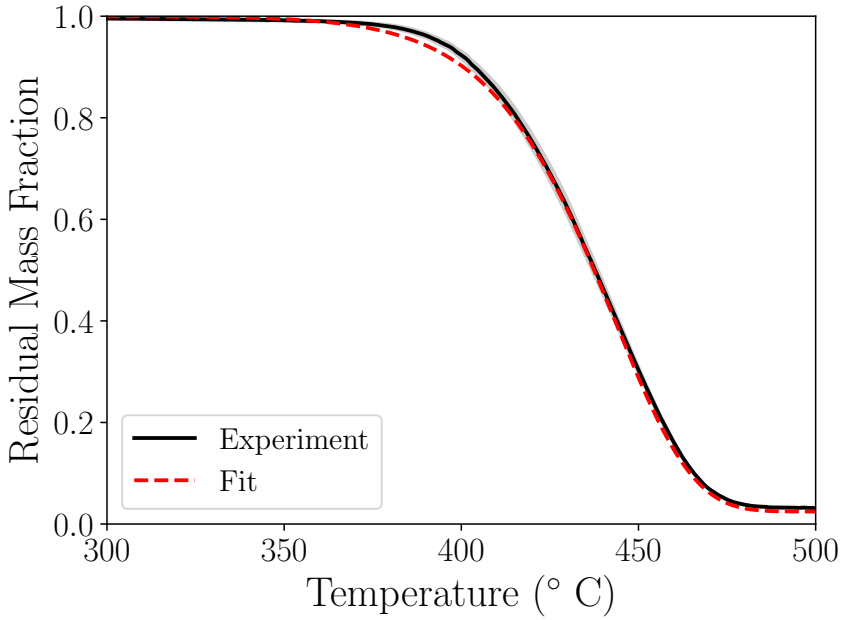
Test Materials:

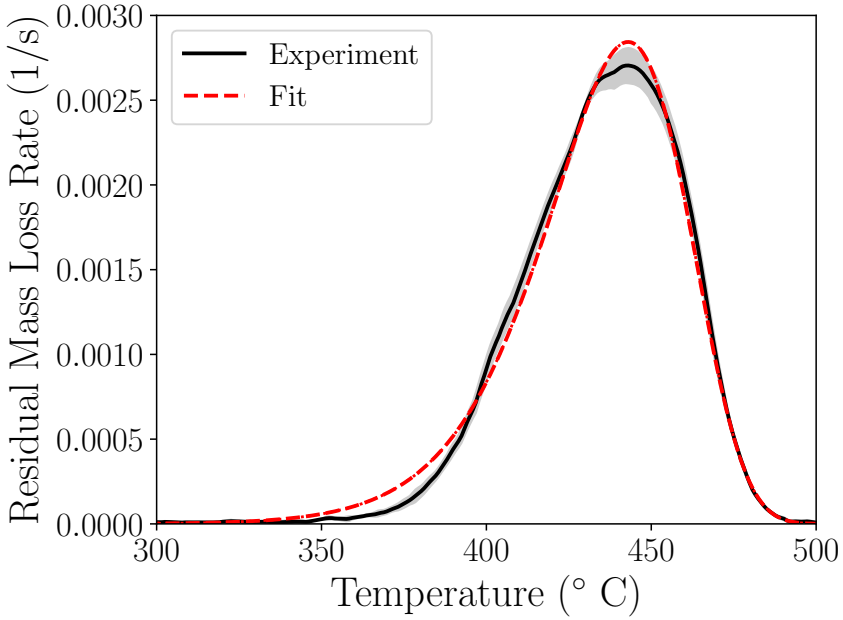
1. Nylon 6,6
2. Flexible polyurethane (PU) foam
3. Polyvinyl Chloride (PVC)

Procedure:

- In nitrogen
- Samples: 3-5.5 mg
- Isothermal heating for 20-30 min
- Dynamic heating at 10 K/min

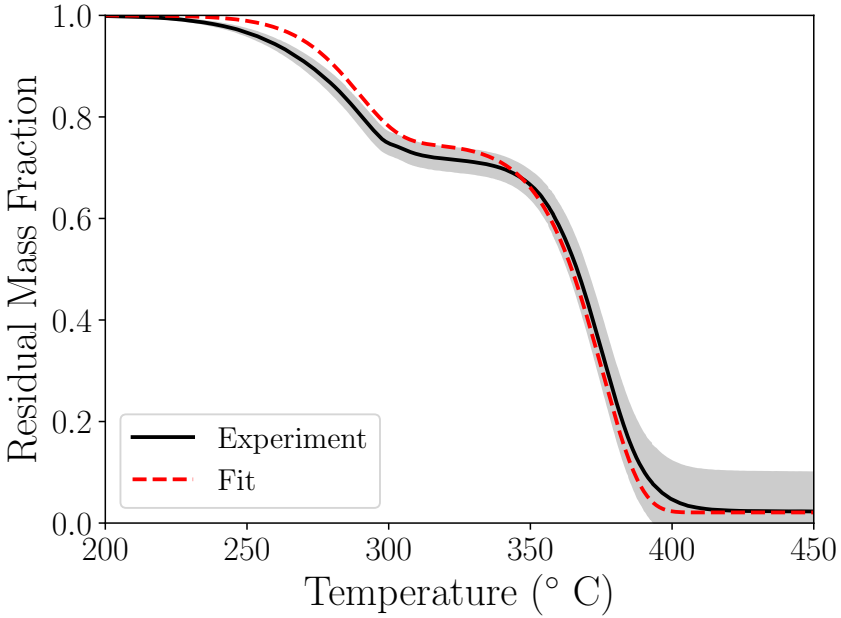
Validation: Nylon 6,6

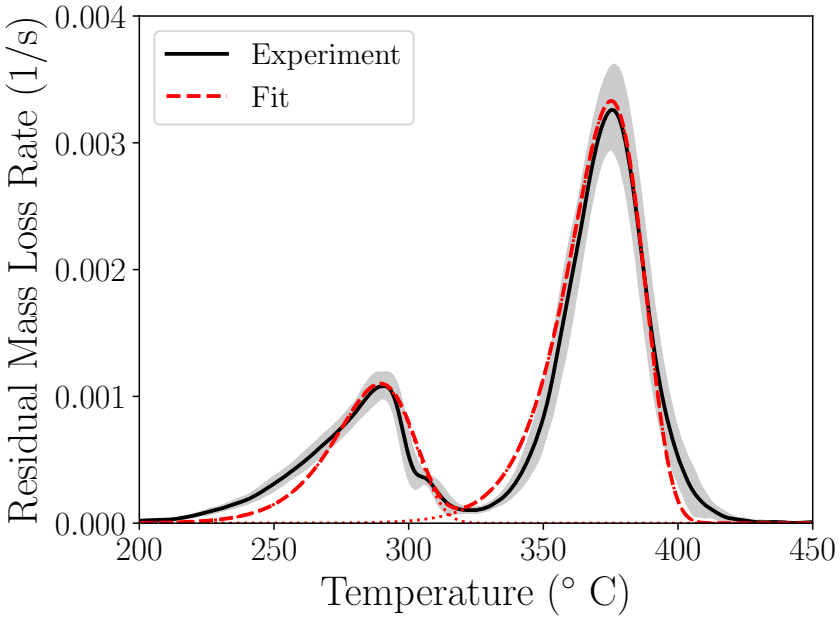




Kinetic Parameter	Reaction 1
T_p (K)	716.3
ΔT (K)	22.11
Δm	0.9754
ξ	0.03087
$\ln[A\ (s^{-1})]$	27.50
E (kJ/kmol)	192.9×10^3

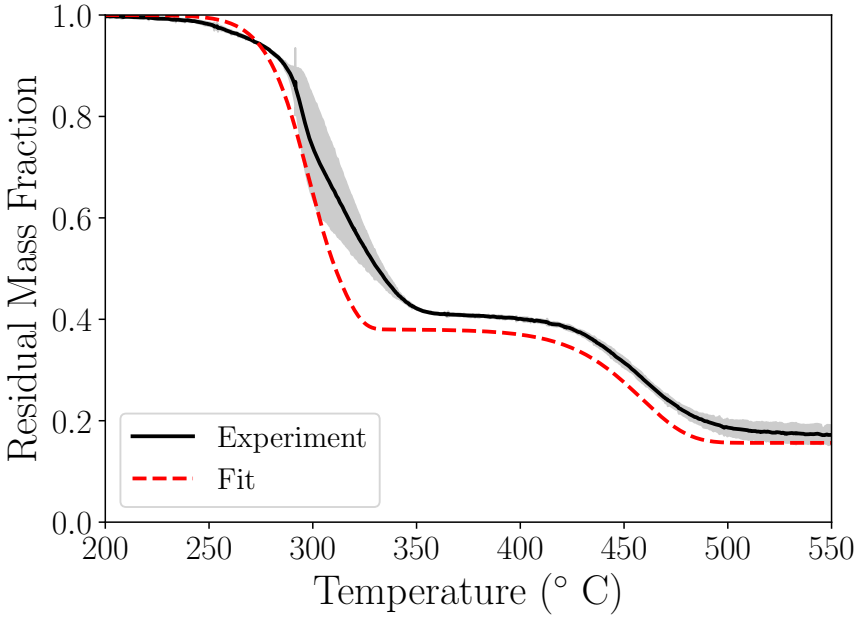
Validation: Polyurethane Foam

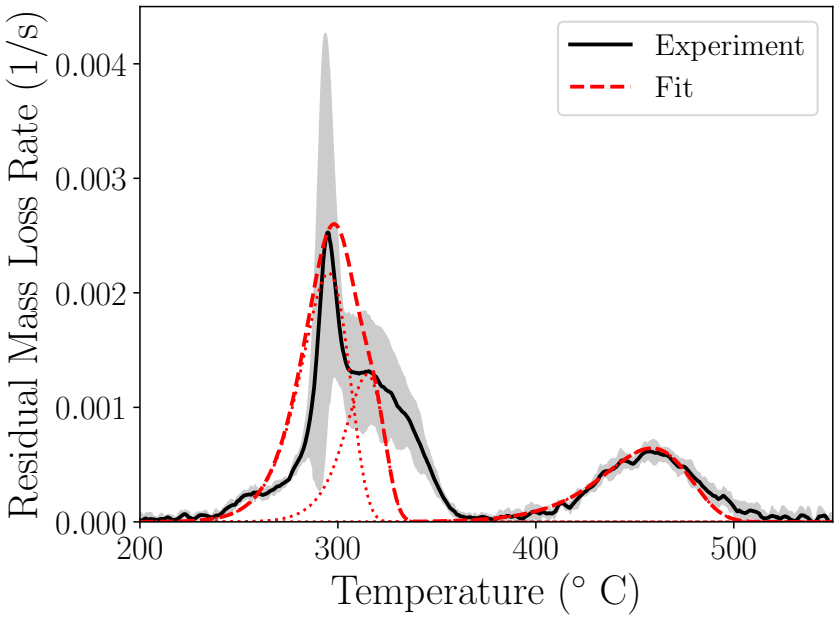




Kinetic Parameter	Reaction 1	Reaction 2
T_p (K)	562.7	648.5
ΔT (K)	14.50	13.69
Δm	0.2511	0.7280
ξ	0.02577	0.02112
$\ln[A\ (s^{-1})]$	34.34	42.95
E (kJ/kmol)	181.5×10^3	255.3×10^3

Validation: PVC



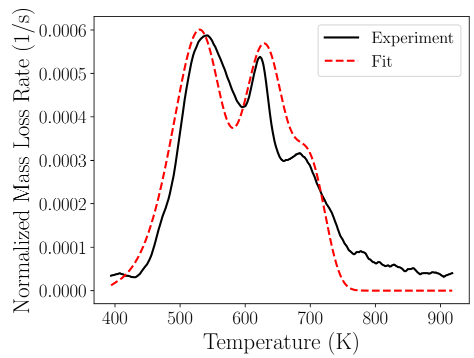


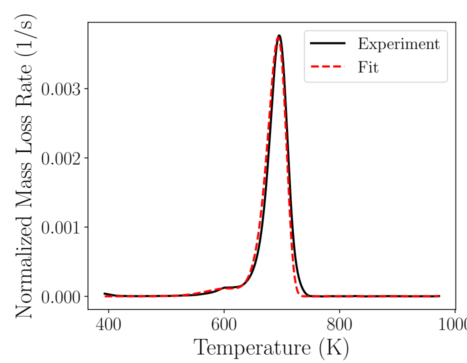
Kinetic Parameter	Reaction 1	Reaction 2	Reaction 3
T_p (K)	568.5	731.7	588.1
ΔT (K)	12.15	22.39	9.62
Δm	0.4200	0.2238	0.1999
ξ	0.02138	0.03060	0.01636
$\ln[A\ (s^{-1})]$	42.49	27.78	57.06
E (kJ/kmol)	221.1×10^3	198.8×10^3	298.8×10^3

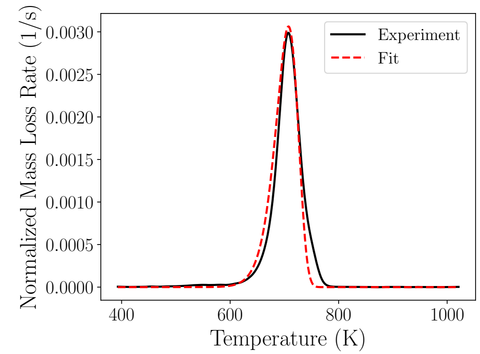
Validation Summary

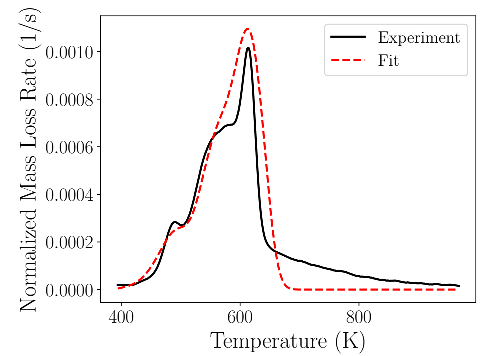
25 materials:

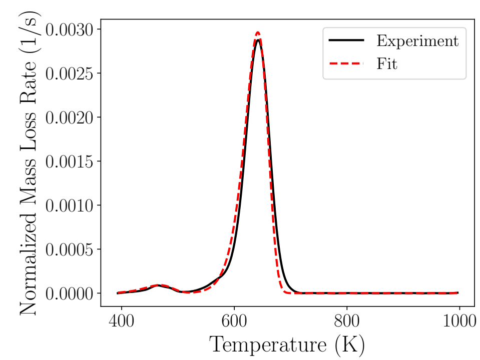
```
# list of all current TGA test series
tga_tests = [
    'ABS_Expt_TGA_N2_10K',
    'BigBerry-Leaf_Expt_TGA_N2_10K',
    'BigBerry-Stem_Expt_TGA_N2_10K',
    'Chamise-Leaf_Expt_TGA_N2_10K',
    'Chamise-Stem_Expt_TGA_N2_10K',
    'Chaparral-Leaf_Expt_TGA_N2_10K',
    'Chaparral-Stem_Expt_TGA_N2_10K',
    'DesertCeanothus-Leaf_Expt_TGA_N2_10K',
    'DesertCeanothus-Stem_Expt_TGA_N2_10K',
    'DouglasFir-Leaf_Expt_TGA_N2_10K',
    'HDPE_Expt_TGA_N2_10K',
    'HIPS_Expt_TGA_N2_10K',
    'Kydex_Expt_TGA_N2_10K',
    'LodgepolePine-Leaf_Expt_TGA_N2_10K',
    'LodgepolePine-Stem_Expt_TGA_N2_10K',
    'MaCFP_PMMA_Expt_TGA_N2_10K',
    'PolyIso1_Expt_TGA_N2_10K',
    'PolyIso2_Expt_TGA_N2_10K',
    'PolyIso05_Expt_TGA_N2_10K',
    'POMGF_Expt_TGA_N2_10K',
    'XPSgreen_Expt_TGA_N2_10K',
    'XPSpink_Expt_TGA_N2_10K'
]
```



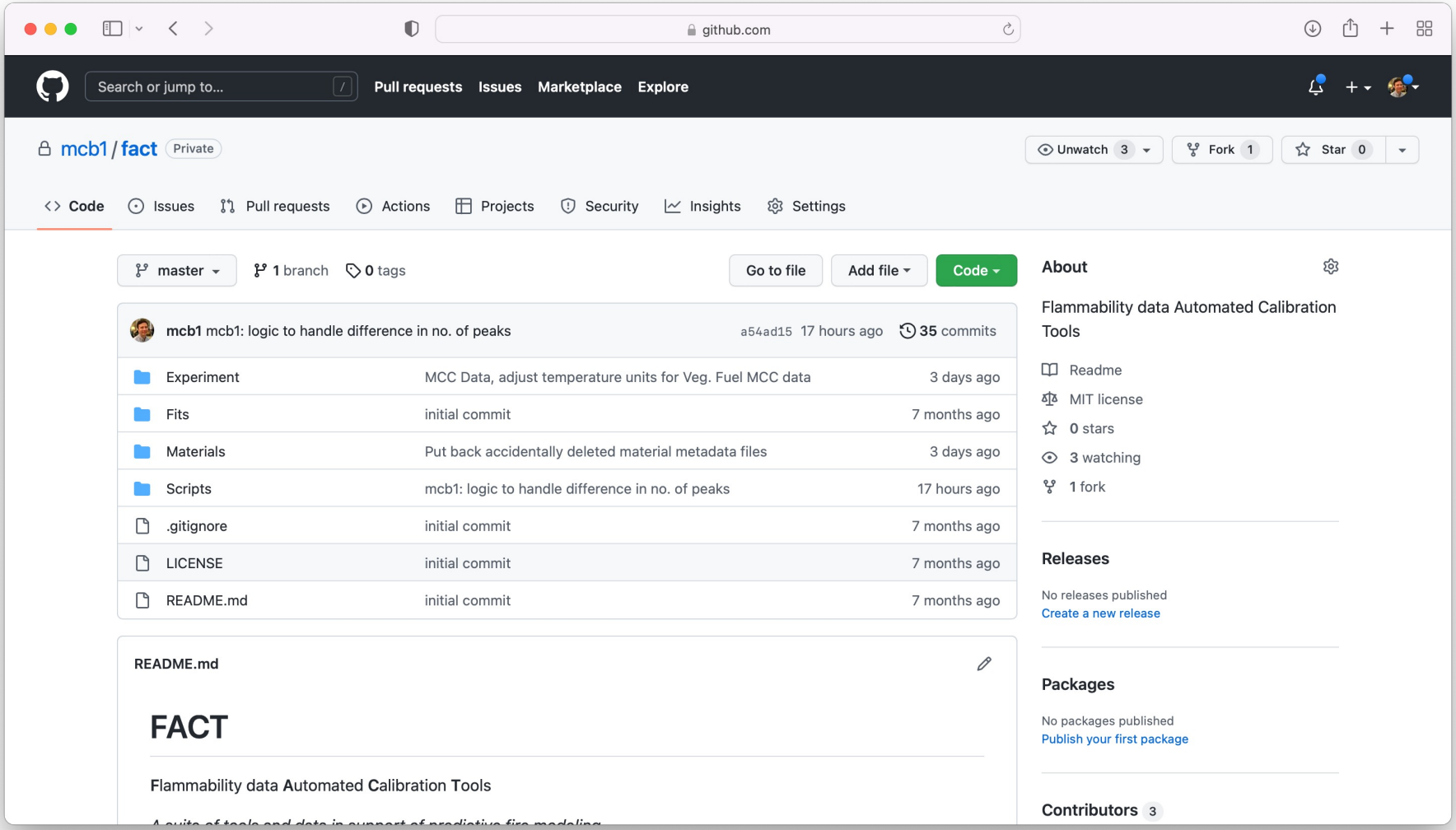




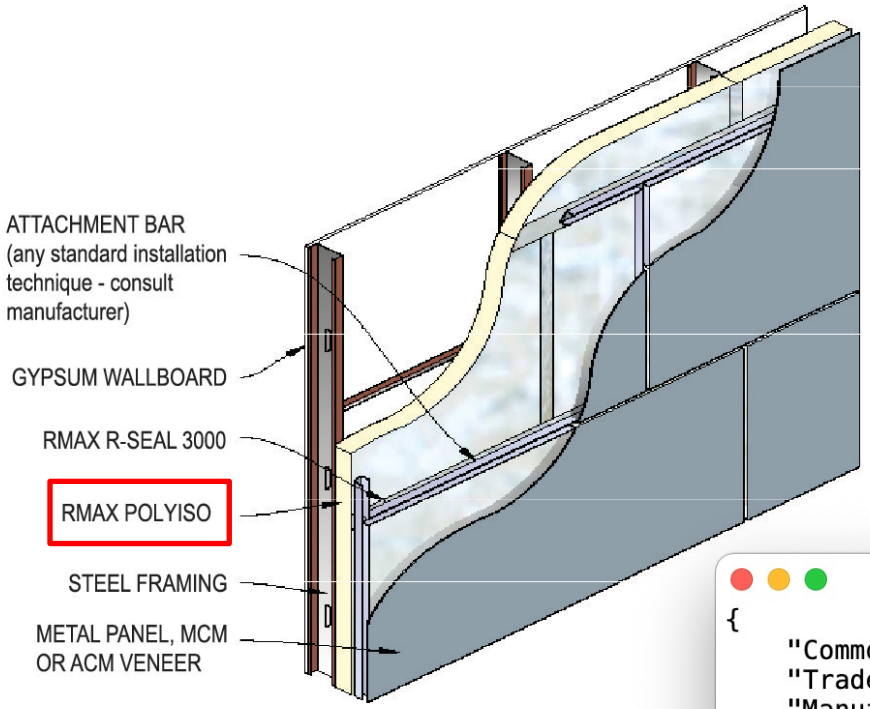




FACT: **F**lammability data **A**utomated **C**alibration **T**ools



Example: Polyisocyanurate Board Insulation



www.rmax.com

`fact/Materials/metadata/PolyIso2.json`

PolyIso2.json

```
{
    "Common Names": ["Poly(Isocyanurate) foam", "PolyIso foam"],
    "Trade Name": "Thermasheath",
    "Manufacturer": "RMAX",
    "Distributor": "Lowe's",
    "Date Acquired": "February 2020",
    "Description": "Yellow polyiso foam core bonded to Kraft-paper-
reinforced aluminum facers on each side; both sides have a reflective
surface; nominal thickness 2in. (50.5 to 51.7 mm)",
    "Categories": ["Synthetic Polymer", "Porous Foam", "Thermoset"]
}
```

Replicate TGA Data Files:

```
Time,Temperature,Mass
[s],[K],[mg]
0,300.772,5.64900711774
4.998,300.77222,5.65034706054
9.996,300.77115,5.64897096414
14.994,300.77005,5.64900768264
19.992,300.77194,5.64766717494
24.99,300.77516,5.64650687034
29.988,300.79185,5.64423088824
34.986,300.8111,5.64203116764
39.984,300.87397,5.63949985074
```

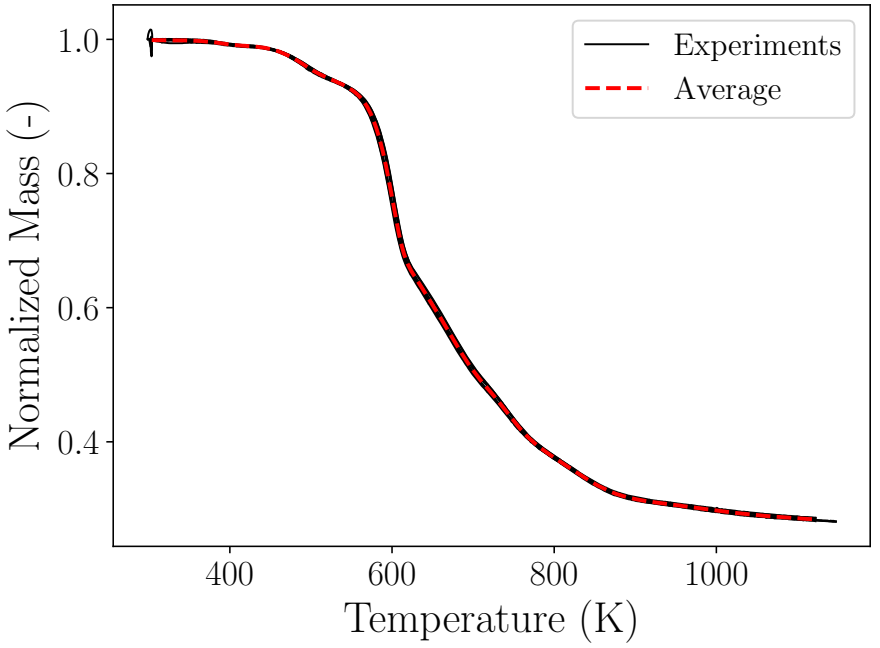
```
Time,Temperature,Mass
[s],[K],[mg]
0,303.653,4.53640016592
4.998,303.64491,4.53640016592
9.996,303.6319,4.53640016592
14.994,303.62205,4.53606994512
19.992,303.609,4.53472955712
24.99,303.60149,4.53220890192
29.988,303.591,4.52989826352
34.986,303.57958,4.52413981152
39.984,303.57796,4.51468270512
```

```
Time,Temperature,Mass
[s],[K],[mg]
0,298.818,4.88188150002
4.998,298.82011,4.88322139522
9.996,298.81941,4.88378928812
14.994,298.81898,4.88289179272
19.992,298.83343,4.88321602392
24.99,298.85833,4.88321700052
29.988,298.90316,4.88323457932
34.986,298.98718,4.88329171042
39.984,299.0697,4.88474342632
```

```
Time,Temperature,Mass
[s],[K],[mg]
0,301.008,4.23159800954
4.998,301.00631,4.23159800954
9.996,301.00344,4.23025805184
14.994,301.00297,4.23025805184
19.992,301.00235,4.23128787724
24.99,301.00844,4.22795131064
29.988,301.01631,4.22486945024
34.986,301.03529,4.22067695234
39.984,301.09055,4.21446457504
```

• • •

```
(base) Scripts $ python average_tga_series.py PolyIso2_Expt_TGA_N2_10K
============================================================

Reading data from:

   PolyIso2_Expt_TGA_N2_10K_r7.csv
   PolyIso2_Expt_TGA_N2_10K_r6.csv
   PolyIso2_Expt_TGA_N2_10K_r4.csv
   PolyIso2_Expt_TGA_N2_10K_r5.csv
   PolyIso2_Expt_TGA_N2_10K_r2.csv
   PolyIso2_Expt_TGA_N2_10K_r3.csv
   PolyIso2_Expt_TGA_N2_10K_r8.csv

Number of data sets in series =  7

============================================================
```

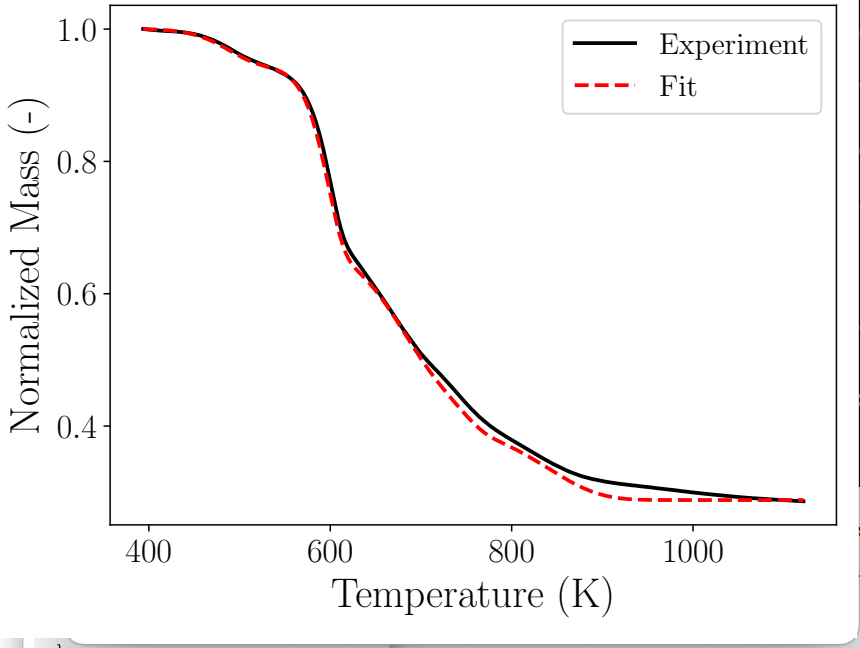


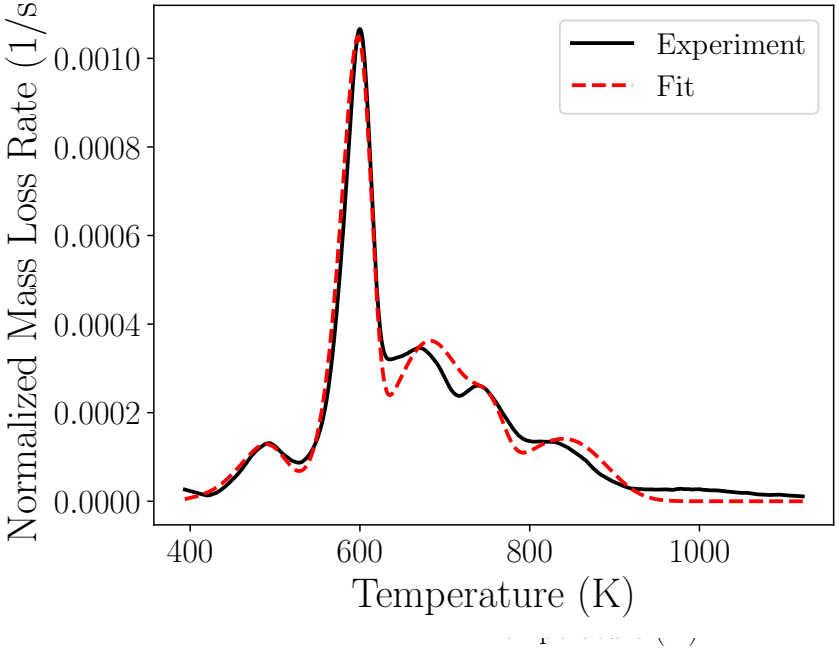
```
(base) Scripts $ python tga_fit.py PolyIso2_Expt_TGA_N2_10K_avg
```

PolyIso2_props.json


```
{
    "A": {
        "Name": "Pre-exponential Factor",
        "Units": "s^-1",
        "Values": [
            117257.20357330737,
            8420315447744.545,
            29625.162033341265,
            371893548781.6816,
            7241.320706107077
        ]
    },
    "E": {
        "Name": "Activation Energy",
        "Units": "kJ kmol^-1",
        "Values": [
```

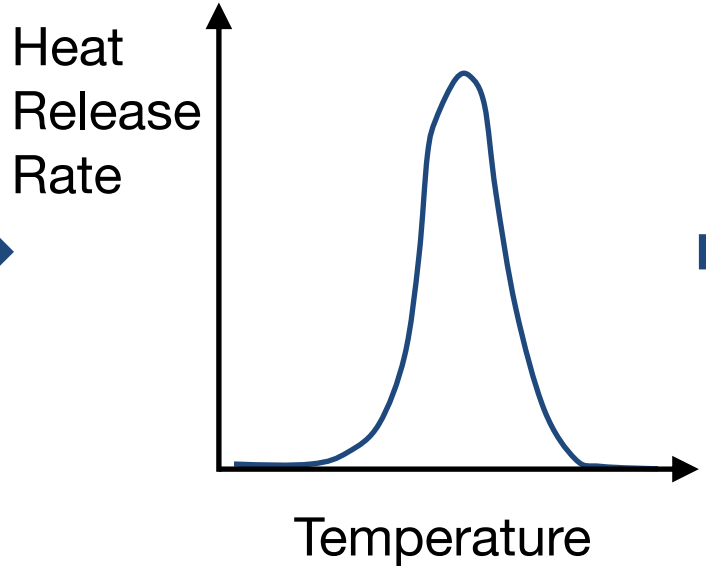

```
TGA/data/PolyIso2_Expt_TGA_N2_10K_avg.csv

42739
68e-05

 676.65 747.65 839.65]
7.36943641 42.71081662 23.66168942 57.03020686]
```





Analysis of MCC Data

How should we estimate individual reaction heats of combustion ($\Delta h_{c,i}$) from raw MCC data?



$\Delta h_{c,i}$

Single Reaction

$$\dot{Q}\left(T\right) = \dot{m}\left(T\right)\Delta h$$

1) Value at Peak Temperature: T_{p}

$$\Delta h = \frac{\dot{Q}\left(T_{\mathrm{p}}\right)}{\dot{m}\left(T_{\mathrm{p}}\right)}$$

2) Simple Average: N_{d} data points

$$\Delta h = \frac{1}{N_{\mathrm{d}}} \sum_{k=1}^{N_{\mathrm{d}}} \frac{\dot{Q}\left(T_k\right)}{\dot{m}\left(T_k\right)}$$

Multiple Reactions

$$\dot{Q}(T) = \sum_{i=1}^{N_\mathrm{r}} \dot{m}_i(T)\,\Delta h_i$$

1) Linear System: N_r equations, N_r unknowns

$$\sum_{i=1}^{N_\mathrm{r}} \dot{m}_i(T_{\mathrm{p},j})\,\Delta h_i = \dot{Q}(T_{\mathrm{p},j}),\ j = 1,\ldots,N_\mathrm{r}$$

2) Multiple Linear Regression: N_d data points

$$\sum_{i=1}^{N_\mathrm{r}} \dot{m}_i(T_k)\,\Delta h_i = \dot{Q}(T_k),\ k = 1,\ldots,N_\mathrm{d} > N_\mathrm{r}$$

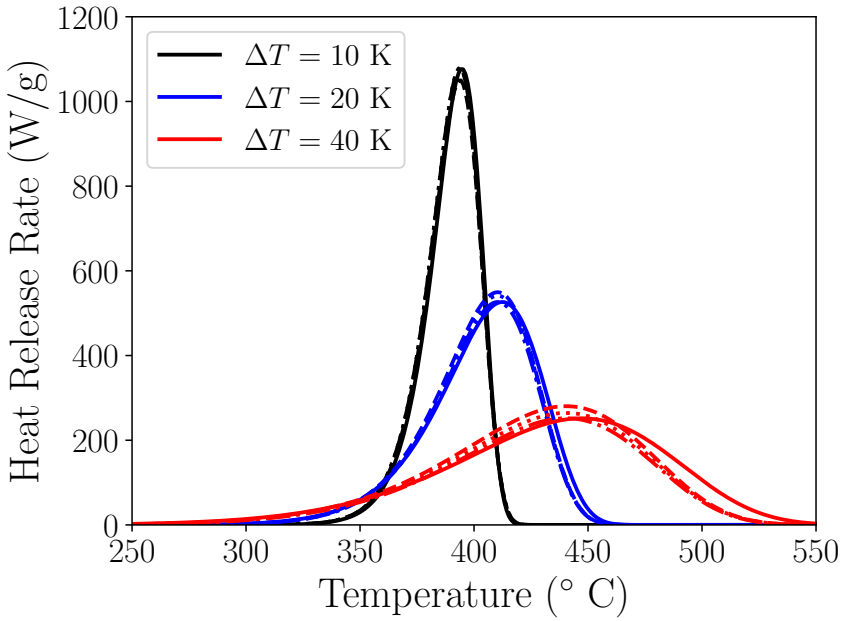
MCC Fit Verification

1. Assume **kinetic parameters** and **heats of combustion**
2. Generate TGA data
3. Use TGA fit algorithm to find kinetic parameters
4. Use TGA predictions and MCC data to find heats of combustion

Purpose:

1. Check implementation
2. Test validity of approximate solution

MCC: Single Reaction Verification



Solid: Simulated Data
Dash: Total HRR/mass
Dash-Dot: Peak Match
Dot: Simple Average

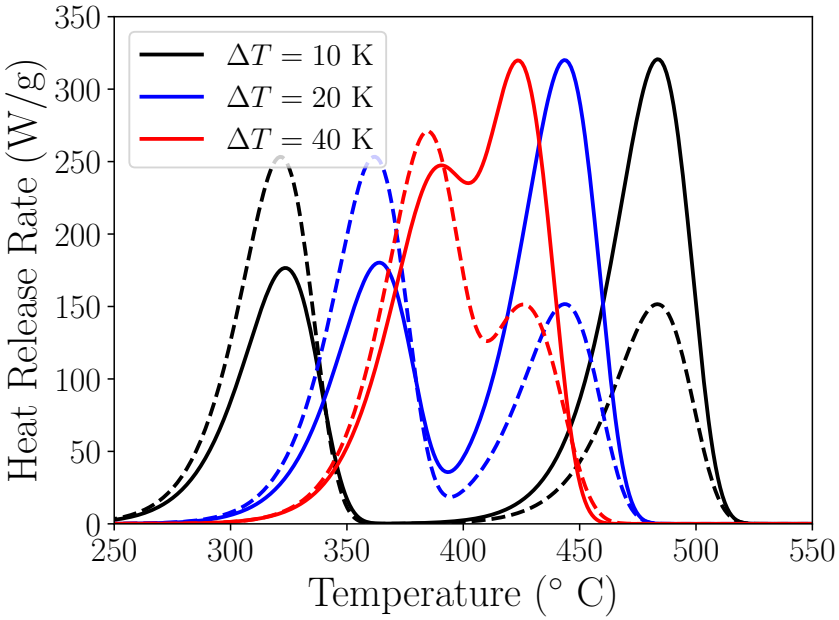
- TGA Data
  - 10 K/min
  - $T_{\mathrm{p}} = 650$ K
- MCC Data
  - 60 K/min
  - $\Delta h = 30$ kJ/g

MCC: Single Reaction Verification

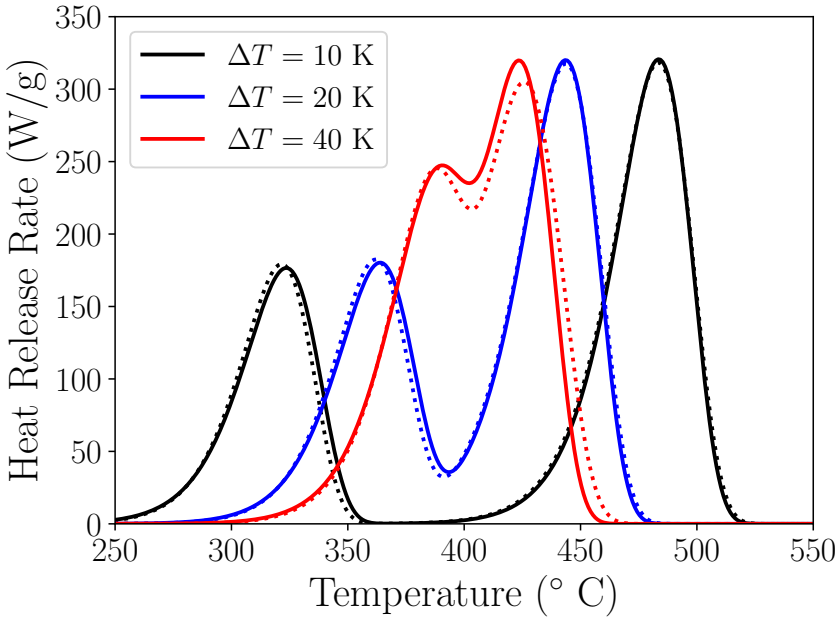
Scenario	Δh (kJ/g) (Total HR/mass)	Method 1: Peak Ratio Δh (kJ/g)	Method 2: Simple Average Δh (kJ/g)
ΔT = 10 K	30.026	30.792	30.849
ΔT = 20 K	29.997	28.731	29.556
ΔT = 40 K	29.997	26.949	28.291

- Total HR/mass not applicable to multiple reaction
- Method 2 performs better than Method 1

MCC: Two Reactions Verification



Evenly distributed heat release



Method 2: Multiple linear regression

MCC: Two Reactions Verification

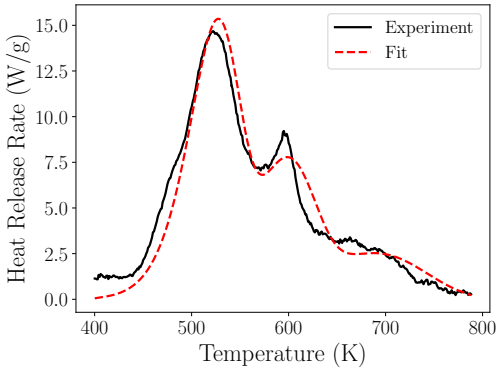
		$-\Delta h_1$ (kJ/g)	$-\Delta h_2$ (kJ/g)	$-\Delta h_{total}$ (kJ/g)
Specified Value		15	45	21
ΔT = 10 K	Simple Integration	--	--	20.998
	Linear Regression	14.854	44.085	21.021
ΔT = 20 K	Simple Integration	--	--	20.998
	Linear Regression	14.953	43.973	21.061
ΔT = 40 K	Simple Integration	--	--	20.998
	Linear Regression	15.415	42.304	21.501

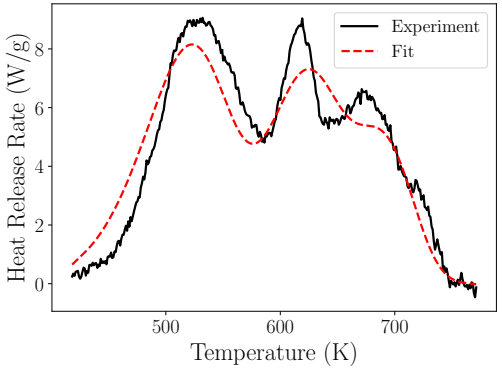
- Accuracy decreases with “broader” reactions
- Future work: correct individual reaction values to force match of total value

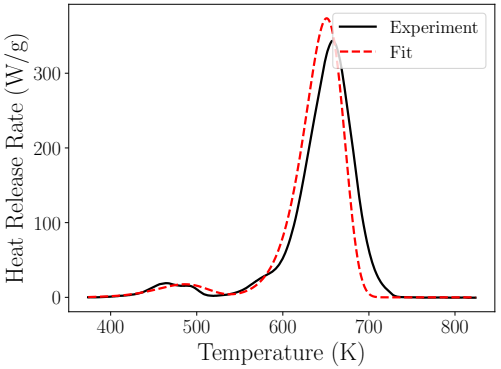
MCC Validation

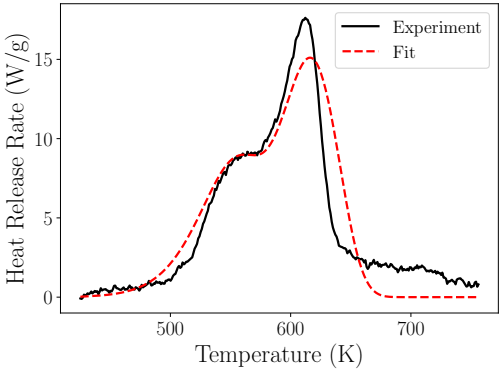
12 materials:

```
# list of all current MCC test series
mcc_tests = [
    'BigBerry-Leaf_Expt_MCC_N2_10K',
    'BigBerry-Stem_Expt_MCC_N2_10K',
    'Chamise-Leaf_Expt_MCC_N2_10K',
    'Chamise-Stem_Expt_MCC_N2_10K',
    'Chaparral-Leaf_Expt_MCC_N2_10K',
    'Chaparral-Stem_Expt_MCC_N2_10K',
    'DesertCeanothus-Leaf_Expt_MCC_N2_10K',
    'DesertCeanothus-Stem_Expt_MCC_N2_10K',
    'DouglasFir-Leaf_Expt_MCC_N2_10K',
    'LodgepolePine-Leaf_Expt_MCC_N2_10K',
    'LodgepolePine-Stem_Expt_MCC_N2_10K',
    'MaCFP_PMMA_Expt_MCC_N2_60K',
]
```









Example: Lodgepole Pine Stems

fact/Materials/metadata/LodgepolePine-Stem.json

LodgepolePine-Stem.json

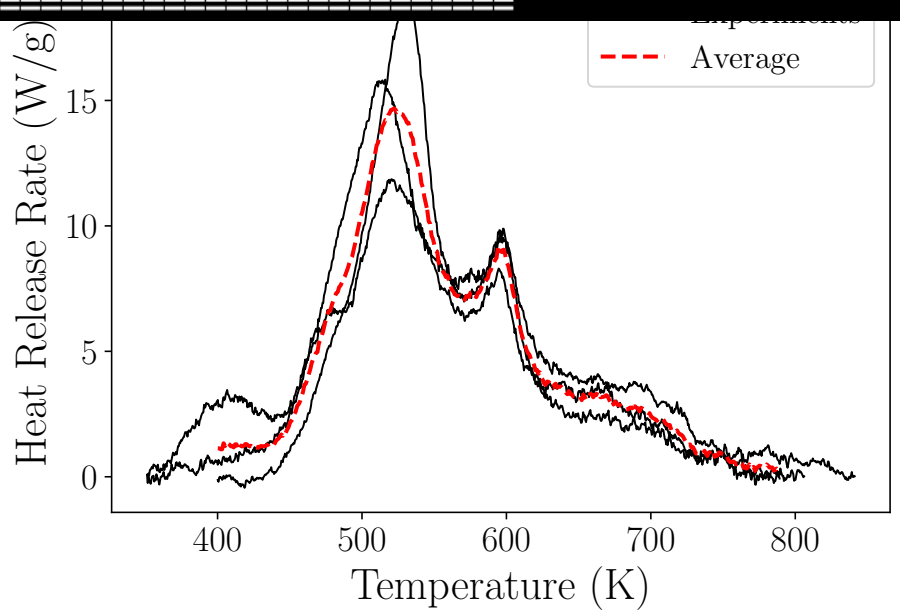

```
{
    "Common Names": "Lodgepole Pine Leaf",
    "Trade Name": "Pinus Contorta",
    "Manufacturer": "Natural Fuel",
    "Distributor": "Rocky Mountain Research Station (Missoula, Montana)",
    "Date Acquired": "May-July 2017",
    "Description": "Thin (<0.75 mm) flat slices of small branches picked
from a series of randomly selected individual Lodgepole Pine trees",
    "Categories": "Vegetation"
}
```

Replicate MCC Data Files:

```
(base) Scripts $ python average_mcc_series.py LodgepolePine-Stem_Expt_MCC_N2_10K
================================================================

 Reading data from:

    LodgepolePine-Stem_Expt_MCC_N2_10K_1.csv
    LodgepolePine-Stem_Expt_MCC_N2_10K_2.csv
    LodgepolePine-Stem_Expt_MCC_N2_10K_3.csv

 Number of data sets in series =  3

================================================================
```

```
Time,Temperature,HRR
[s],[K],[W/g]
3,400.15,-0.13
5.8,400.65,-0.2
8.7,401.15,-0.03
11.9,401.65,-0
14.8,402.15,-0.05
17.7,402.65,-0.03
21,403.15,-0.12
23.8,403.65,-0.09
26.9,404.15,0.04
```

```
Time,Temperature,HRR
[s],[K],[W/g]
0.5,352.15,0.09
6.5,352.65,-0.12
11.6,353.15,-0.21
17.1,353.65,-0.28
22.3,354.15,-0.12
27.2,354.65,0.01
32.3,355.15,-0
37.4,355.65,0.04
42.2,356.15,-0.19
```

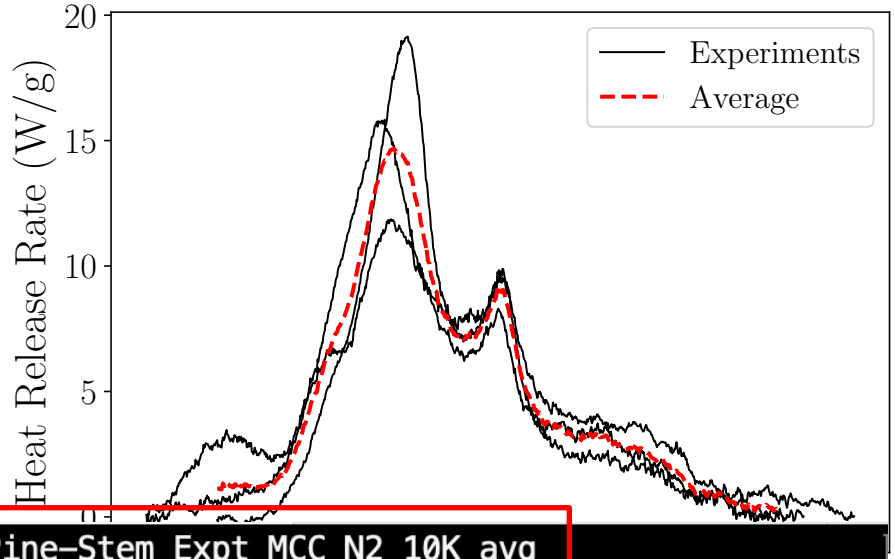


Pyrolysis Kinetics from TGA

LodgepolePine-Stem_props.json


```
{
    "A": {
        "Name": "Pre-exponential Factor",
        "Units": "s^-1",
        "Values": [
            4895170.775500201,
            235982.41393676633,
            241.86226531218318
        ]
    },
    "E": {
        "Name": "Activation Energy",
        "Units": "kJ kmol^-1",
        "Values": [
            90468.95723804967,
            88696.41047329734,
            65820.96613844081
        ]
    },
```


Average MCC Data




```
(base) Scripts $ python mcc_fit.py LodgepolePine-Stem_Expt_MCC_N2_10K_avg
------------------------------------------------------------

 Fitting MCC data from file:  ../Experiment/MCC/data/LodgepolePine-Stem_Expt_MCC_N2_10K_avg
.csv
   at heating rate of  10.0  K/min.

------------------------------------------------------------

Results:
  RMS HRR Error     =  0.9460753645395685
  dh_c_tot (J/g)    =  11054.7026255
  dh_c (J/g)        =  [19534.18875694 11315.38066012 11669.52953085]

============================================================
```

```
(base) Scripts $ python mcc_fit.py LodgepolePine-Stem_Expt_MCC_N2_10K_avg
============================================================

 Fitting MCC data from file:  ../Experiment/MCC/data/LodgepolePine-Stem_Expt_MCC_N2_10K_avg
.csv
   at heating rate of  10.0  K/min.

------------------------------------------------------------

Results:
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============================================================
```

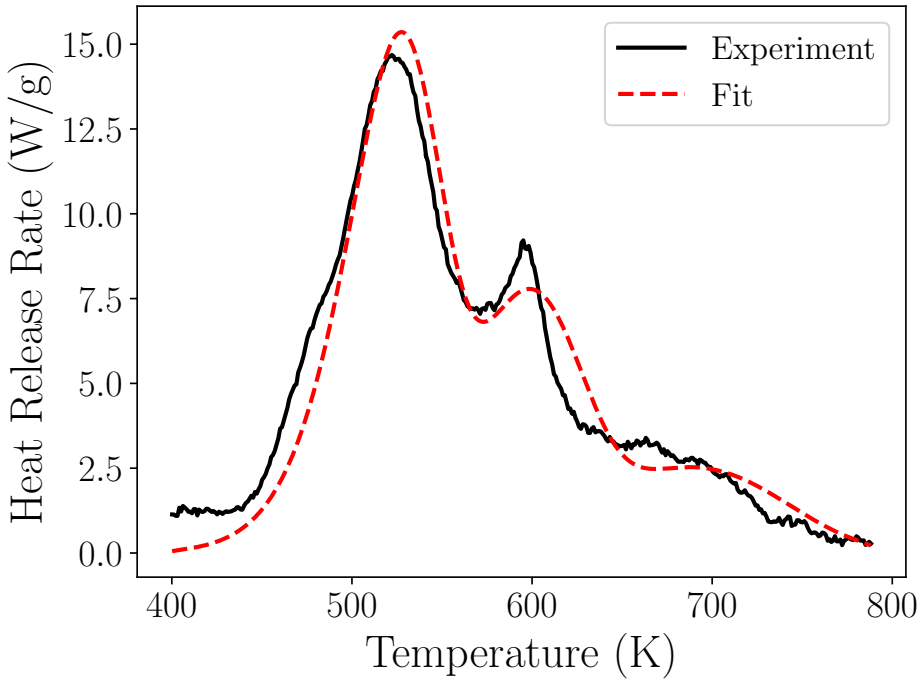

LodgepolePine-Stem_props.json


```
{
    "A": {
        "Name": "Pre-exponential Factor",
        "Units": "s^-1",
        "Values": [
            4895170.775500201,
            235982.41393676633,
            241.86226531218318
        ]
    },
    "E": {
        "Name": "Activation Energy",
        "Units": "kJ kmol^-1",
        "Values": [
            90468.95723804967,
            88696.41047329734,
            65820.96613844081
        ]
    },
    "dmu": {
        "Name": "Normalized Mass of Reaction",
        "Units": " - ",
        "Values": [
            [
                0.2755842737690579,
                0.3073389550813397,
                0.18798788151838927
            ]
        ]
    },
    "dh_c": {
        "Name": "Heat of Combustion",
        "Units": "J g^-1",
        "Values": [
            19534.188756943473,
            11315.380660123741,
            11669.52953084592
        ]
    }
}
```

Summary

- **Predicting** fire growth requires material properties
- To obtain material properties:
  - Small-scale tests (TGA, MCC, DSC, etc.)
  - **Calibration algorithms**
- Calibration algorithms are presented for obtaining
  - pyrolysis kinetic parameters from TGA data
  - individual reaction heats of combustions from MCC data
- Algorithms performs well for
  - Manufactured solution verification cases
  - Multiple reaction materials with well-separated reaction peaks
- Algorithms implemented in **FACT:** **https://github.com/mcb1/fact/**