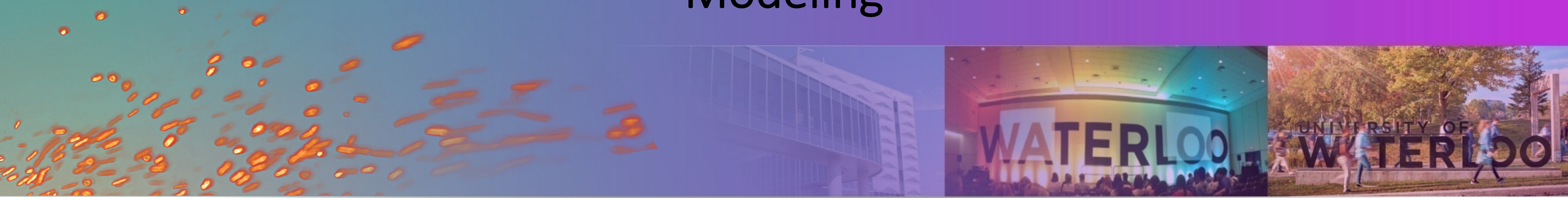
13th International Symposium on Fire Safety Science

Measurement and Computation of Fire Phenomena
The MaCFP Condensed Phase Working Group

Modeling



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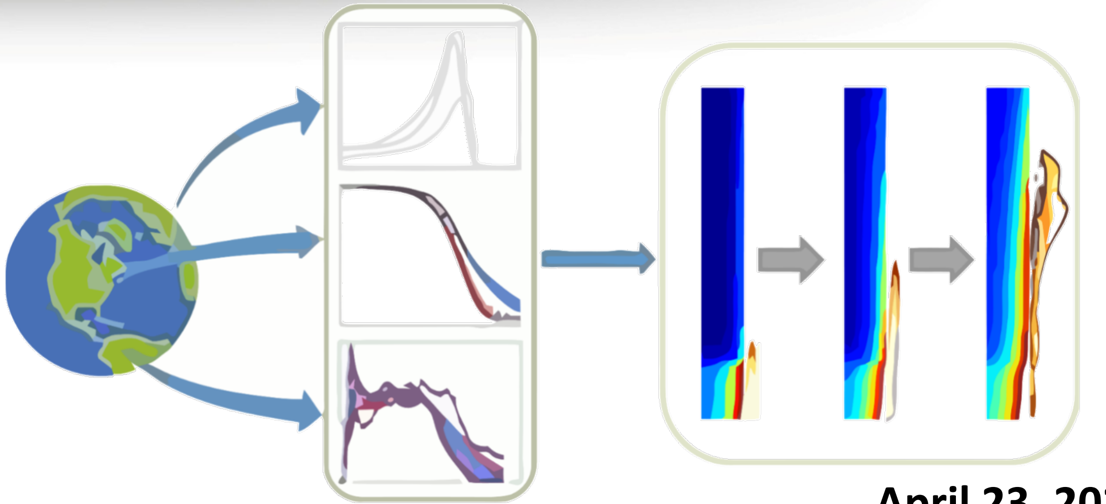


April 23, 2021

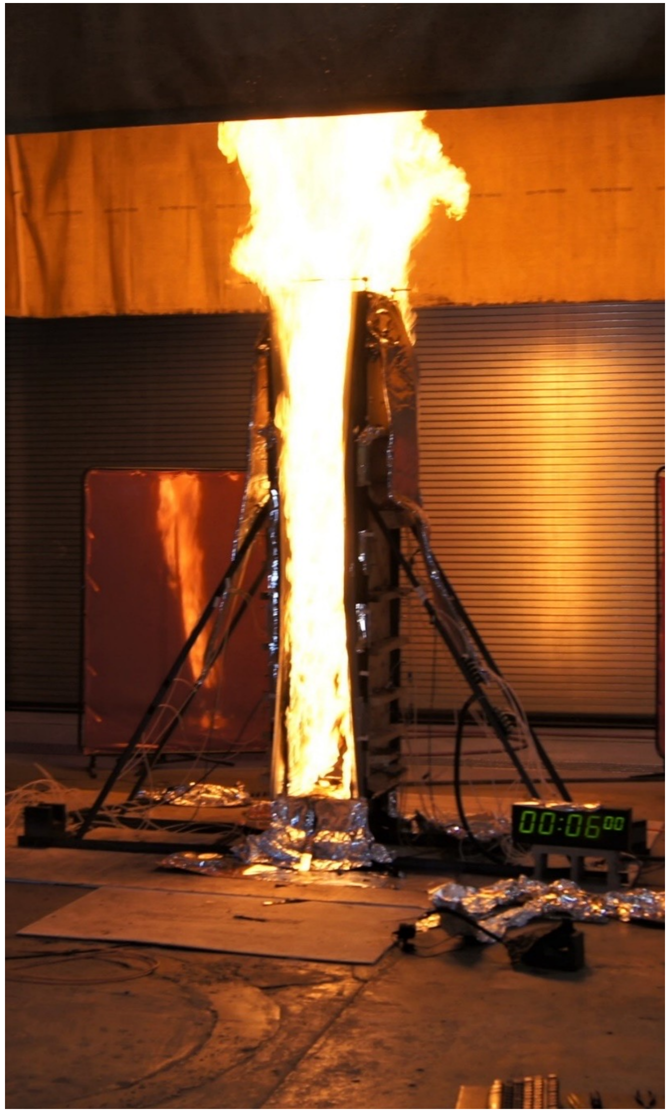
Overview

1. Purpose
2. Material Properties
3. Target Simulation Predictions
   - Thermogravimetric Analysis (TGA)
   - Gasification
4. Discussion

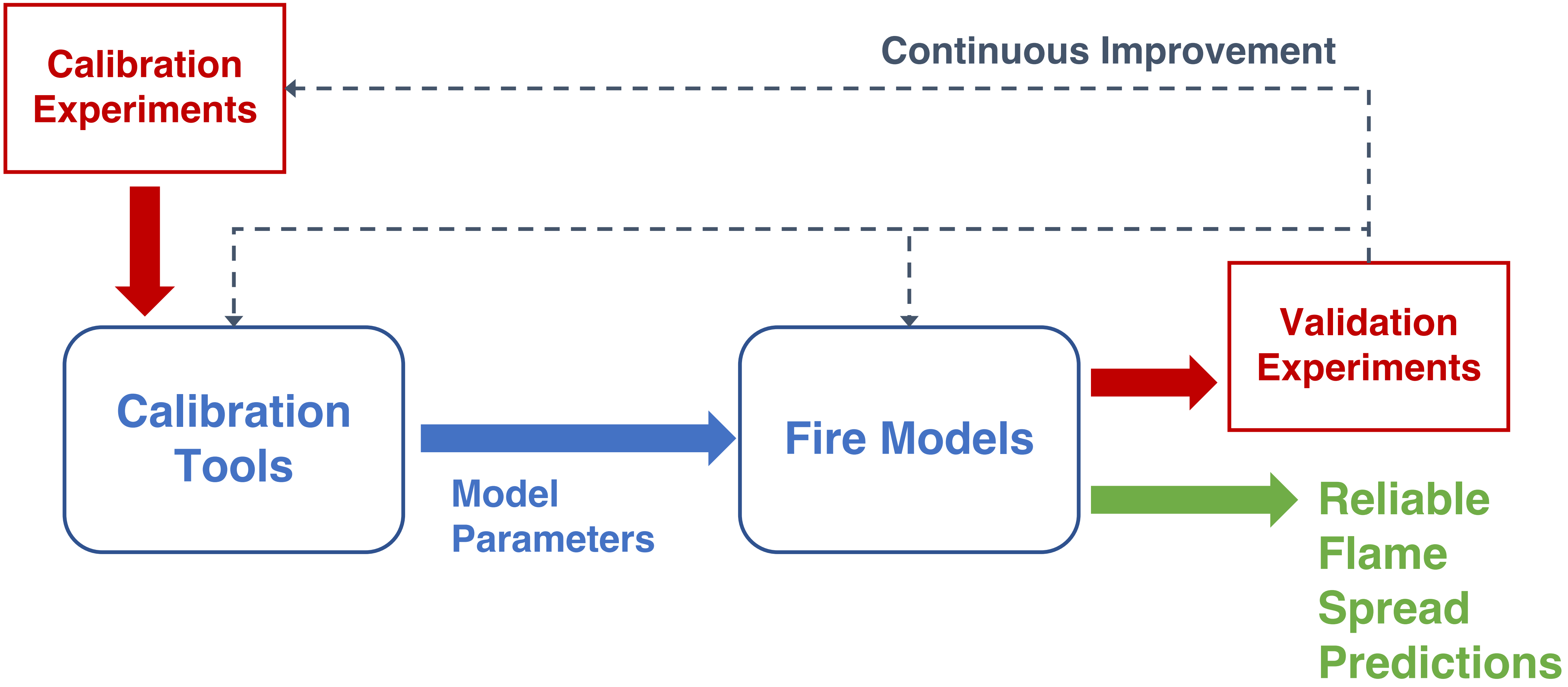
1. Purpose

Why are we here?

- Final destination: reliable predictions of flame spread and fire growth
- Barriers to getting there
  - Complex physics
  - Material variability
  - Scenario variability
- **MaCFP provides a forum for collaboration**



Fire Model Development Process



MaCFP Condensed Phase Modeling Phase

- Objectives from, “Guidelines for Participation in the 2021 MaCFP Condensed Phase Workshop”:
  - To catalogue current approaches used to parameterize pyrolysis models;
  - To quantify the interlaboratory variability for comparable experimental datasets;
  - To assess the impact of the variability of model parameters on predictions of sample burning rate; and
  - To present a rigorous analysis of these results in the *Fire Safety Journal*.

Note

- **Validation** asks: “Do model *predictions* agree with experiments?”
  - Must compare with experimental data
  - Experimental data cannot be same data used for calibration
- **Not showing true model validation today**
- **Code-to-code Comparison** asks: “Do different model predictions agree with each other?”

Contributors to Modeling Phase

1. **Aalto**—Aalto University, 🇫🇮 Finland
2. **BoWFZJ**—University of Wuppertal and Forschungszentrum Jülich, 🇩🇪 Germany
3. **DBI**—Danish Institute of Fire and Security Technology, 🇩🇰 Denmark
4. **GIDAZE+**—Imperial College of London, 🇬🇧 United Kingdom
5. **NIST**—National Institute of Standards and Technology, 🇺🇸 United States
6. **Sandia**—Sandia National Laboratories, 🇺🇸 United States
7. **UCLAN**—University of Central Lancashire, 🇬🇧 United Kingdom
8. **UMD**—University of Maryland, 🇺🇸 United States
9. **UMET**—EDF, Université de Lille, and Université de Toulouse, 🇫🇷 France

2. Material Properties

Requested Model Parameters

Symbol	Units	Name
	Degradation Kinetics	
A	s^{-1}	Pre-exponential constant
E	$J\ mol^{-1}$	Activation energy
n	[-]	Reaction order
ν	[-]	Stoichiometric coefficient
	Thermodynamic Properties	
c_p	$J\ kg^{-1}\ K^{-1}$	Heat capacity
h_r	$J\ kg^{-1}$	Heat of reaction
ρ	$kg\ m^{-3}$	Density
	Transport Properties	
k	$W\ m^{-1}\ K^{-1}$	Thermal conductivity
$\mathcal{D}$	$m^2\ s^{-1}$	Mass diffusivity
α	m^{-1} or $m^2\ kg^{-1}$	Absorption coefficient
ε	[-]	Emissivity

- Complications
  - Multiple reactions
  - Temperature dependent properties
- Differences
  1. Data
  2. Model
  3. Method

Aalto

1. Data
   - TGA from UMET at 1, 2, 5, 10, 20, and 50 K min^{-1}
   - Gasification from DBI at 25 kW m^{-2} and from Aalto at 65 kW m^{-2}
   - UV-Vis and FTIR for absorption coefficients
   - Density and emissivity from literature
2. Model
   - Gpyro for fitting kinetics, FDS for fitting thermophysical properties
   - Two-step, parallel reaction mechanism with 1^{st} order kinetics
   - Gasification boundary conditions: convective heat transfer at top, ceramic wool at back surface
3. Method
   - Kinetics: Gpyro with shuffled complex evolution optimization
   - Thermophysical Properties: PROPTI + FDS with shuffled complex evolution optimization

BoWFZJ

1. Data
   - TGA from LCCP
   - Gasification (CAPA) from UMD
2. Model
   - FDS
   - Two-step, parallel reaction mechanism with 1st order kinetics
3. Method
   - PROPTI with shuffled complex evolution optimization
   - Method A—Kinetics from TGA **then** other properties from CAPA
   - Method B—All properties from TGA and CAPA **simultaneously**

DBI

1. Data
    - STA (TGA/DSC) from DBI at 20 K min^{-1}
    - Heat Flow Meter (HFM) from DBI
    - Assumed emissivity = 1
2. Model
    - FDS and Gpyro
    - One-step reaction mechanism with 1^{st} order kinetics
3. Method
    - Smoothing filters: LOESS and Savitzgy-Golay
    - Three fitting methods: (1) Monte Carlo sampling, (2) Gpyro, and (3) manual updating

GIDAZE+

1. Data
    - TGA
        - UMET, LCPP, and literature at 5 K min^{-1}
        - UMD, GIDAZE+, LCCP, and UMET at 10 K min^{-1}
        - Literature at 30 K min^{-1}
    - Literature values for other properties
2. Model
    - Gpyro
    - One-step reaction mechanism with 1^{st} order kinetics
3. Method
    - Kinetics by manual updating

NIST

1. Data
   - TGA from NIST at 10 K min^{-1}
   - Literature values for other properties
2. Model
   - FDS
   - One-step reaction mechanism with 1^{st} order kinetics
3. Method
   - Algebraic estimation of kinetics based on peak parameters

Sandia

1. Data
   - TGA
     - Sandia (S) at 1 K min^{-1} and 5 K min^{-1}
     - UMET (U) at 1 K min^{-1}, 2 K min^{-1}, 5 K min^{-1}, and 50 K min^{-1}
2. Model
   - Sierra Thermal/Fluids (Sandia)
   - Three reaction mechanisms (n^{th} order kinetics) :
     1. One-step
     2. Two-step in series
     3. Two-step in parallel
3. Method
   - MatCal + Dakota using gradient-based optimization of least squares residual

UCLAN

1. Data
   - TGA from UCLAN
2. Model
   - ThermaKin
   - One-step reaction mechanism with 1st order kinetics
3. Method
   - Manual updating

UMD

1. Data
    - TGA/DSC from UMD at 10 K/min
    - Gasification (CAPA) from UMD at 25 kW m^{-2}
2. Model
    - ThermaKin2D
    - Two-step in series reaction mechanism with 1^{st} order kinetics
3. Method
    - Hill climbing optimization with least squares objective function

UMET

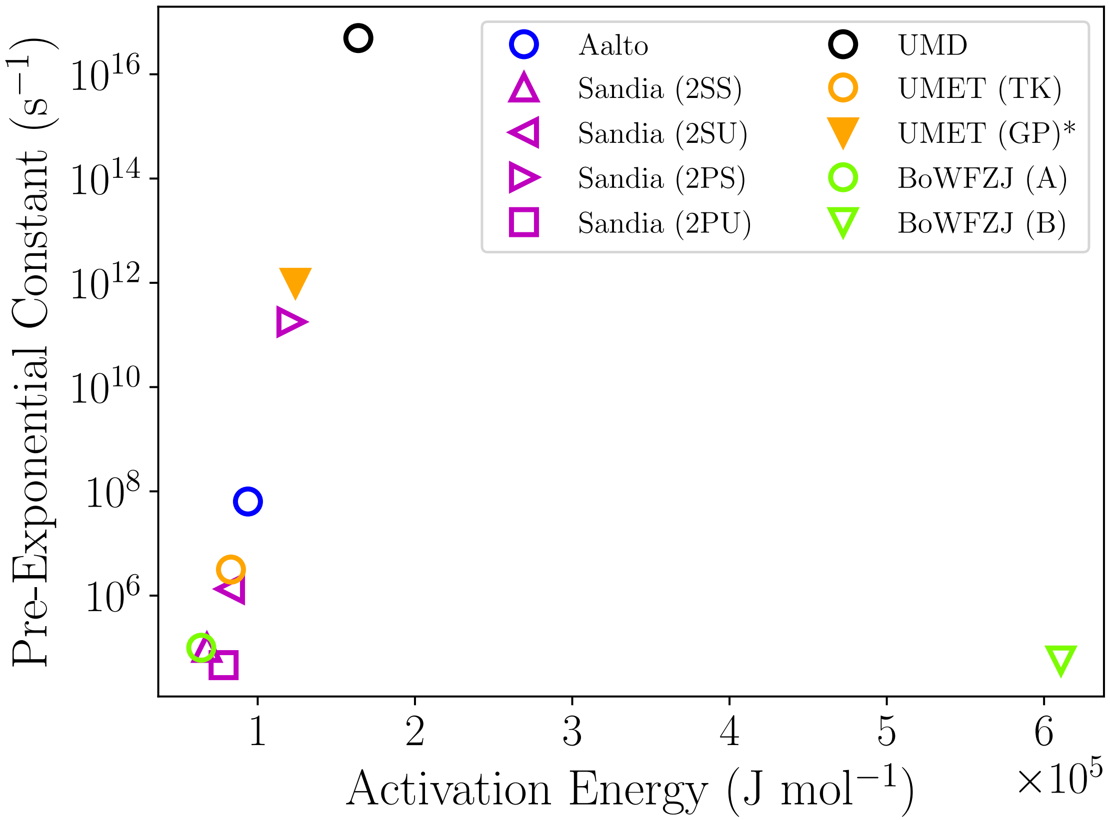
1. Data
   - TGA from UMET at 1 K min^{-1}, 2 K min^{-1}, 5 K min^{-1}, 20 K min^{-1}, 50 K min^{-1}, and 100 K min^{-1}
   - DSC (STA) from UMET
   - Hot Disk Analyzer (Transient Plane Source) from UMET
   - Literature data for density, emissivity, and absorption coefficient
2. Model
   - ThermaKin (TK)
   - Gpyro (GP)
   - Two-step reaction mechanism with 1^{st} order (TK) and n^{th} order (GP) kinetics
3. Method
   - Hybrid regularized Gauss-Newton or Marquardt optimization of TGA

Calibration Method Summary

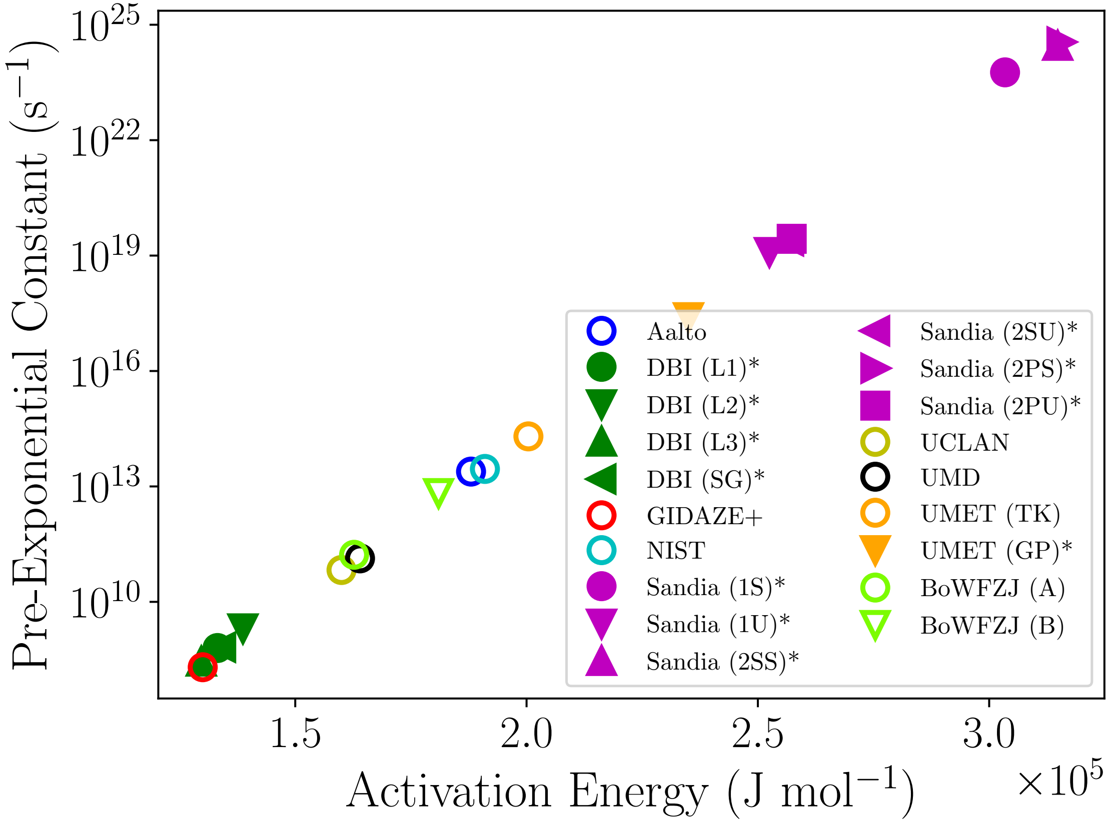
Data	Models	Methods
• TGA at many heating rates • Gasification/CAPA • STA (TGA/DSC) • Heat flow meter • Hot disk • UV-Vis and FTIR • Literature data and values	• FDS, Gpyro, ThermaKin, Sierra Thermal/Fluids • One-step, two-step (series and parallel) reaction mechanism • 1^{st} order and n^{th} order kinetics	• PROPTI, Gpyro, MatCal+Dakota tools • Shuffled complex evolution • Other optimization • Algebraic • Monte Carlo sampling • Manual updating • Direct measurment

Kinetic Properties

1st Reaction



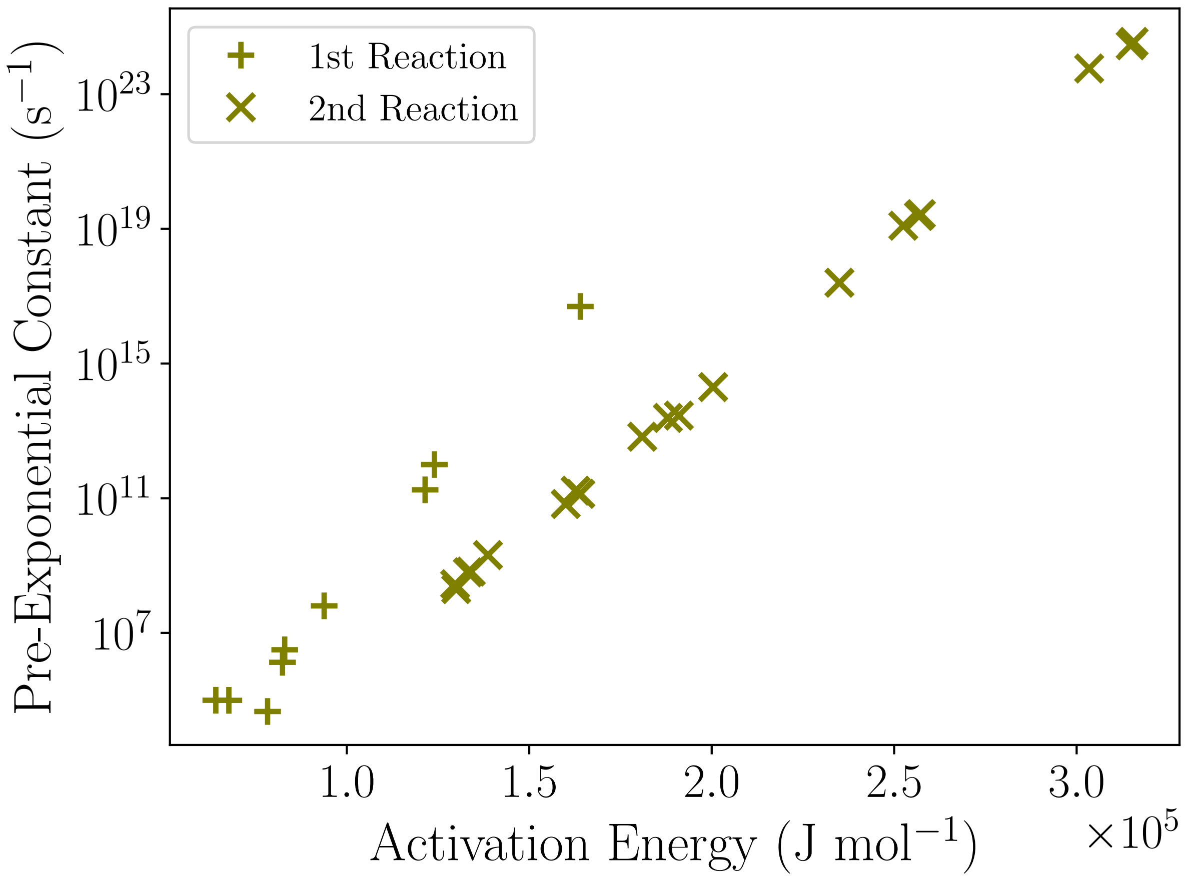
2nd Reaction



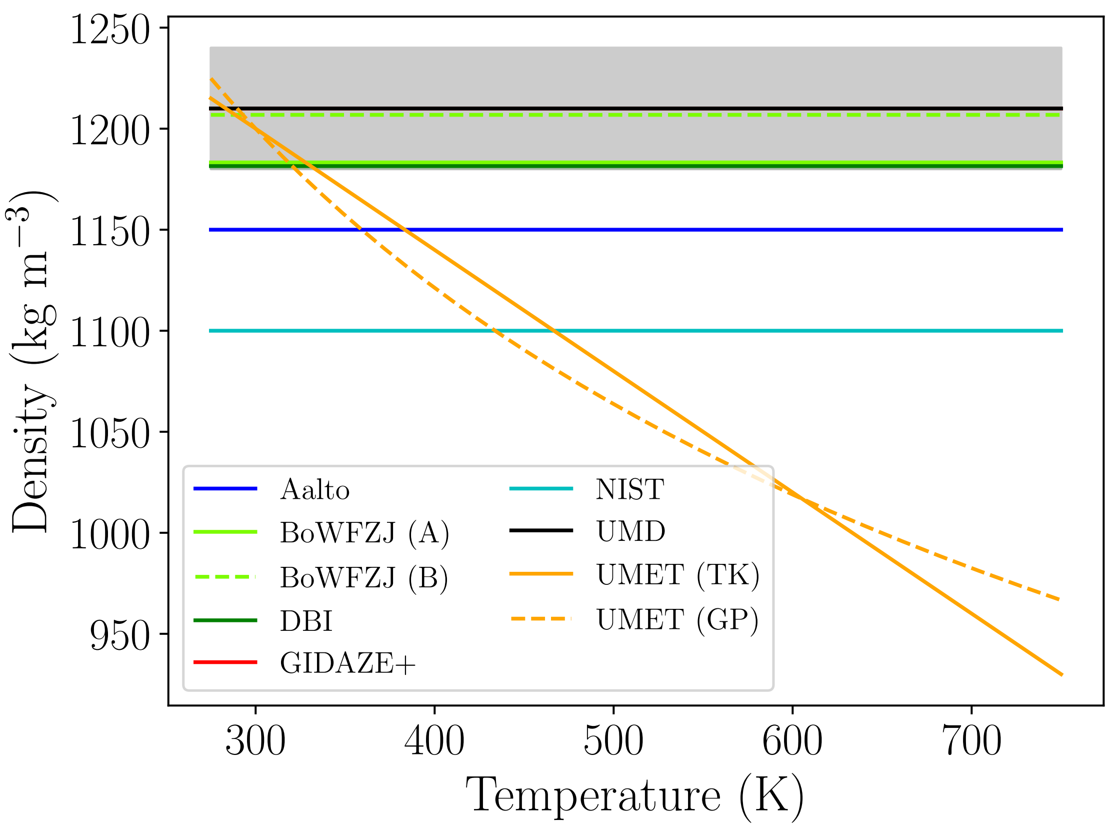
Hollow markers: 1st Order Kinetics; Solid Markers: nth Order Kinetics

Kinetic Properties

- Clear kinetic compensation
- Large range of values
- Location on line affects width of mass loss curve
- Questions
  - Does this spread matter?
  - Are two reactions necessary?
  - Are 1st order models sufficient?



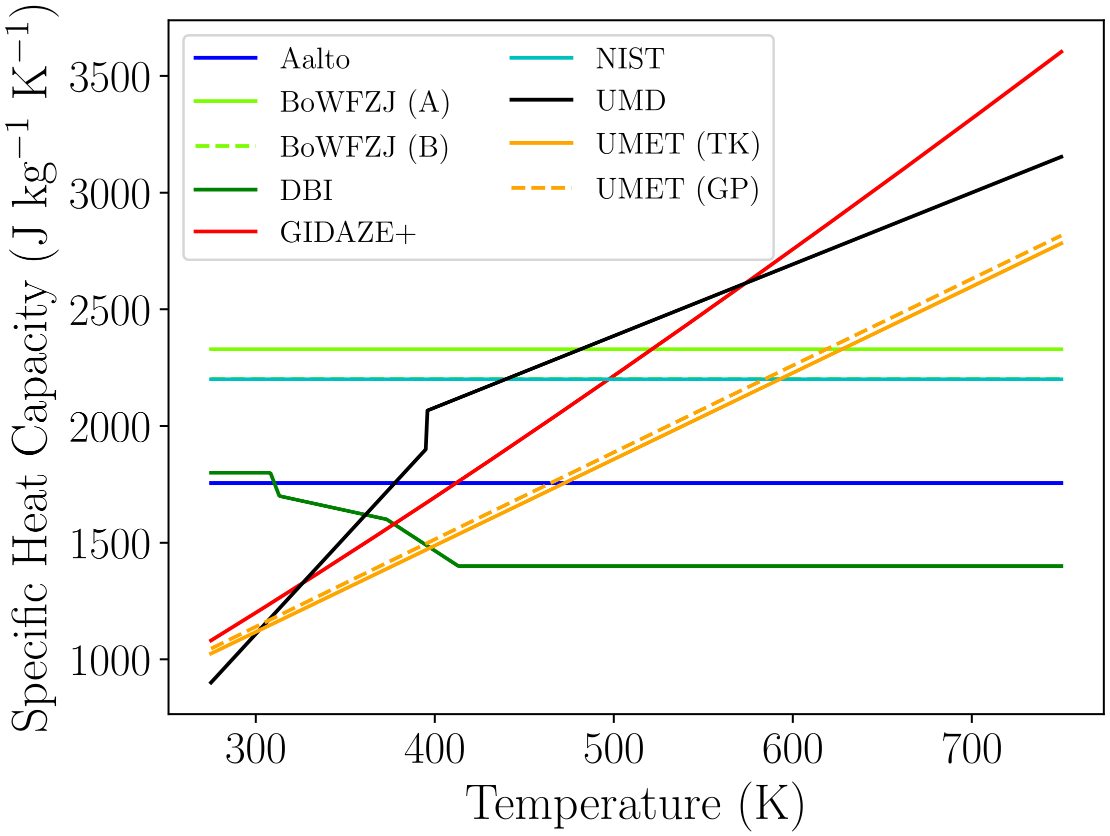
Density

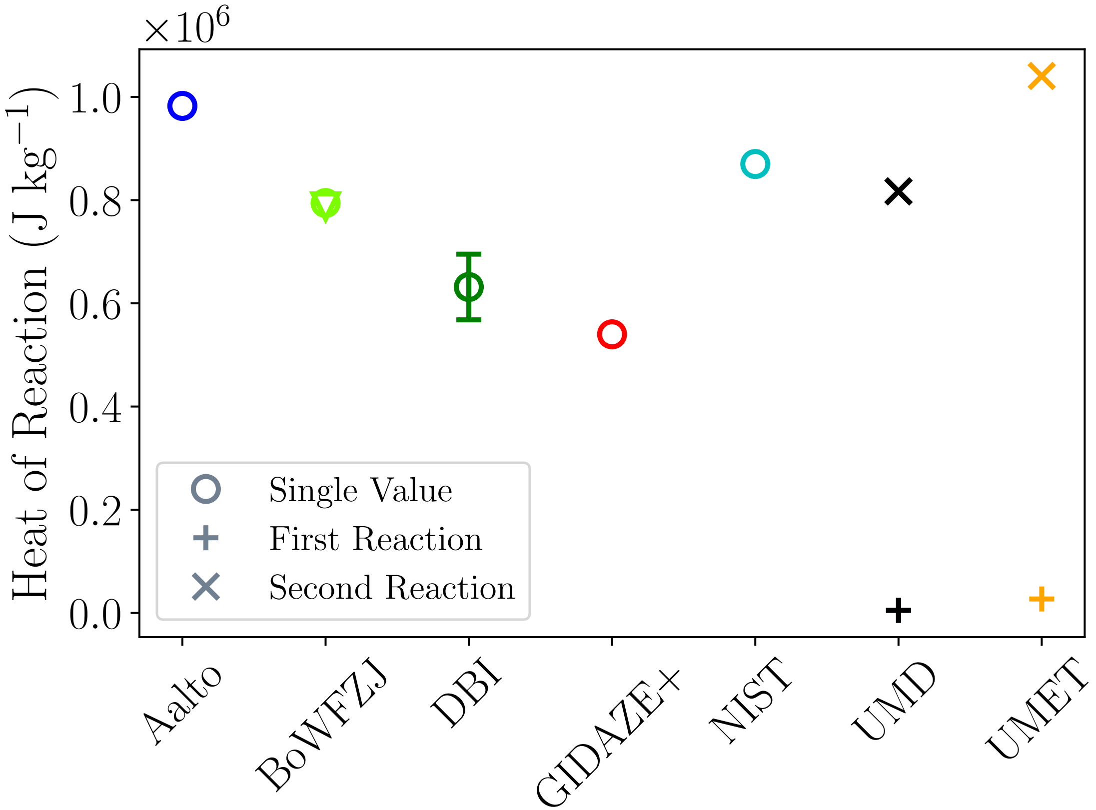


Shaded area is reported uncertainty by UMD

- All except UMET assume constant density
- Aalto and NIST both use literature values
- BoWFZJ gets density by optimization

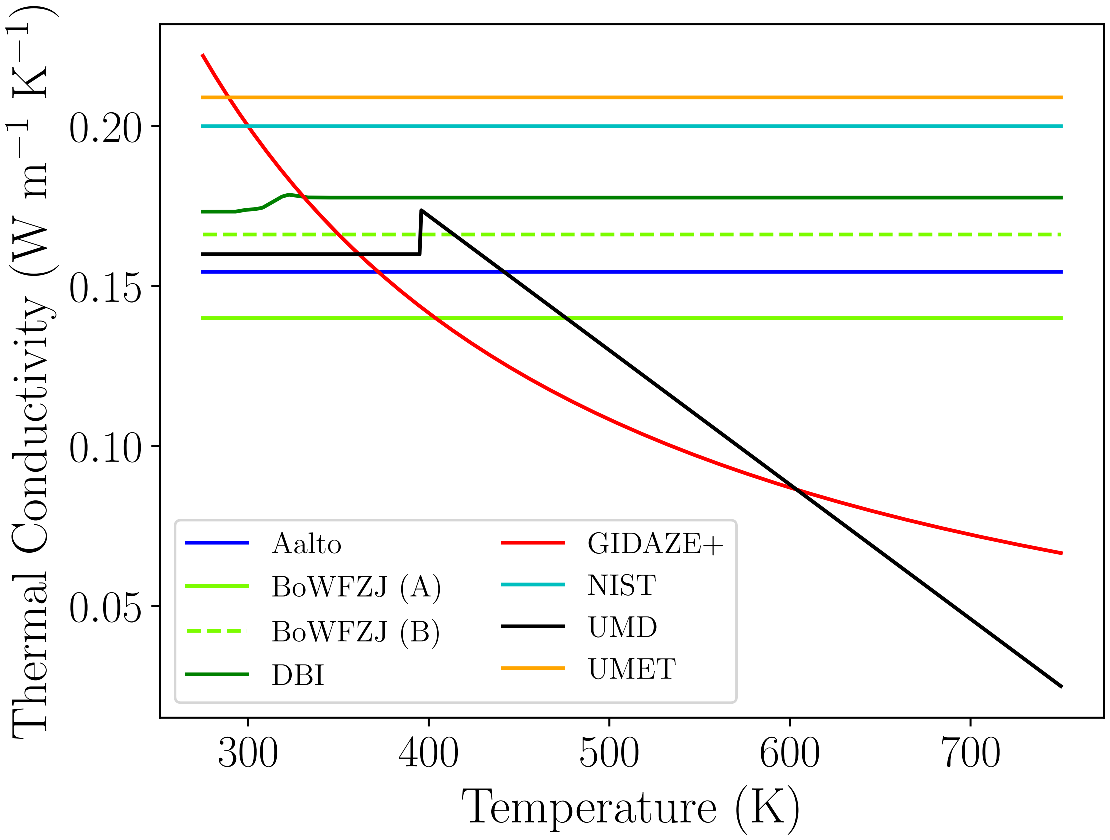
Thermodynamic Properties

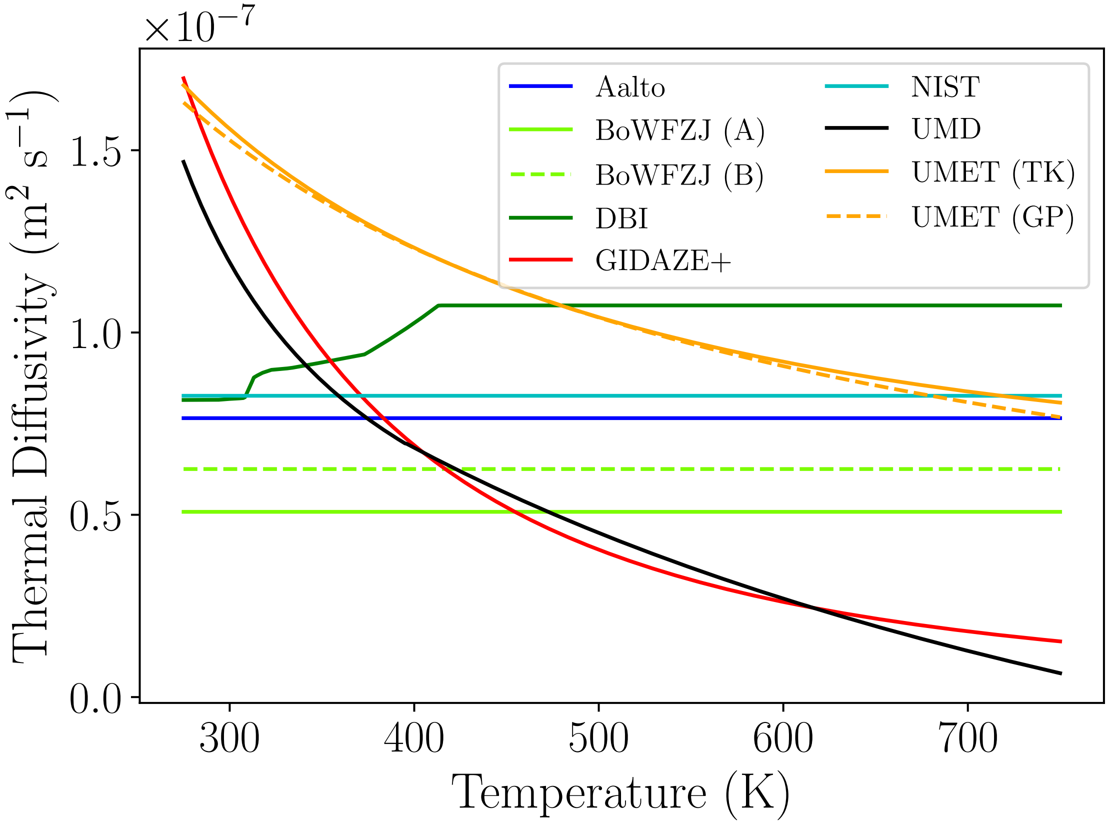




Question: Is heat of reaction for first reaction necessary?

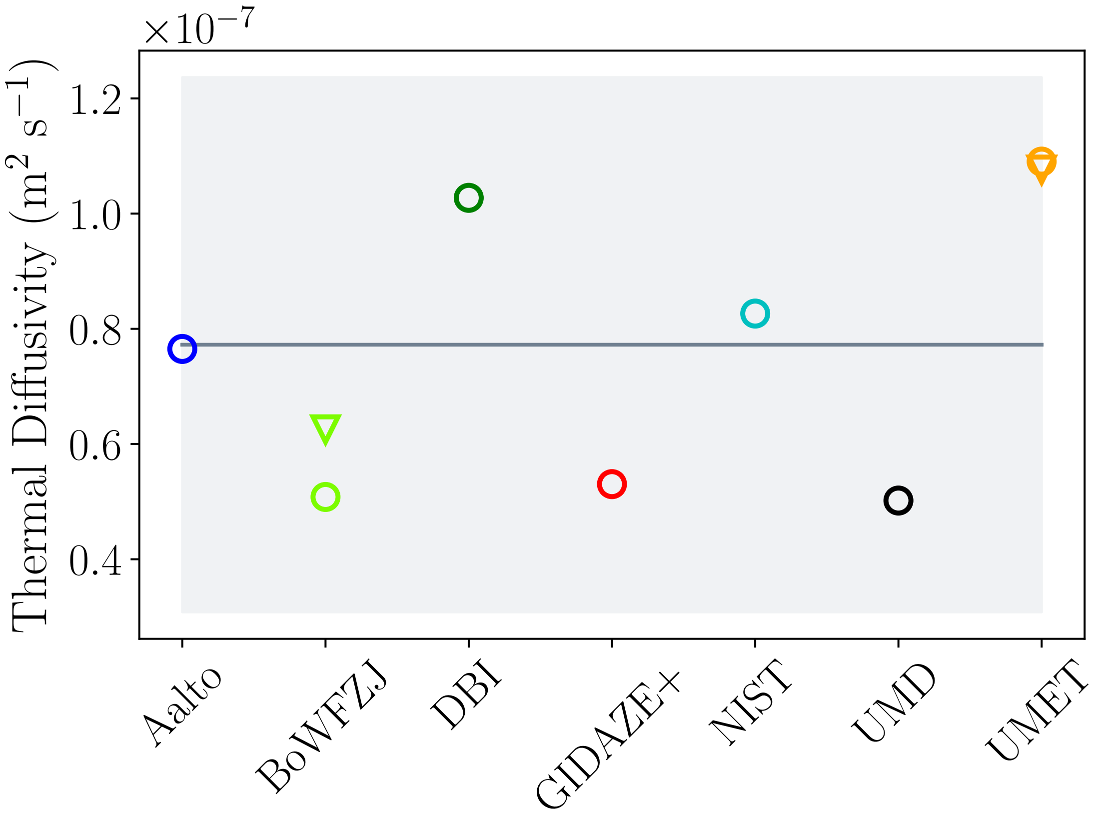
Transport Properties



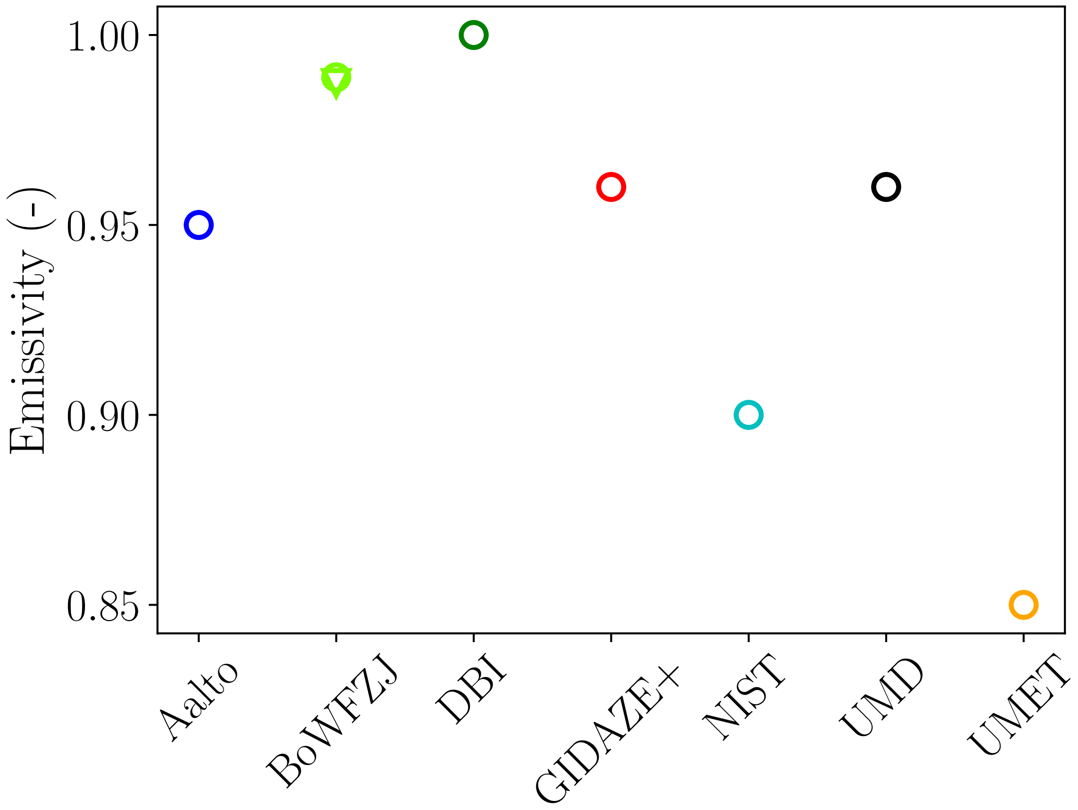


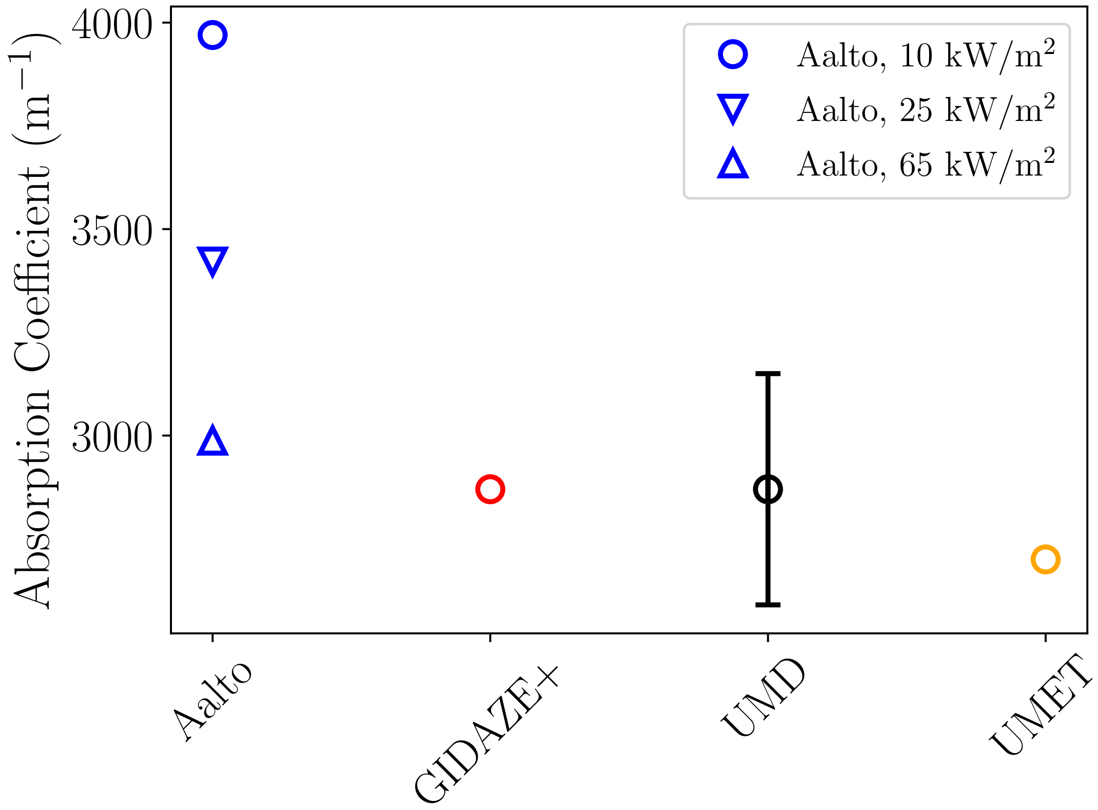
Average Thermal Diffusivity

- Averaged over entire temperature range (275 K to 750 K)
- Shaded area represents +/- two standard deviations
- Do not see clear compensation between thermal conductivity and heat capacity



Radiative Properties





- Large absorption coefficients expected for black PMMA
- Emissivity should affect top surface temperature

Properties Summary

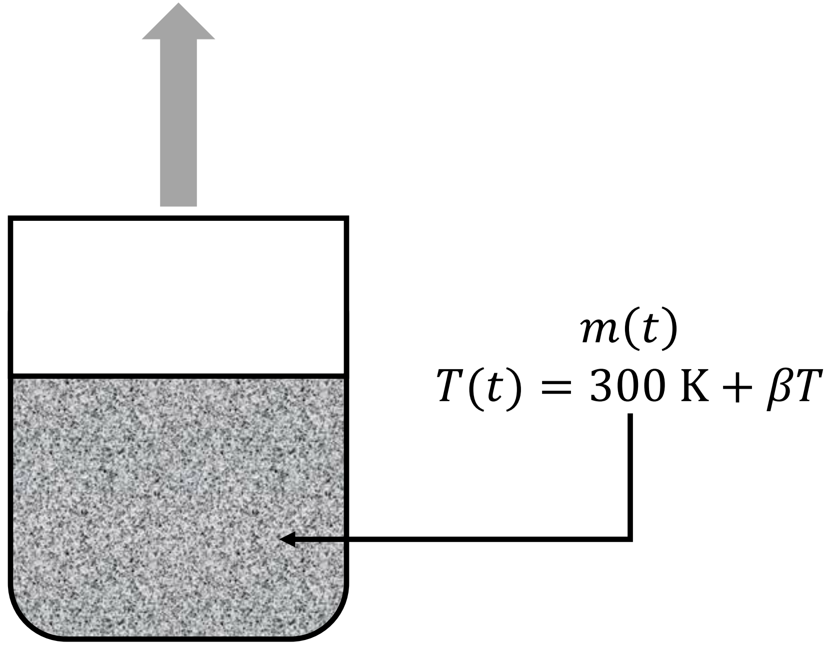
- Typical variability within 10 % to 50 % of averages
- No order of magnitude differences
- Questions
    - Are predictions sensitive to changes within this variability?
    - What are the most influential properties?
    - How do parameter estimates vary with methods?
    - Do we need more calibration experiments or fewer?

3. Target Simulation Predictions

TGA Target Simulations

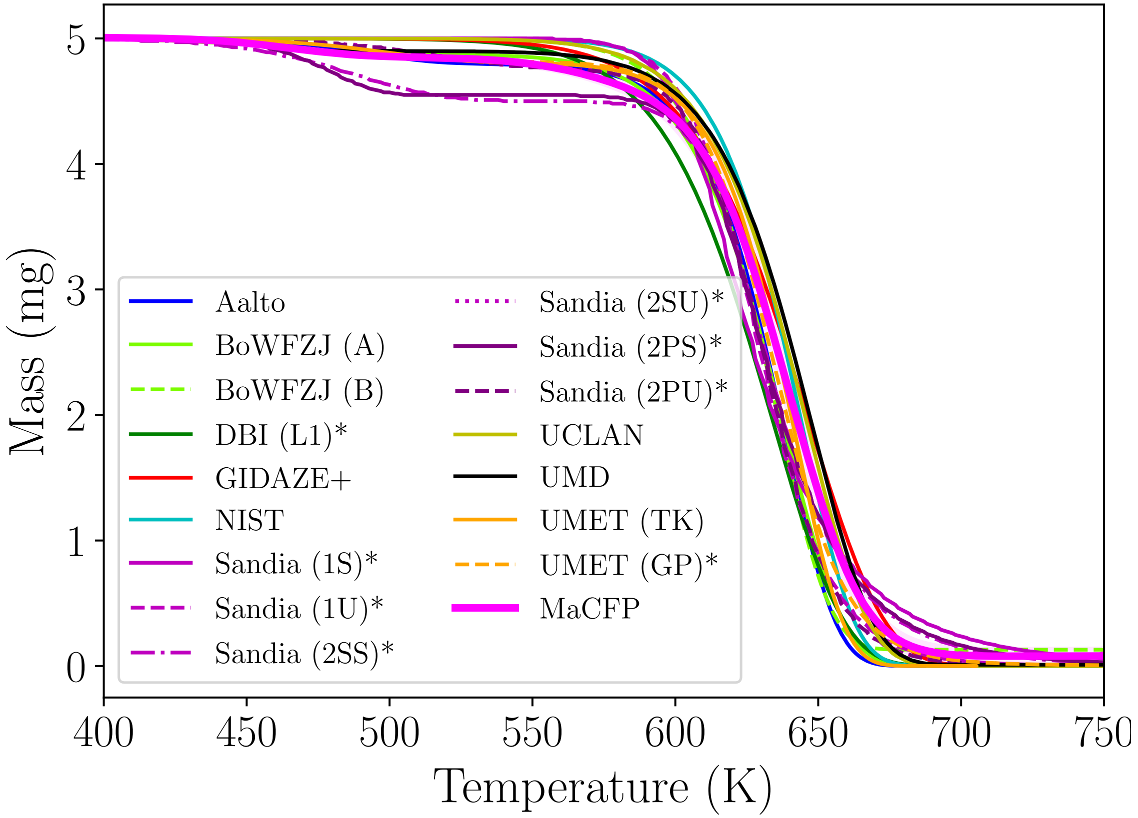
Temperature Range:	300 K to 1000 K
Heating Rates:	10 K min^{-1} and 100 K min^{-1}
Initial Sample Mass	5 mg
Output:	time [s] Time-resolved Sample Temperature [K] Time-resolved Sample Mass [mg]
Test Description:	Simulations of idealized TGA experiments in which sample temperature must remain spatially uniform.

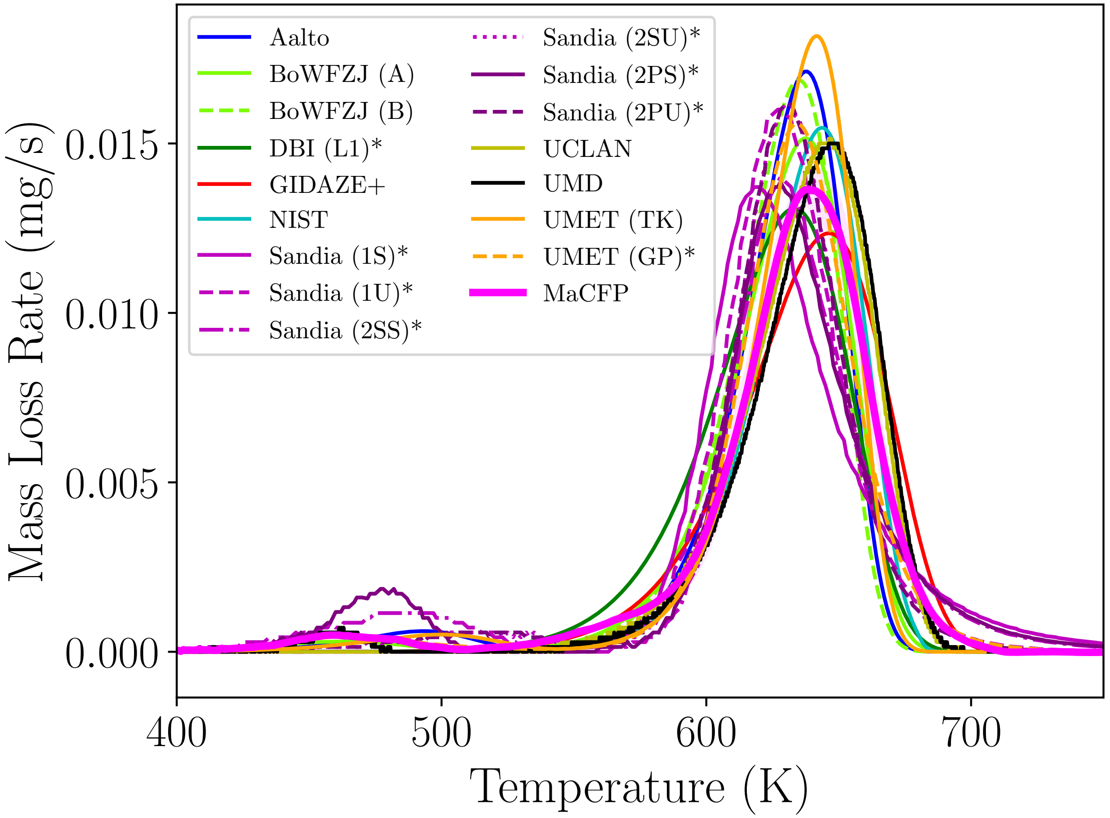
- Two total simulations
- Validation data for 10 K min^{-1}
- TGA data at 100 K min^{-1} is possibly problematic



$$m(t=0) = 5\ \mathrm{mg}$$
$$\beta = 10\ \mathrm{K\ min^{-1}}, 10\ \mathrm{K\ min^{-1}}$$

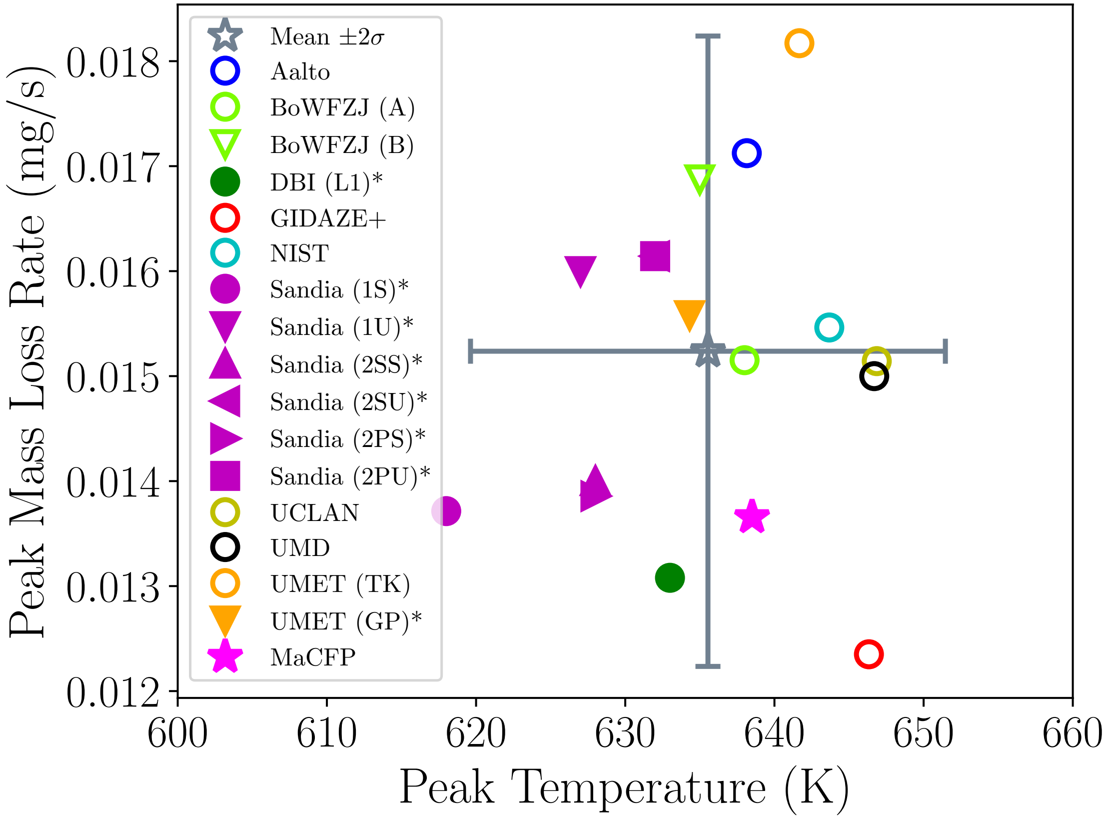
TGA at 10 K/min



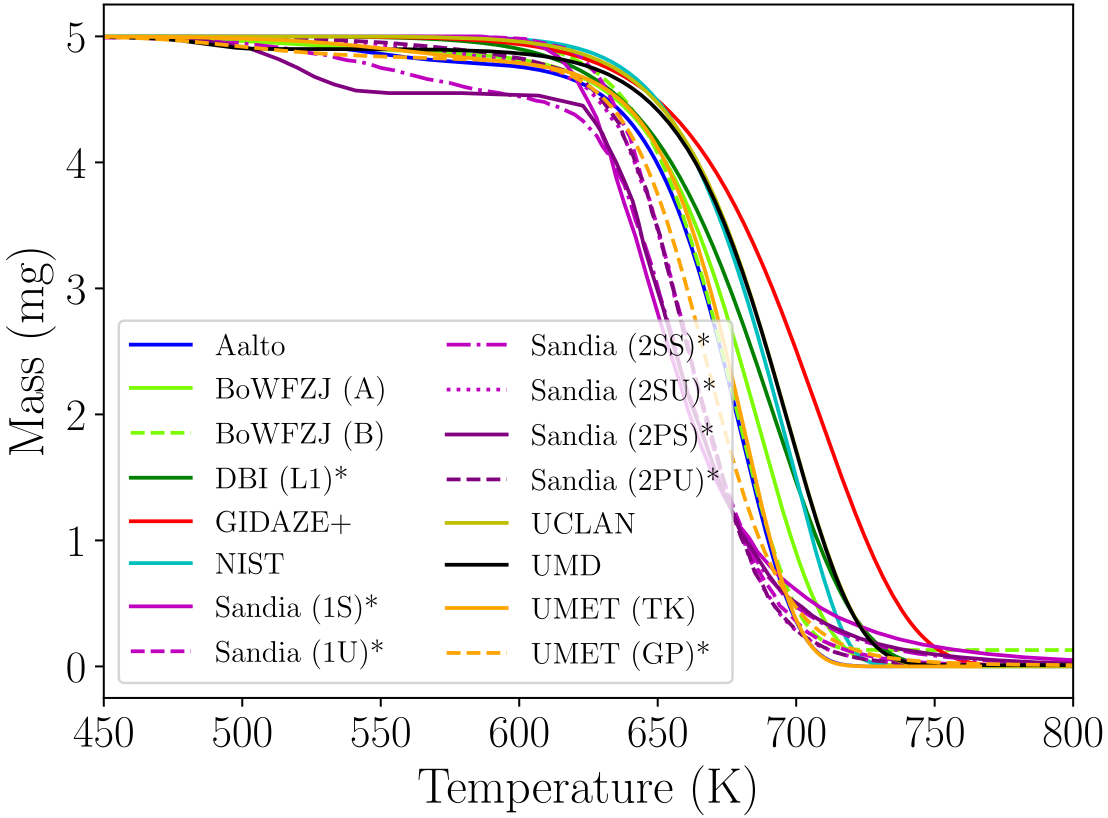


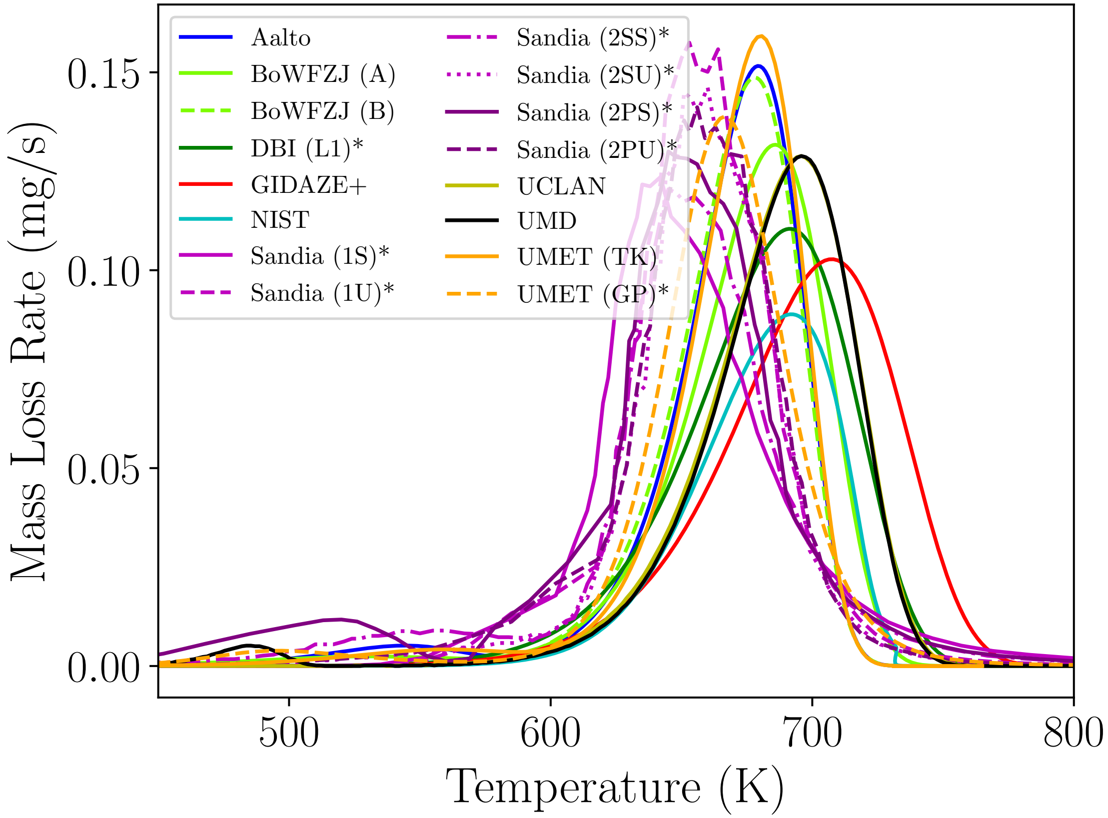
TGA at 10 K min^{-1} Peak Data

- Peak temperature predictions vary by ~30 K
- Peak mass loss rate predictions vary by ~40 %
- Models predict peak temperature very close to MaCFP mean
- Scatter is about twice what we see in experimental data



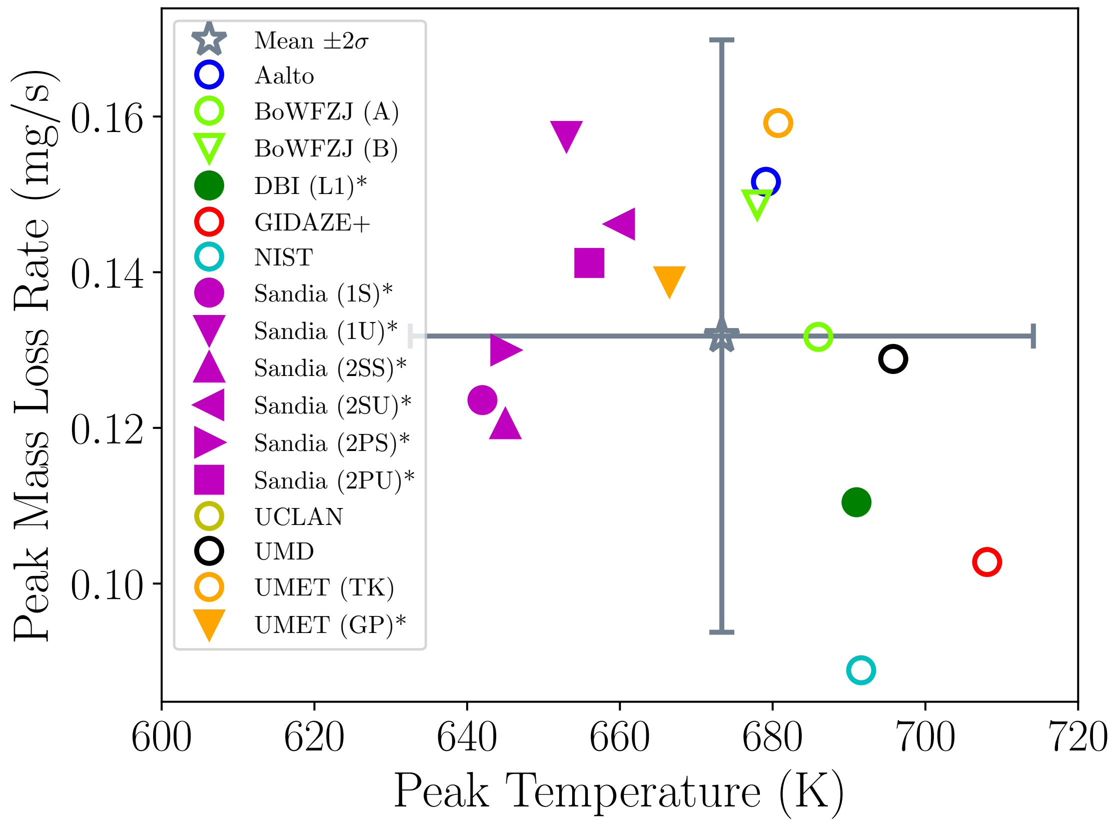
TGA at 100 K/min



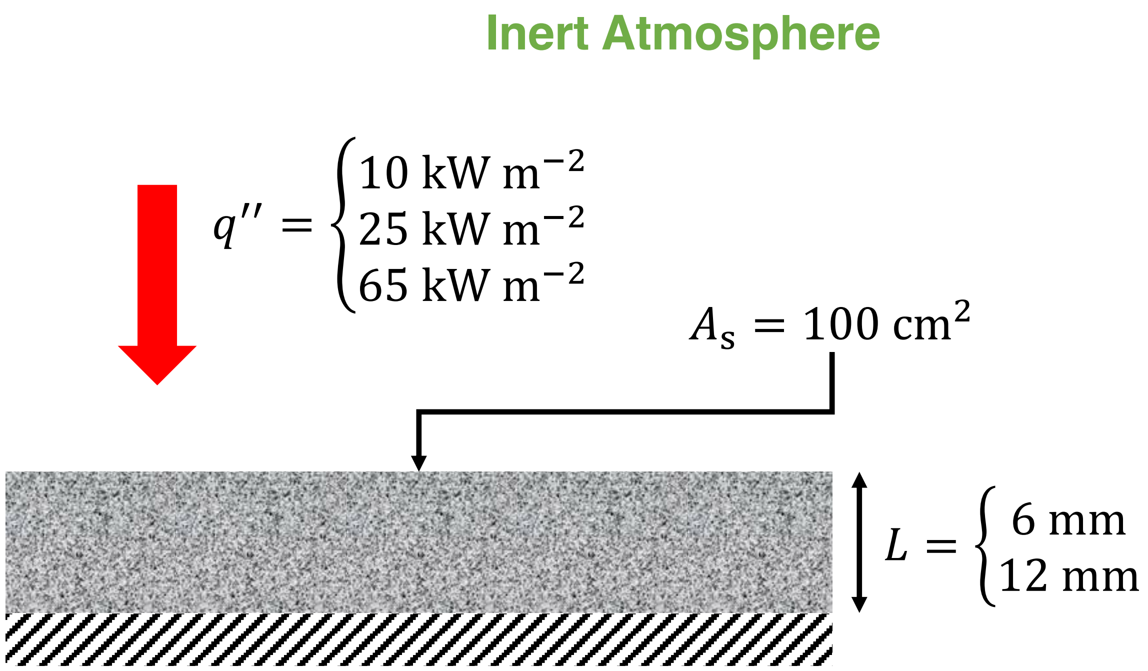


TGA at 100 K/min Peak Data

- Peak temperature predictions vary by ~80 K
- Peak mass loss rate predictions vary by ~60 %
- Not surprising that variability increases with heating rate
- What impact does this have on flame spread predictions?



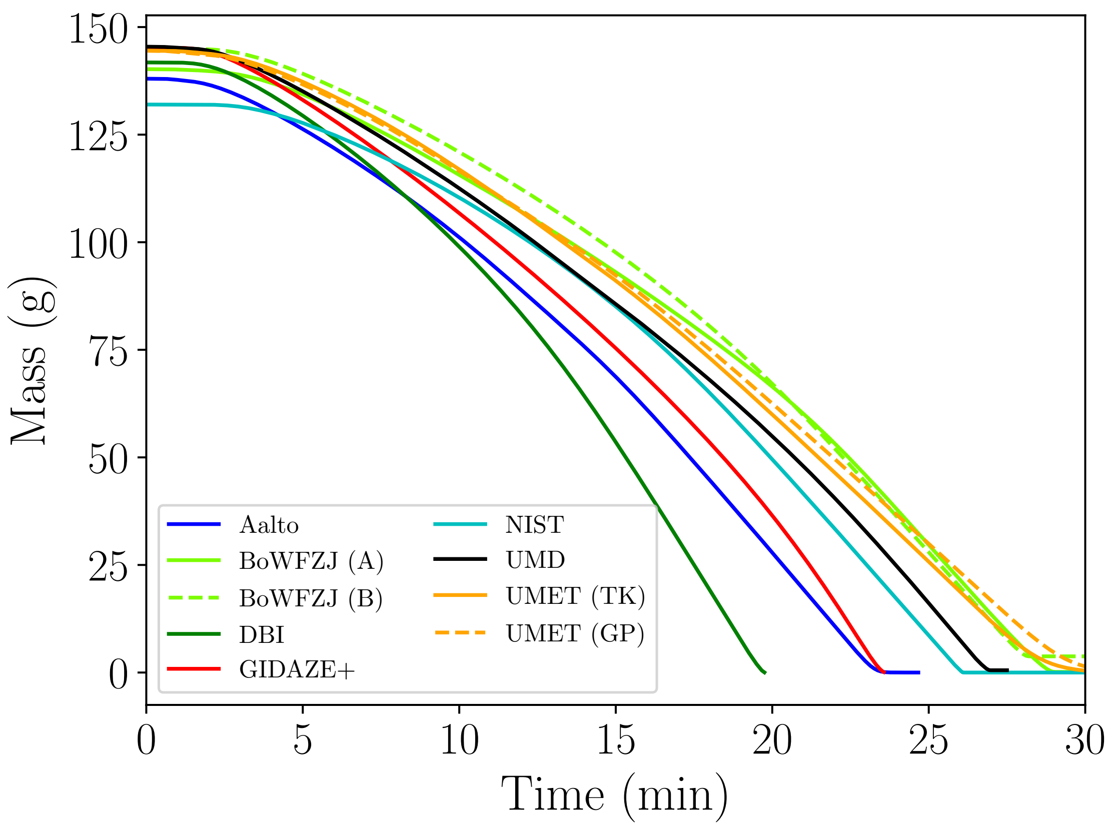
Gasification Target Simulations

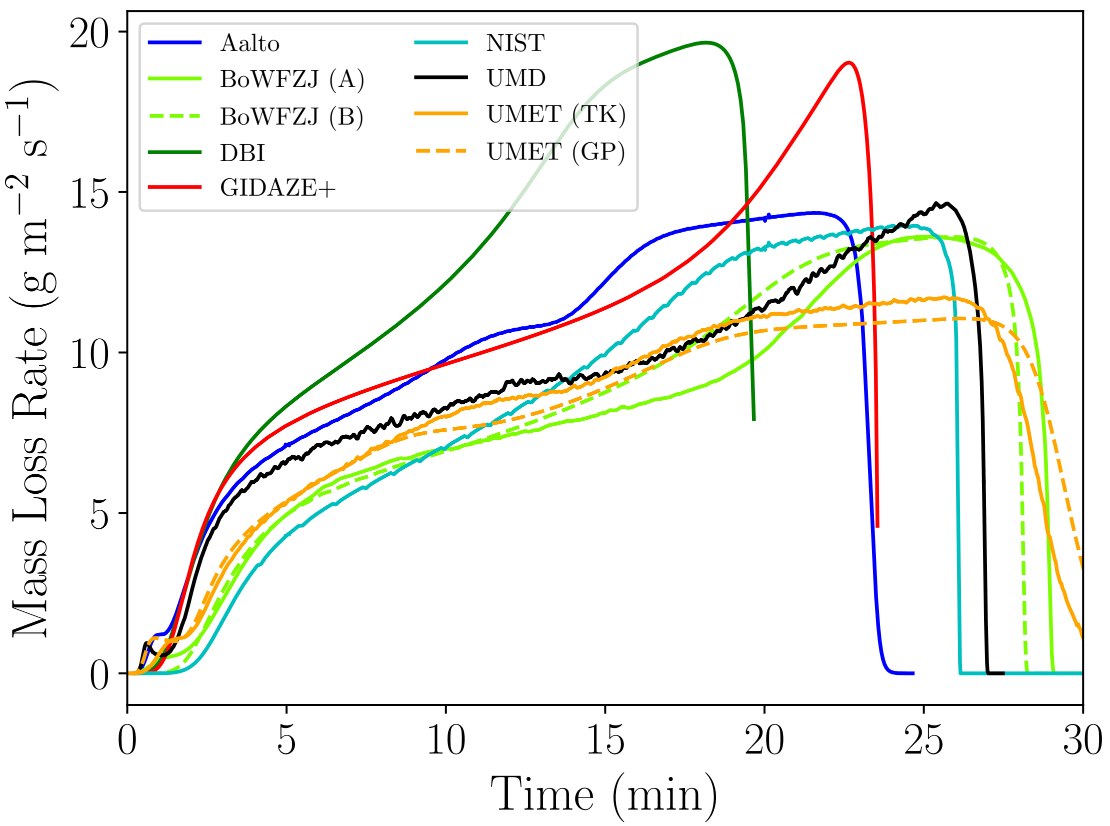


Simulations should be performed using a computational pyrolysis solver.

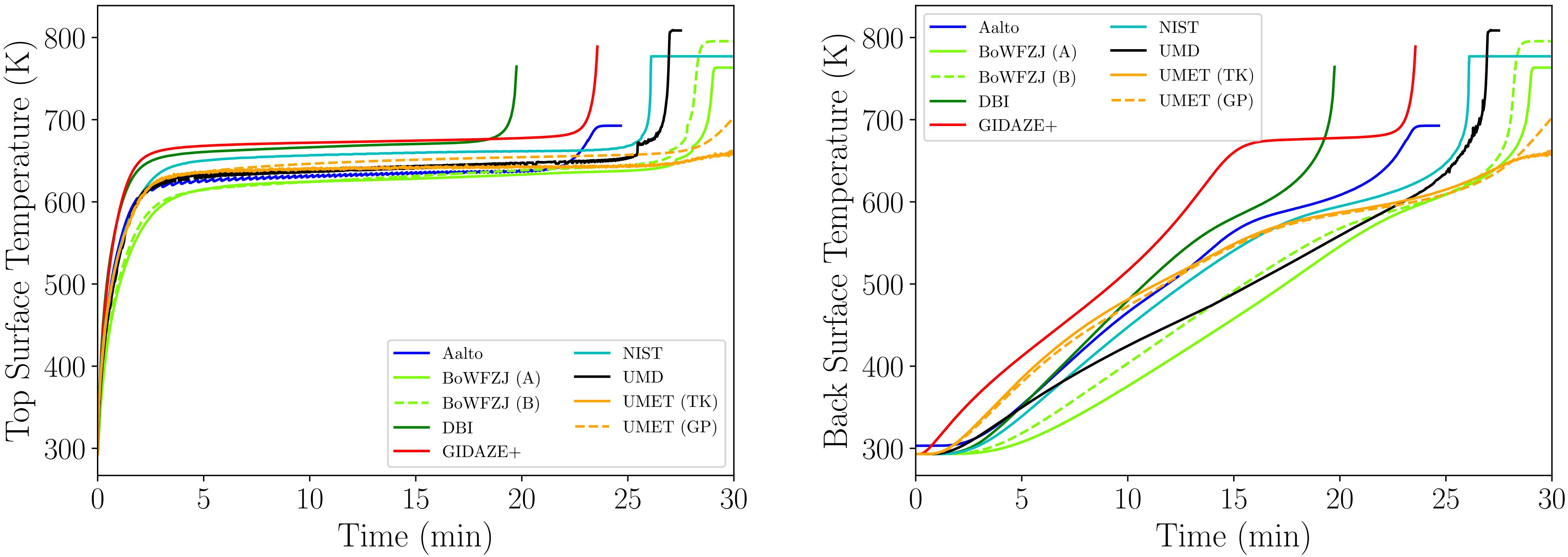
Initial Temperature	Initial ambient and sample temperatures should be 293K.
Top Surface Boundary Conditions:	Sample surface exposed to 10, 25, and 65 kW m^{-2} of incident radiant heat flux; no convection
Bottom Surface Boundary Conditions:	Sample back surface should be perfectly insulated. (i.e., no convection or radiation)
Sample Dimensions:	Simulations should be repeated at each incident heat flux using sample thicknesses of 6 mm and 12 mm. Simulation outputs should be scaled such that samples are initial 10 cm x 10 cm, squares.
Output:	Time [s] Time-resolved Sample Mass [g] Time-resolved Sample Back-Surface Temperature [K] Time-resolved Sample Top-Surface Temperature [K]

Gasification Mass: 25 kW m^{-2}, 12 mm

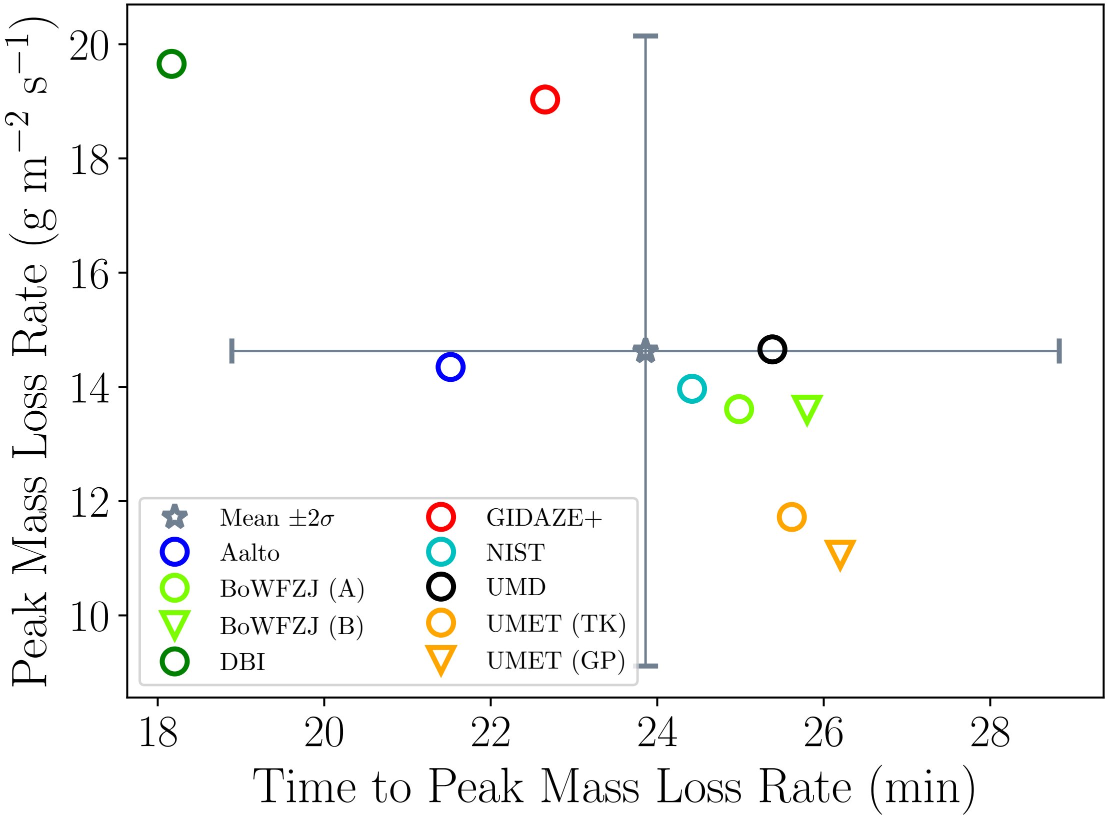




Gasification Temperatures: 25 kW m^{-2}, 12 mm



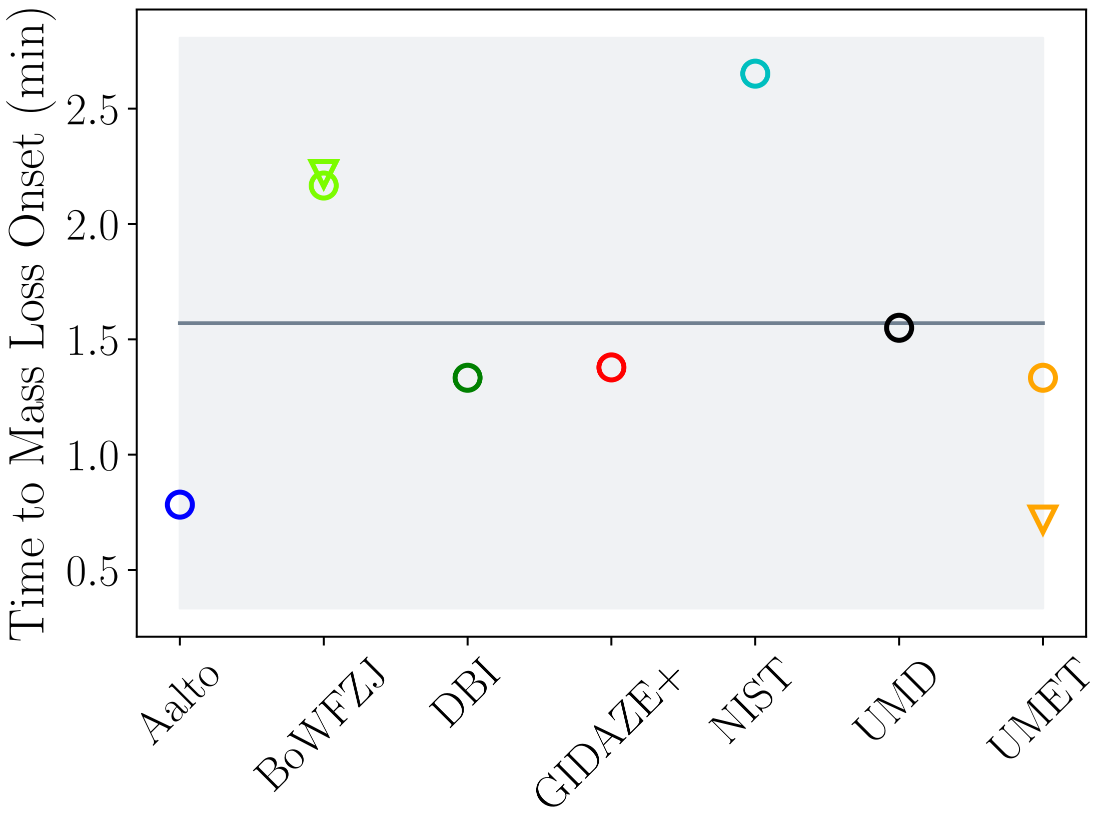
Gasification Peak Data: 25 kW m^{-2}, 12 mm

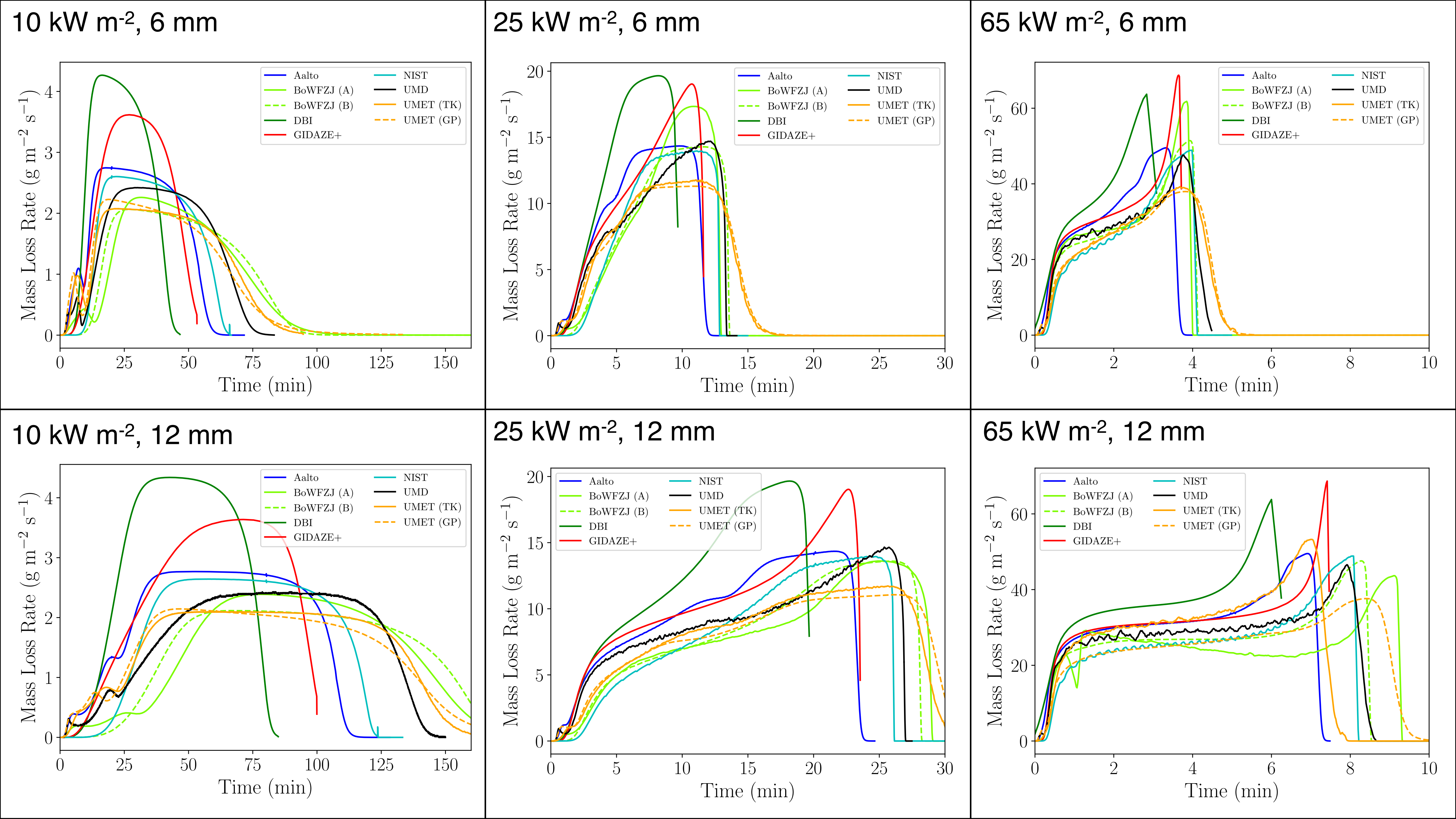


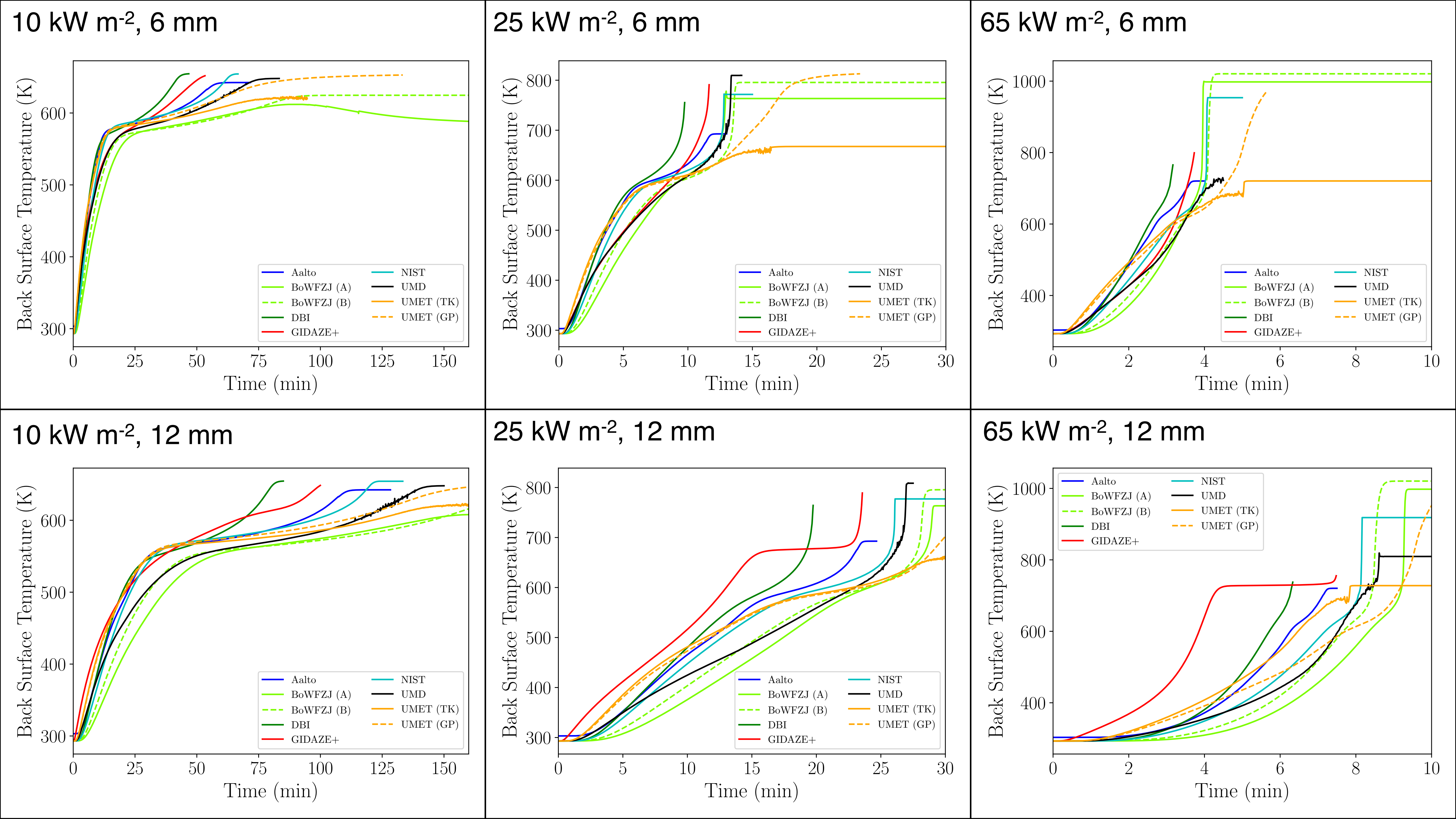
- Peak mass loss rate predictions vary by ~75 %
- Time to peak mass loss rate predictions vary by ~40 %
- Peak rate decreases with time to peak

Gasification Onset: 25 kW m^{-2}, 12 mm

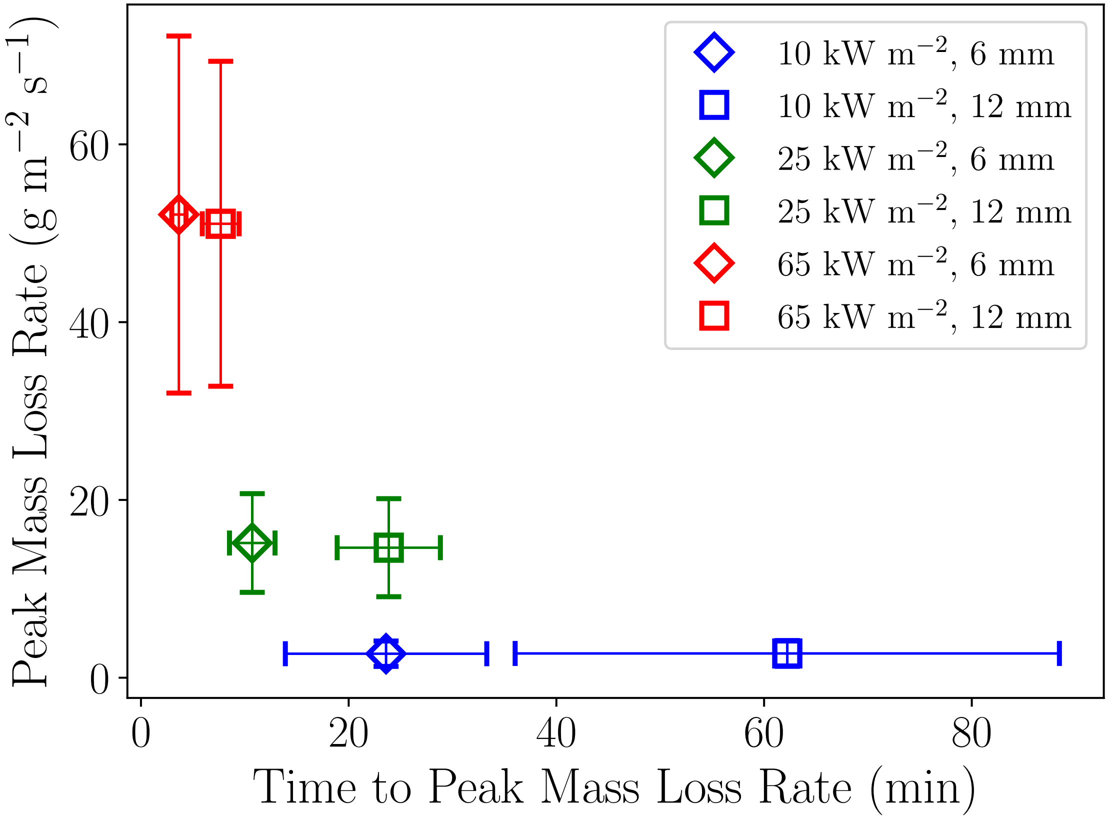
- **Definition**: time where mass loss rate exceeds 1 g m^{-2} s
- Indicative of time to ignition
- Time to gasification onset predictions vary by ~125 %




10 kW m-2, 6 mm
25 kW m-2, 6 mm
65 kW m-2, 6 mm
10 kW m-2, 12 mm
25 kW m-2, 12 mm
65 kW m-2, 12 mm
Mass Loss Rate (g m−2 s−1)
Time (min)
Aalto
BoWFZJ (A)
BoWFZJ (B)
DBI
GIDAZE+
NIST
UMD
UMET (TK)
UMET (GP)


10 kW m-2, 6 mm
25 kW m-2, 6 mm
65 kW m-2, 6 mm
10 kW m-2, 12 mm
25 kW m-2, 12 mm
65 kW m-2, 12 mm
Back Surface Temperature (K)
Time (min)
Aalto
BoWFZJ (A)
BoWFZJ (B)
DBI
GIDAZE+
NIST
UMD
UMET (TK)
UMET (GP)

Gasification Peaks Summary

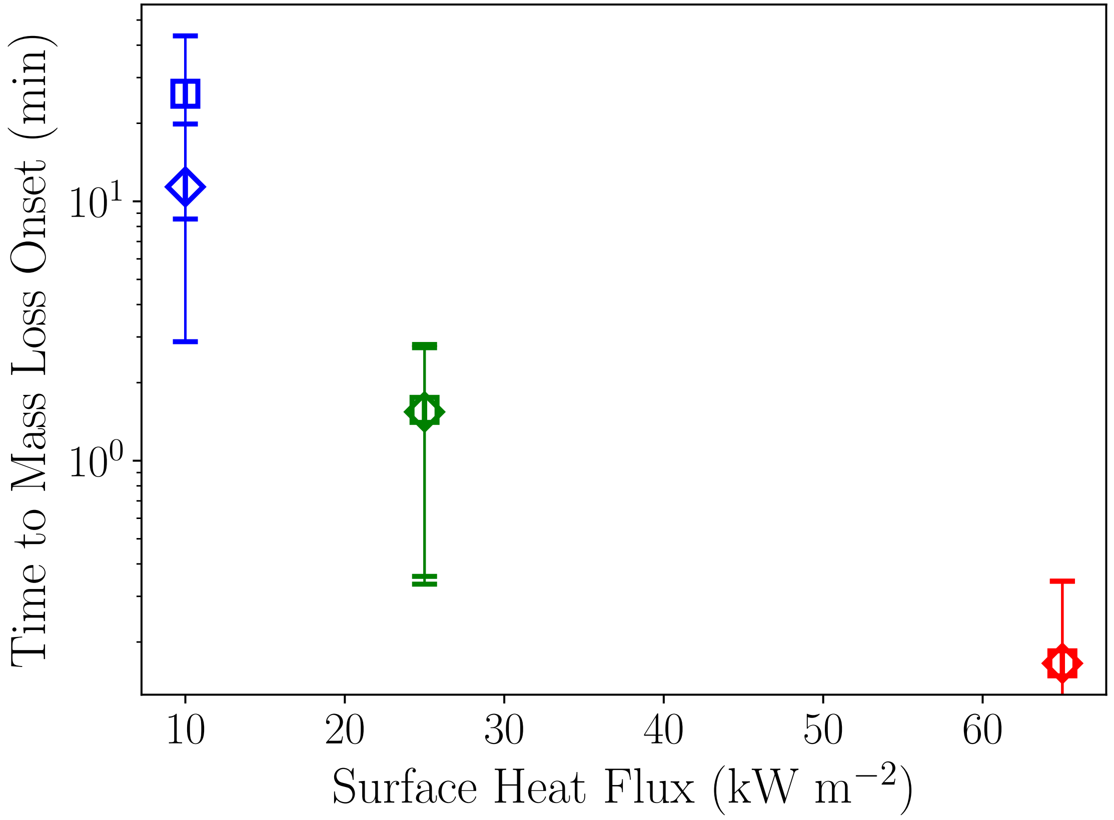


Error bars represent +/- 2 standard deviations

- High heat fluxes: peak mass loss rate predictions vary by up to ~75 %
- Low heat fluxes, time to peak mass loss rate predictions vary by up to ~85 %

Gasification Onset Summary

- Expected trend
- Sample thickness only matters at low heat fluxes
- Substantial (order of magnitude) variations at all heat fluxes



Gasification Summary

- No clear difference between models (FDS, Gpyro, ThermaKin)
- Questions:
  - Are these results good enough?
  - What aspects of this data set should we examine more closely?

4. Discussion

Some Observations

- For these cases, differences between FDS, Gpyro, and ThermaKin seem small
- Variability in model predictions: they can’t all be right, but they could all be wrong
- +/-35 % uncertainty in peak mass loss rate (or peak heat release rate) seems large
- +/-50 % uncertainty in time to mass loss onset (or time to ignition) seems large

Next Steps

- Standard format for material property metadata:
  - (Calibration) Data, Model, and Method
- Standard format for material property data:
  - Different models for temperature dependence
- Share data on GitHub
- Improve plotting scripts
- Investigate data: links between calibration data, methods, and models to predictions
- **Remember purpose: what do we need to do to improve predictions?**

Discussion Topics

- Do we need validation data for gasification predictions? Who will provide it?
- How do we define when a prediction is good enough?
- What can we learn with the results that we currently have?
- Are more calibration experiments necessary?
- Pure validation versus code-to-code comparisons?
- What validation experiments should we do next? Who will perform them?