Evaluation of Critical Temperature via Thermal Runaway Models and Slow Cook-Off Testing

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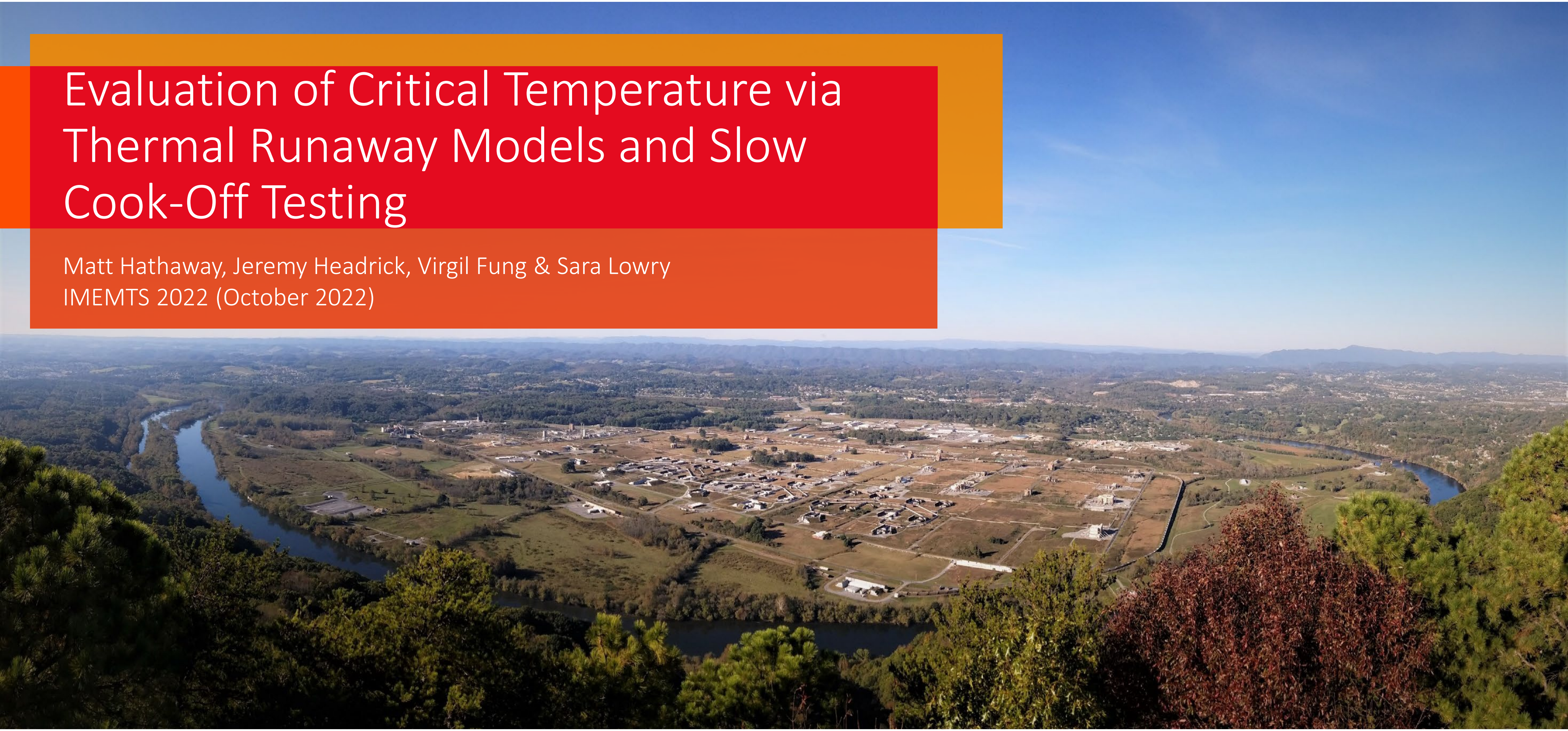

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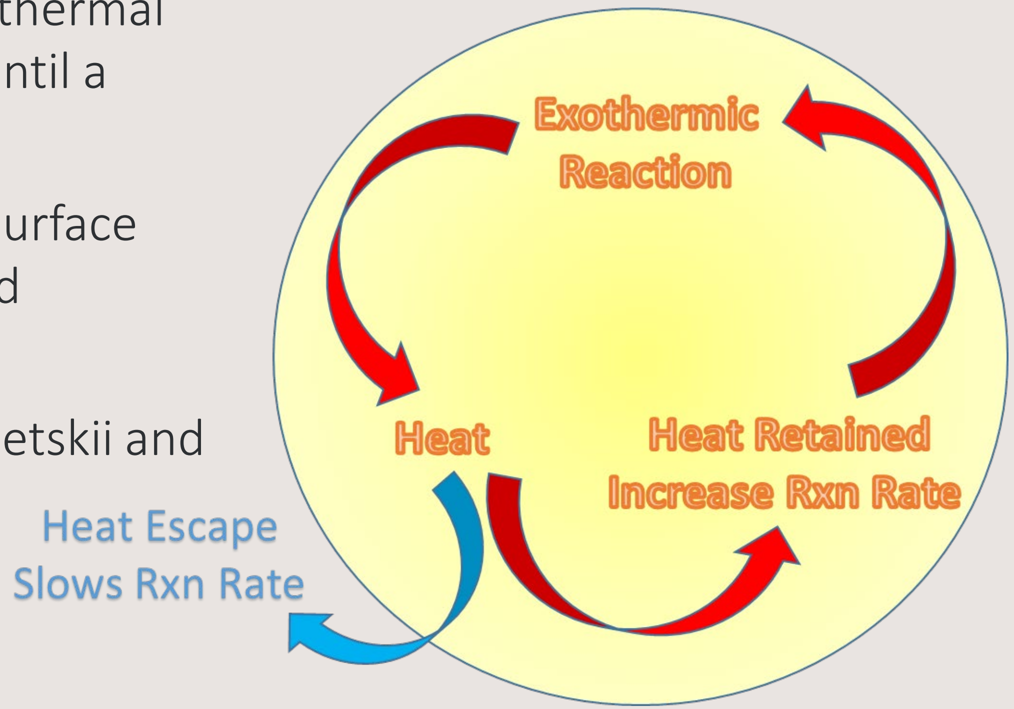
Briefing Outline

- Background – Self Heating & Critical Temperature
- Background – Predictive Models
- Validation of Predictive Models via Slow Cook Off (SCO) Testing
- Results
- Summary
- Acknowledgements

Background – Self-Heating & Critical Temperature of an Explosive Material

- Self-heating is a process where thermal energy is liberated from a material as a results of a slow chemical decomposition.
- If the rate of thermal heat generated from this chemical decomposition exceeds the systems ability to dissipate the thermal energy then the temperature of the material will increase until a catastrophic event occurs.
- The Critical Temperature is defined as the lowest constant surface temperature at which a material in a specific shape, size and composition can begin to self-heat catastrophically.
- Two predictive models of critical temperature Frank-Kamenetskii and Semenov



Background – Frank-Kamenetskii and Semenov Predictive Models

- Frank-Kamenetskii Model
  - Assumes conductive heat transfer
  - Temperature gradient in the reacting mass
  - Worst-case predictive model
  - Mimics a viscous melt with no stirring

$$T_c = \frac{E_a/R}{ln\left[\frac{A^2 \rho Q Z E_a}{T_c^2 \lambda \delta R}\right]}$$

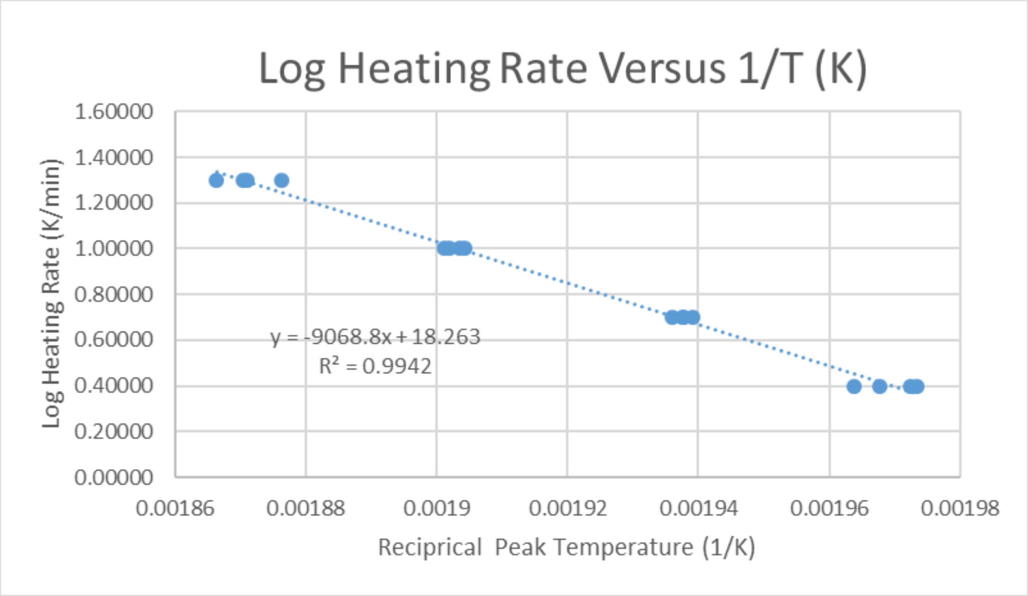
- Semenov Model
  - Assumes perfect stirring
  - Convective heat transfer
  - Uniform temperature in the reacting mass
  - Heat loss to thermal gradient at vessel boundary

$$\frac{E_a}{T_c} = R \ln\left[\frac{V \rho Q Z E_a}{S \alpha R T_c^2}\right]$$

R – gas constant
Q – heat of decomposition
ρ – density
E_a - activation energy
Z – frequency factor
λ – thermal conductivity
A – radius of sphere, cylinder or slab
δ – shape factor
V- volume of charge
S- surface area of charge
α- heat flow coefficient at boundary
T_c- critical temperature

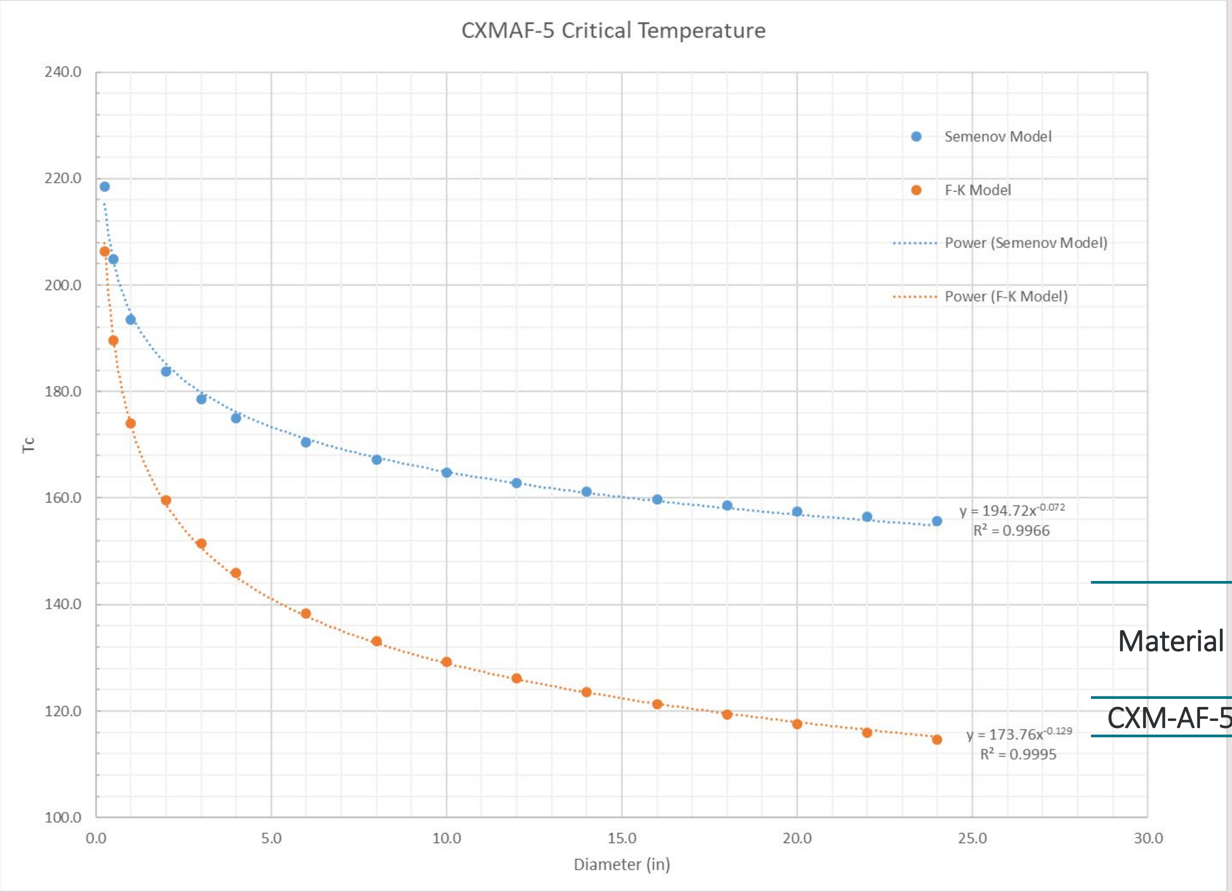
Critical Temperature via Predictive Models

- Heat of decomposition used as 500 cal/g
- Density used were bulk densities for the material.
- Decomposition Kinetic Parameters (E_a & Z) determined by variable ramp rate DSC.



*R – gas constant - 1.987 cal/(mol*K)*
Q – heat of decomposition – 500 cal/g
ρ – density - 1.00 g/cm^3
E_a - activation energy – From DSC
Z – frequency factor – From DSC
*λ – thermal conductivity – 0.000507 cal/cm*S*C*
A – radius of sphere, cylinder or slab
δ – shape factor - 2.75 for right cylinder
V- volume of charge
S- surface area of charge
*α- heat flow coefficient at boundary – 0.0022 cal/(cm^2*s*C) steel*
T_c- critical temperature

Critical Temperatures via Predictive Models: CXM-AF-5



- From parameters the critical temperature for increasing sample diameters were calculated.
- Estimates from the Frank-Kamenetskii model predict at a 20” diameter the critical temperature for this material was 117.5℃
- Estimates from the Semenov model predict at a 20” diameter vessel the critical temperature for this material was 157.5℃

Material	Tc (°C) 1.0” Diameter		Tc (°C) 2.0” Diameter		Tc (°C) 3.0” Diameter		Tc (°C) 20.0” Diameter	
	F-K	Semenov	F-K	Semenov	F-K	Semenov	F-K	Semenov
CXM-AF-5	174.0	193.5	159.5	183.7	151.5	178.6	117.5	157.5

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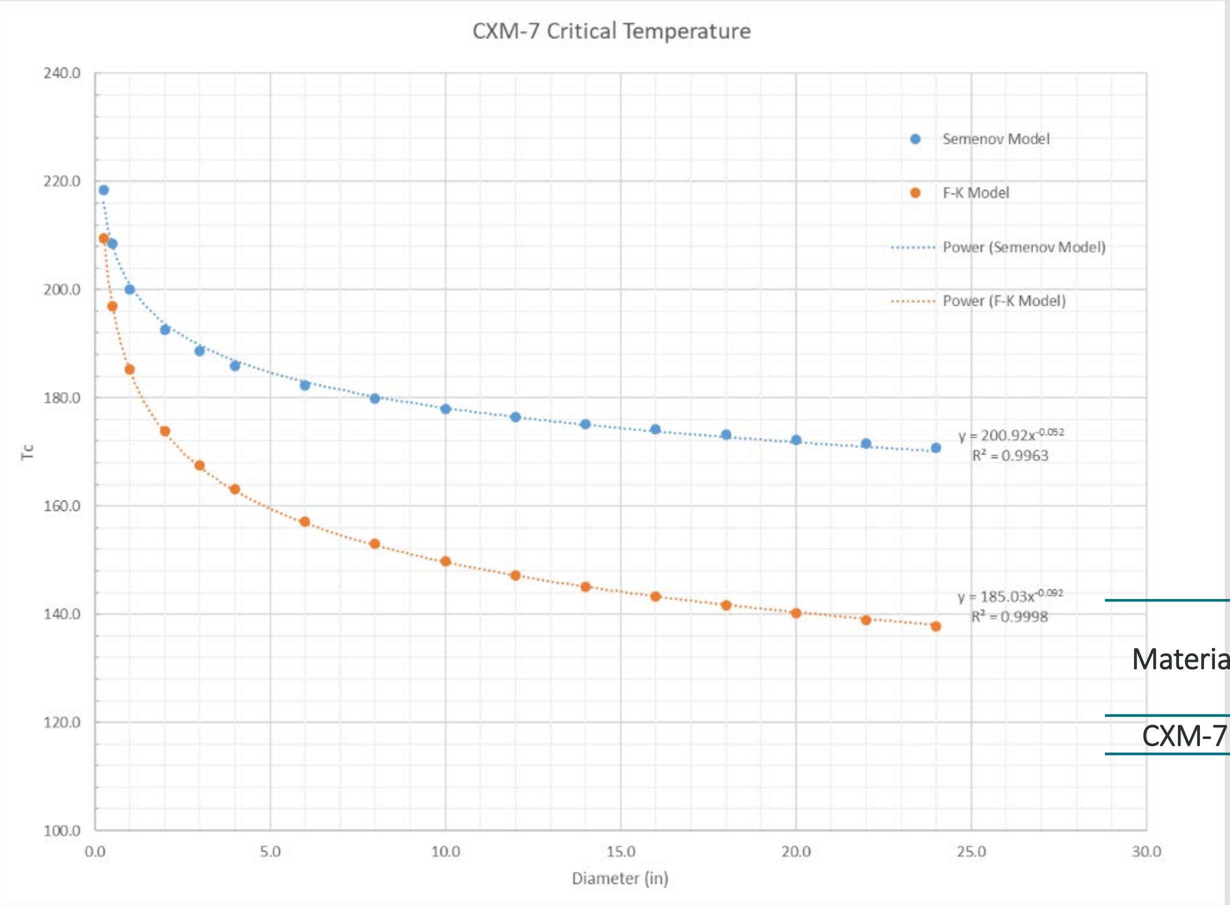
Critical Temperatures via Predictive Models: CXM-7



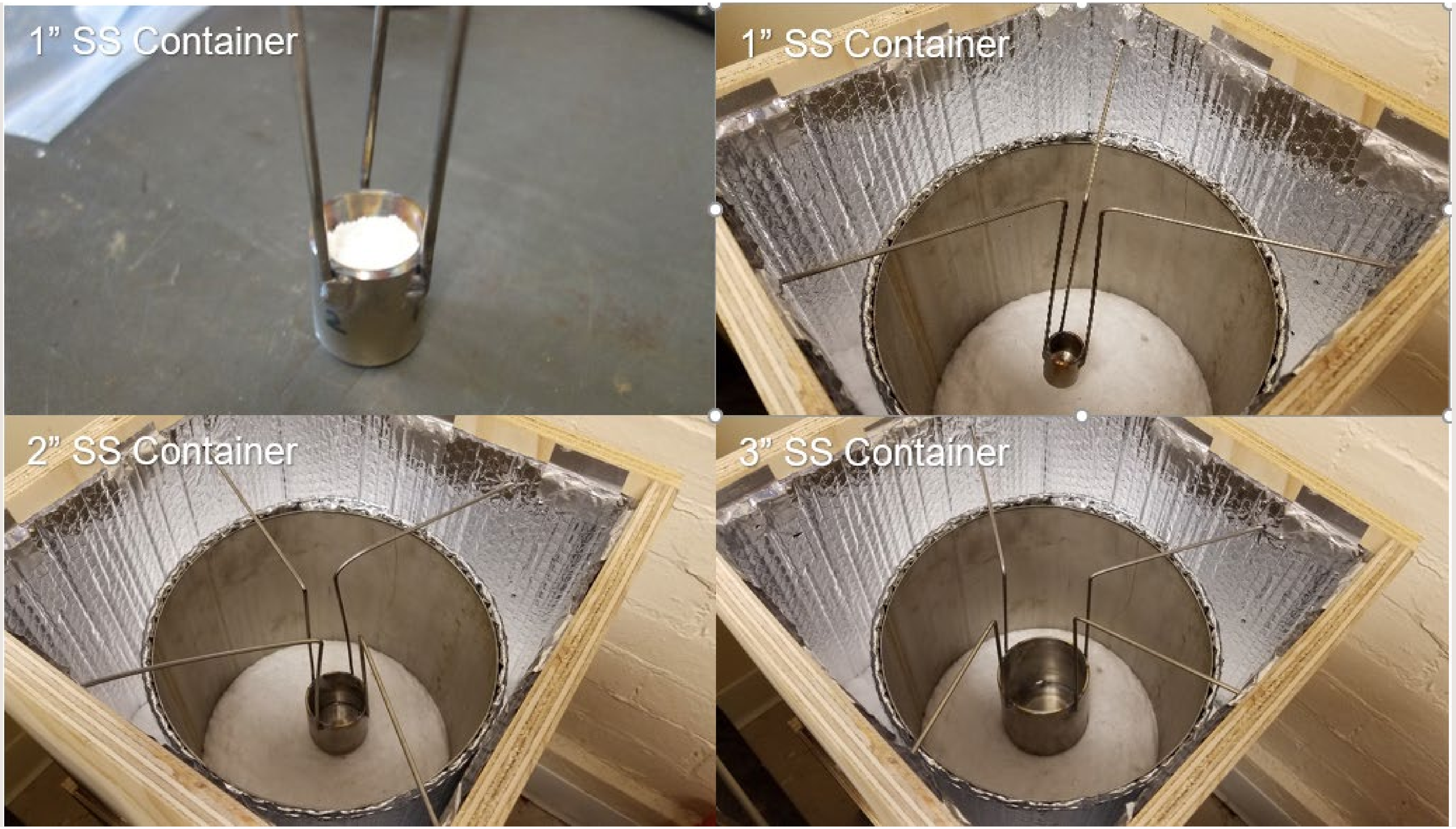
- From parameters the critical temperature for increasing sample diameters were calculated.
- Estimates from the Frank-Kamenetskii model predict at a 20” diameter the critical temperature for this material was 140.2℃
- Estimates from the Semenov model predict at a 20” diameter vessel the critical temperature for this material was 172.3℃

Material	Tc (°C) 1.0” Diameter		Tc (°C) 2.0” Diameter		Tc (°C) 3.0” Diameter		Tc (°C) 20.0” Diameter	
	F-K	Semenov	F-K	Semenov	F-K	Semenov	F-K	Semenov
CXM-7	185.2	200.0	173.9	192.6	167.6	188.6	140.2	172.3

Validation of Values from Thermal Prediction Models

- The results from the predictive models were validated using a series of Slow Cook Off tests.
- In this series of tests the size of the containment vessel used for the explosive was increased between tests.
- The vessel used were right cylinders of 1 in., 2 in., and 3 in. diameters.
- Samples were initially heated to 120 ℃ and then allowed to equilibrate for 6 hours.
- Samples were then heated at 3.3 ℃/min. until an event occurred.
- Post test evaluation of the differences between the oven and sample temperatures were evaluated to measure onset of self-heating within the samples for comparison to the predictive models.

Slow Cook-Off Testing (SCO) – Test Apparatus Setup



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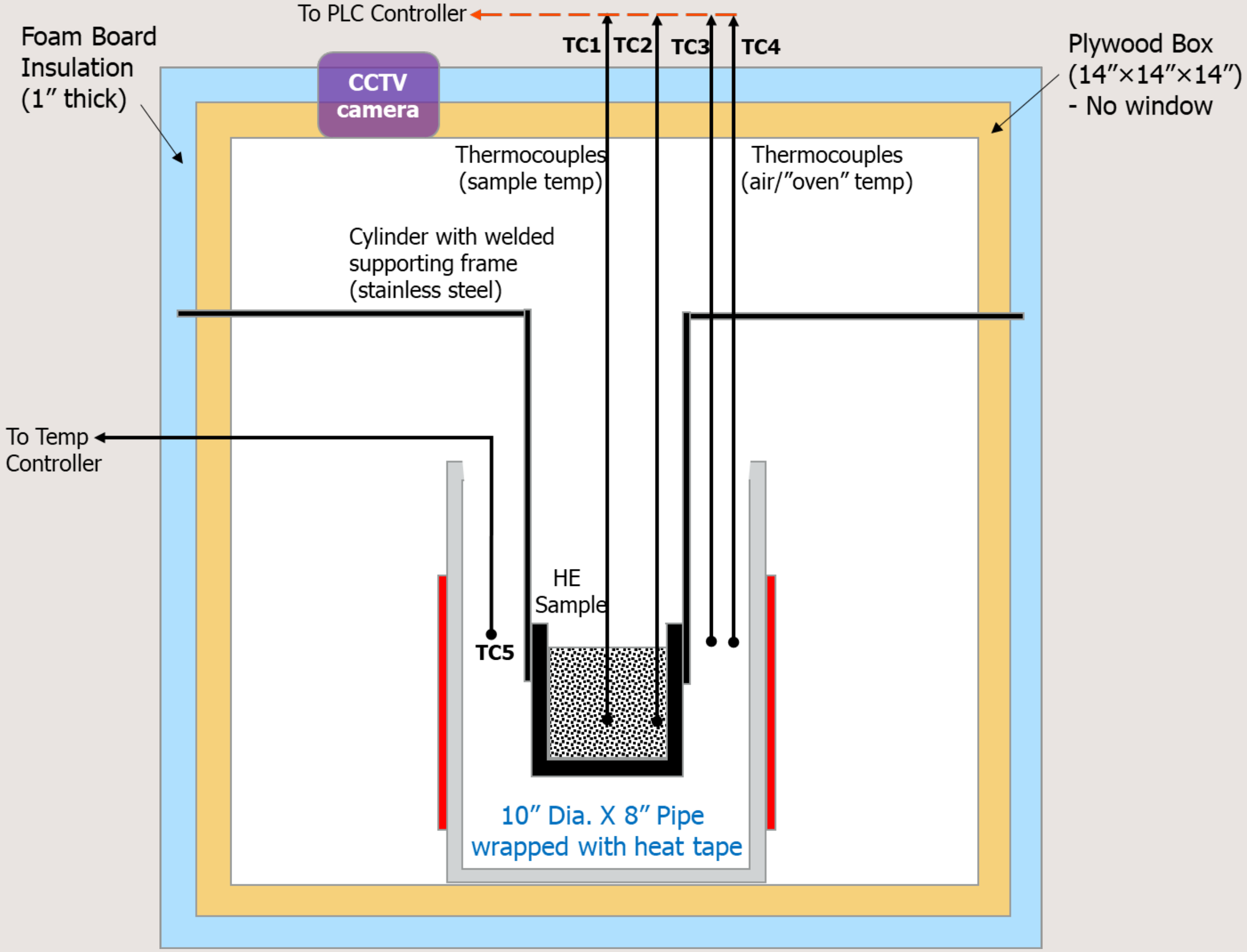
Slow Cook-Off Testing (SCO) – Test Apparatus Setup



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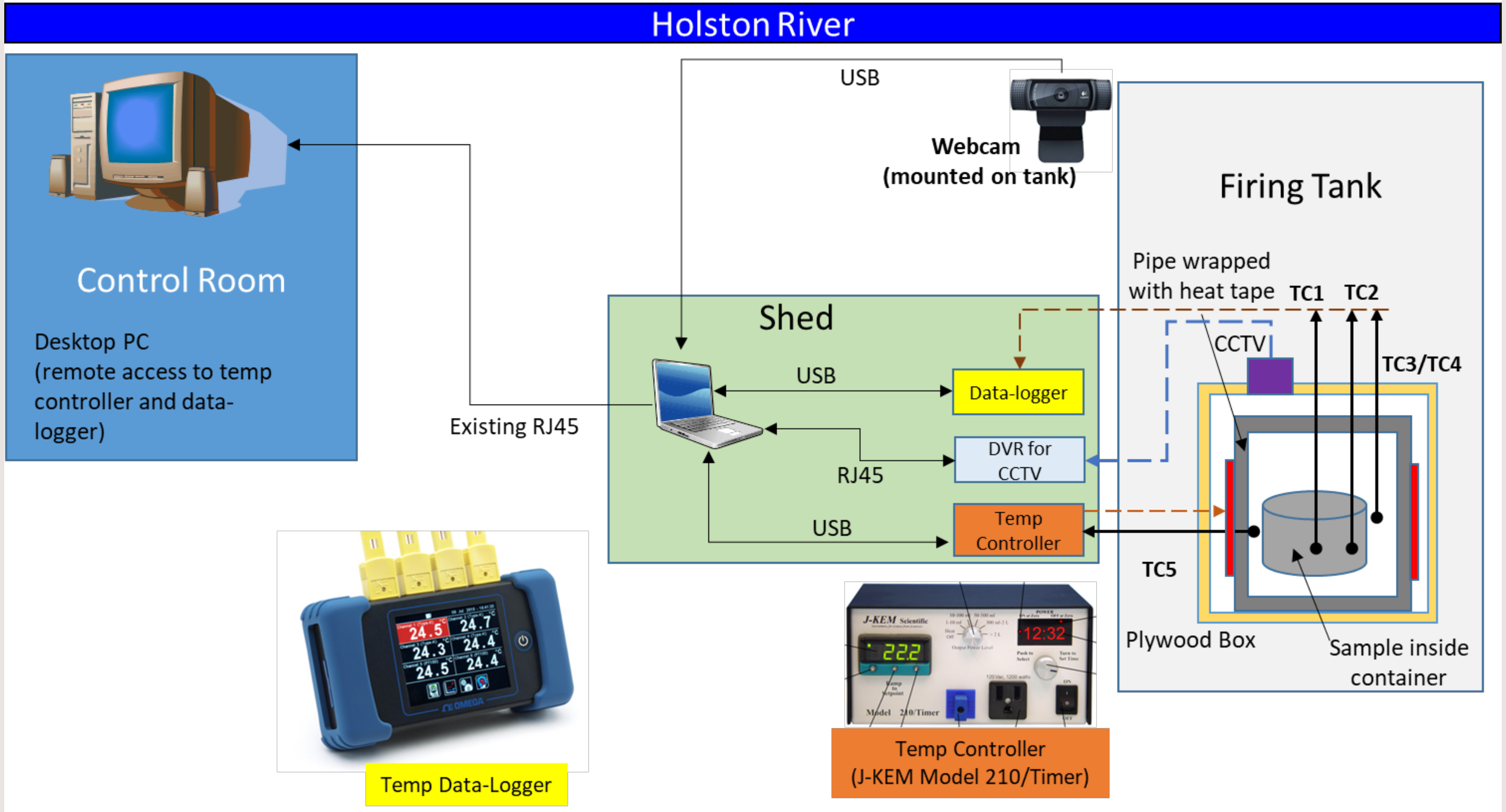
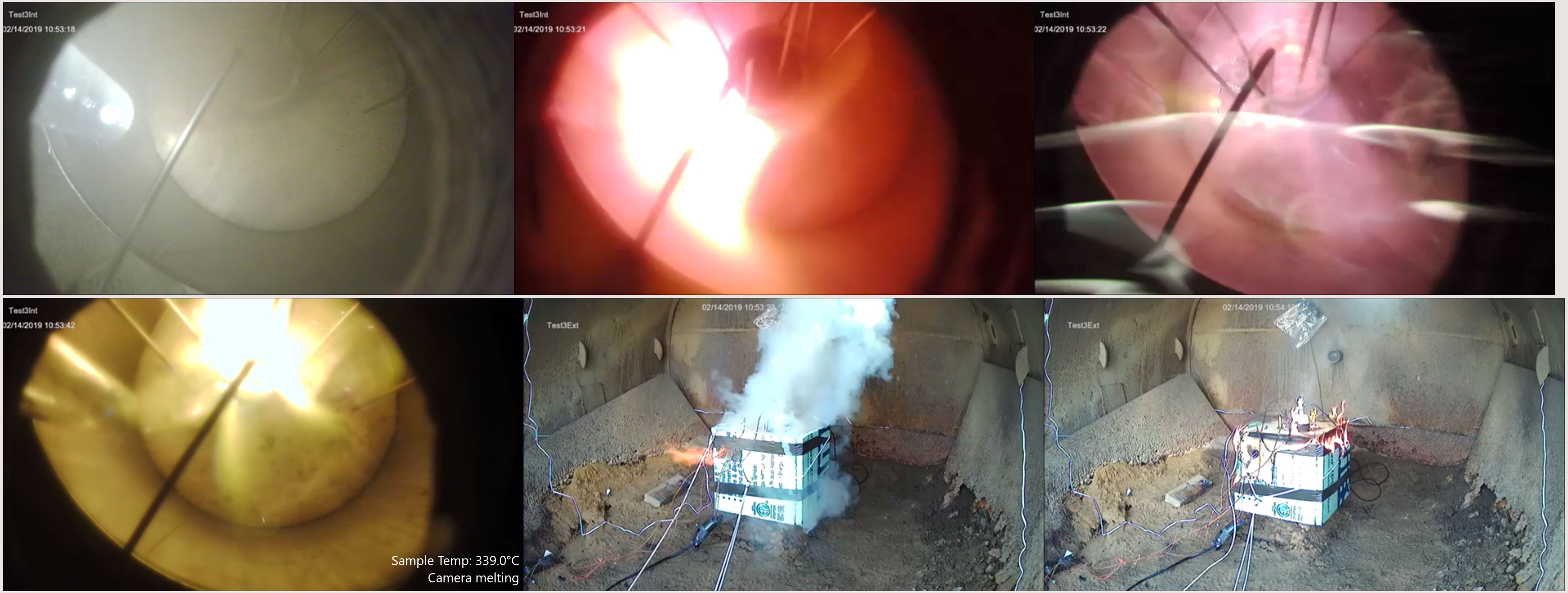
Slow Cook-Off Testing (SCO) – Test Facility Setup



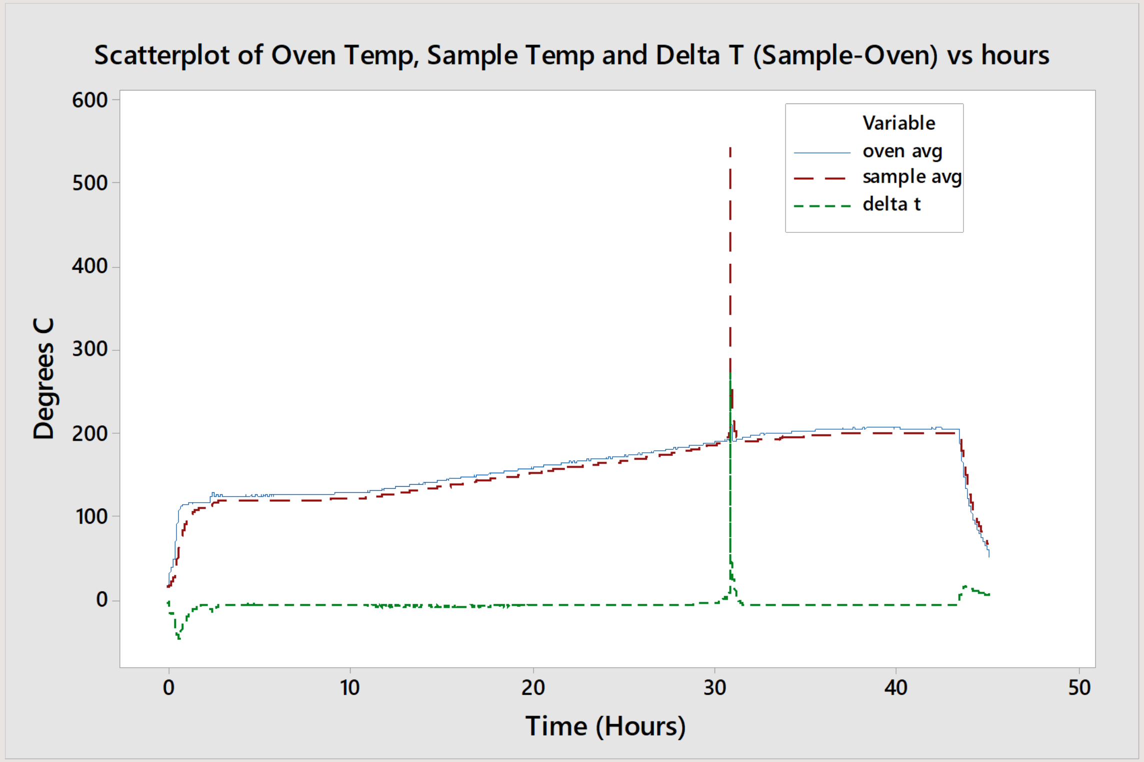
Slow Cook Off (SCO) Test Pictures

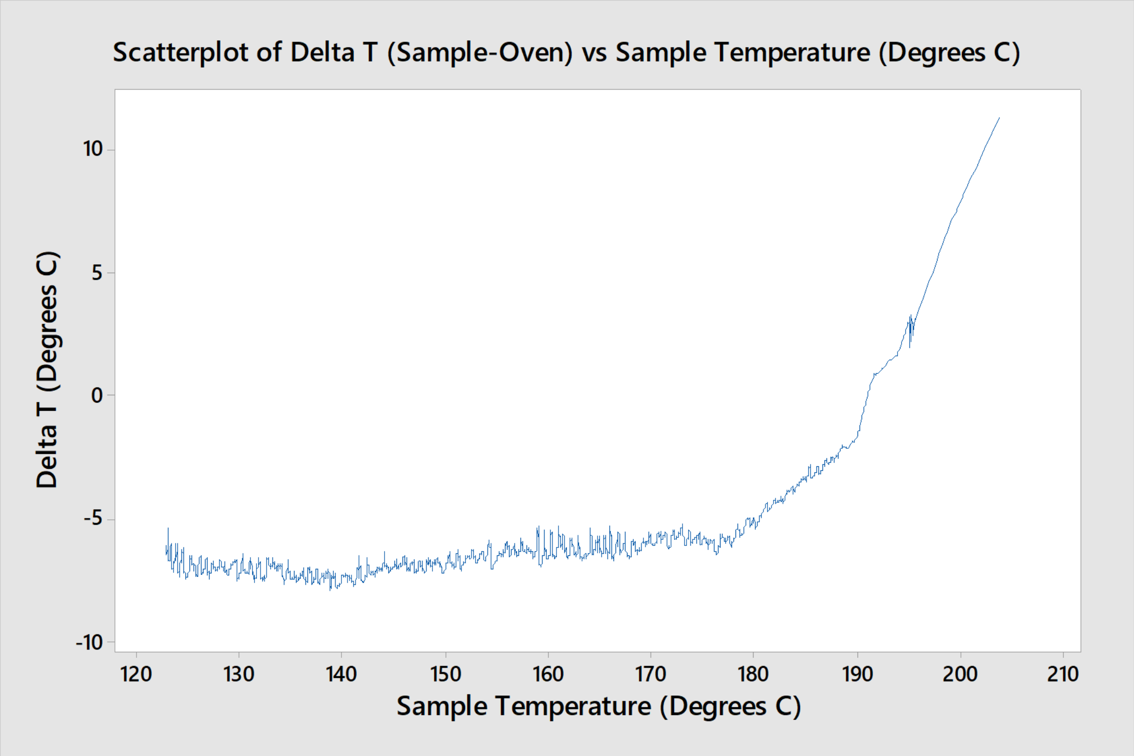
Slow Cook Off (SCO) Test Pictures



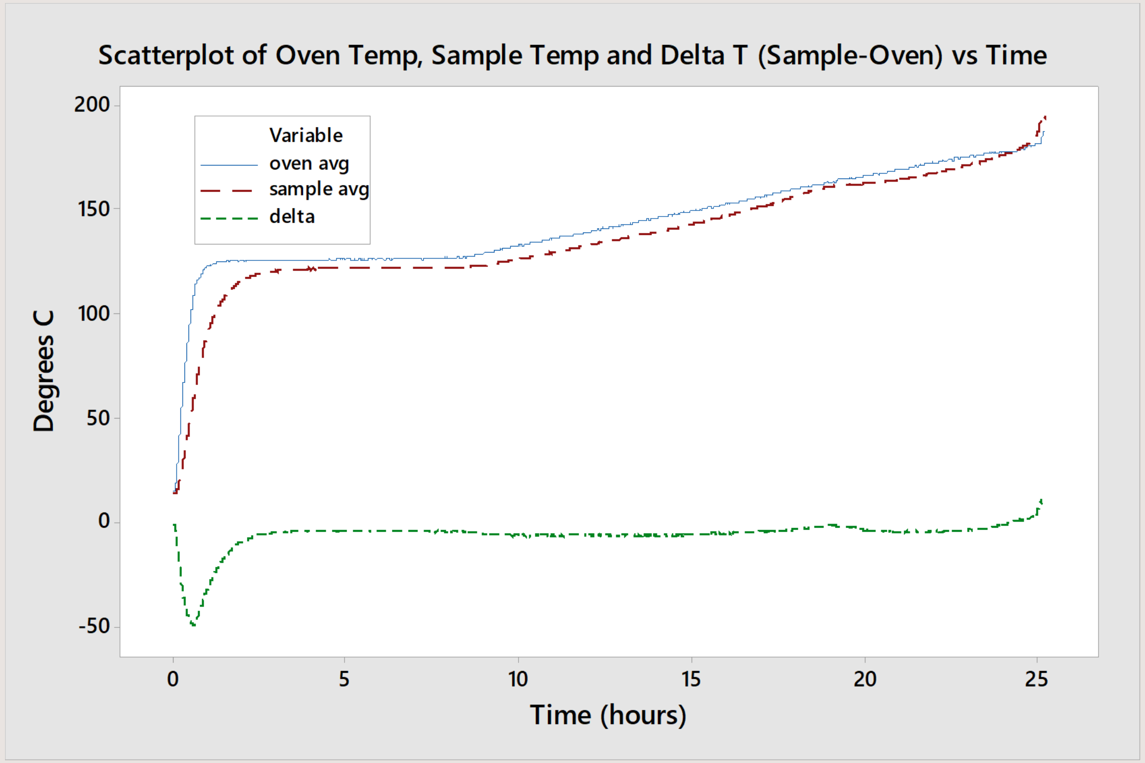
Slow Cook Off (SCO) Test Pictures – Post test

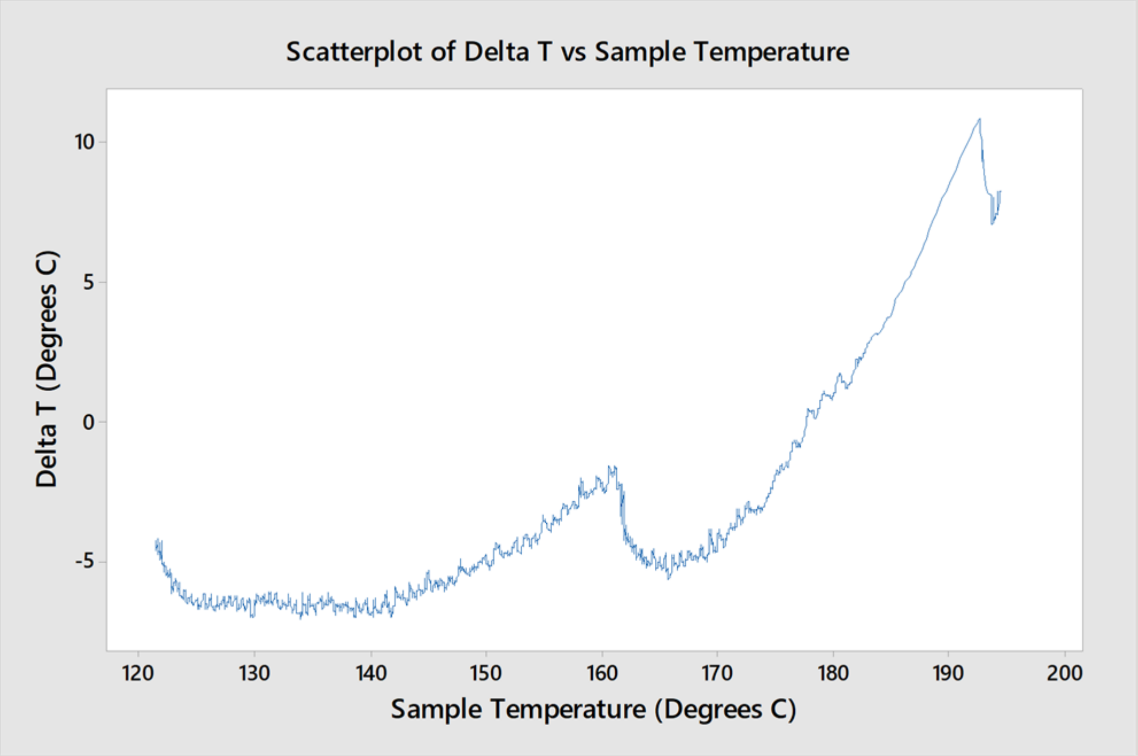
Slow Cook off (SCO) with 1” Diameter Right Cylinder Test Sample





Slow Cook off (SCO) with 2” Diameter Right Cylinder Test Sample





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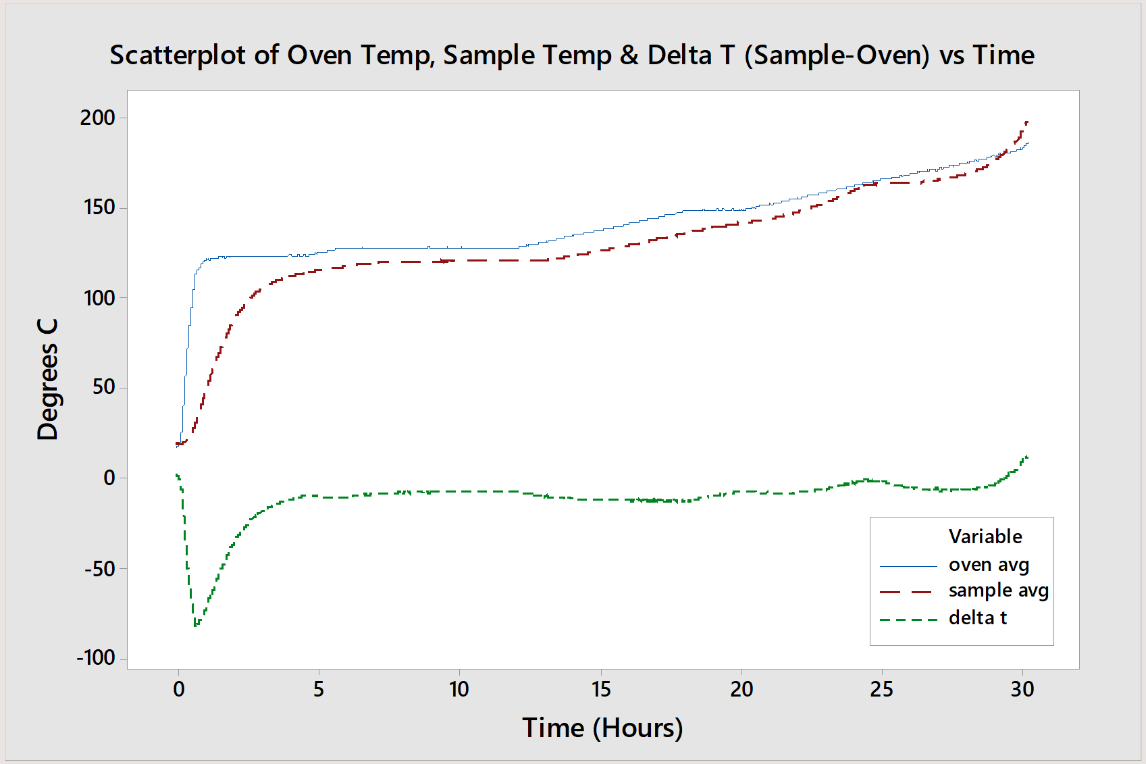
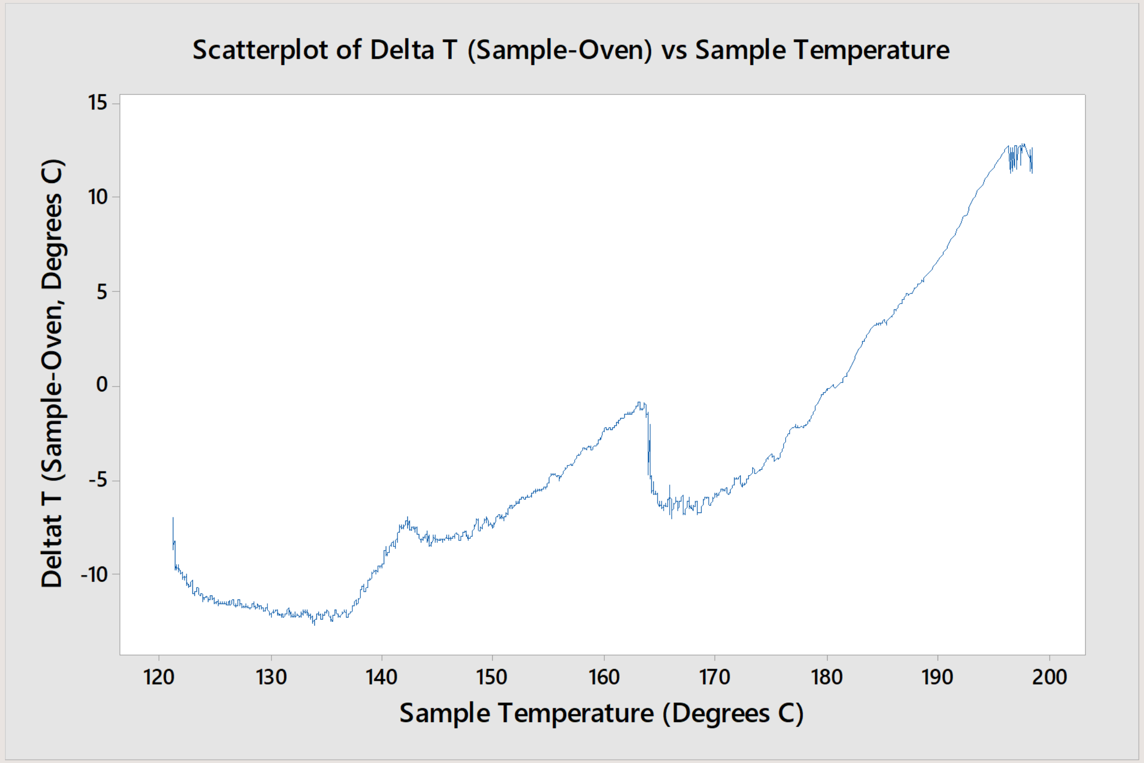
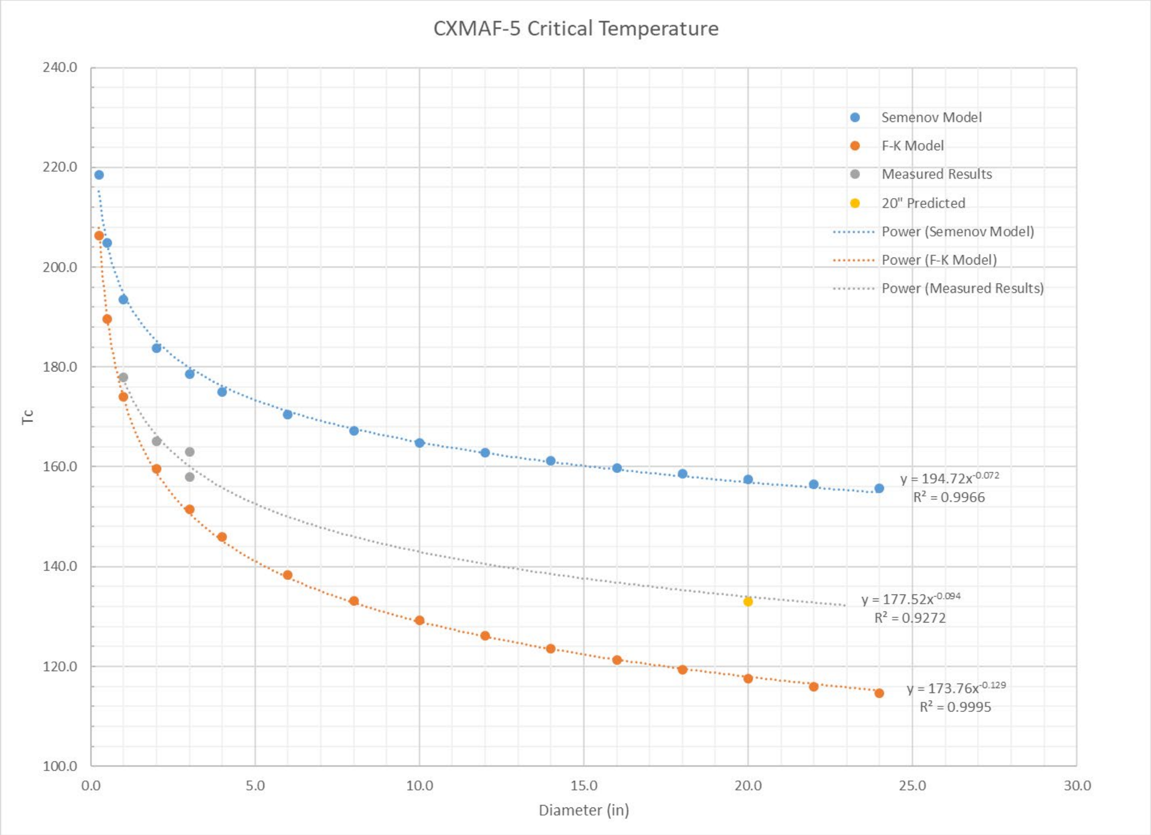
Slow Cook off (SCO) with 3” Diameter Right Cylinder Test Sample





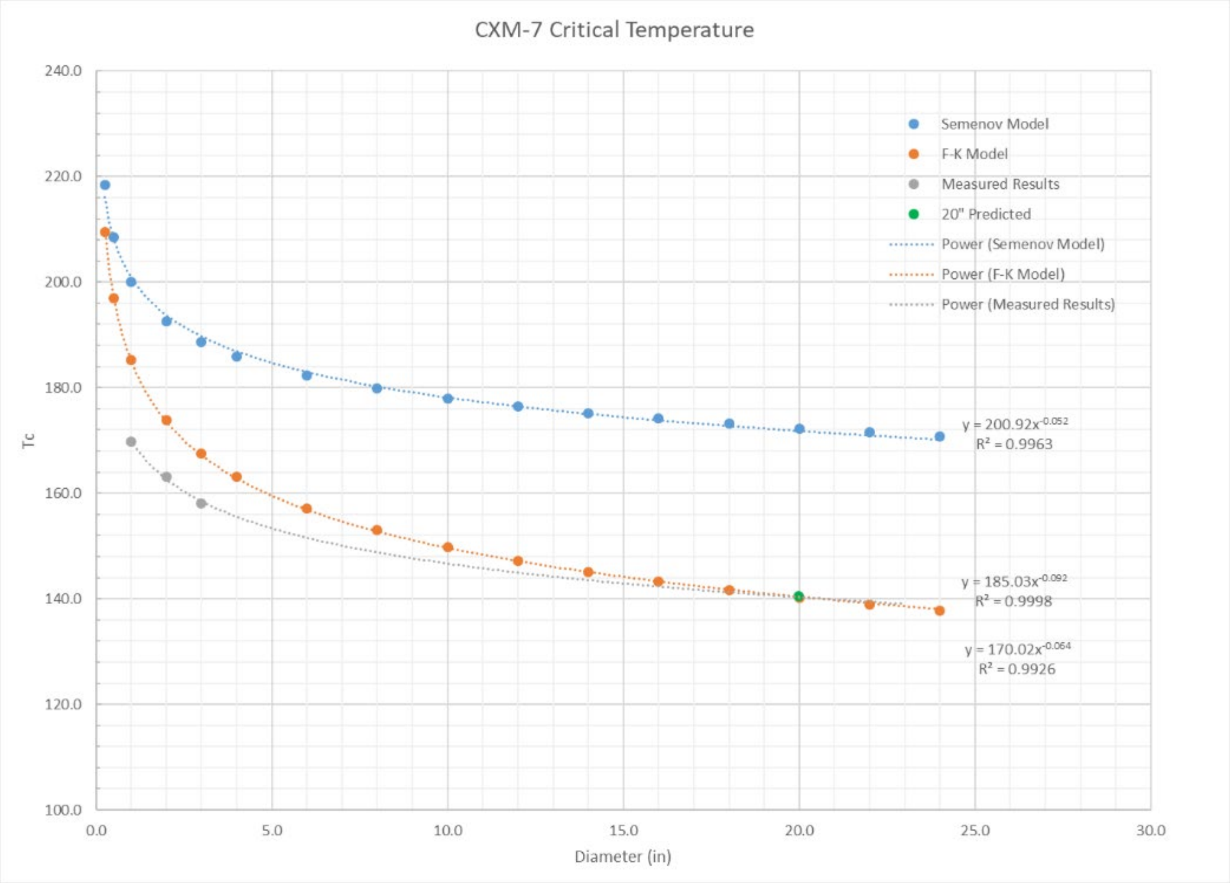
Comparison of SCO Testing to Predictive Models: CXMAF-5



Diameter	F-K Model (T_c °C) Predicted	F-K Model (T_c °C) Measured	% Error from Predicted
1 inch	174.0	178.0	2.3
2 inch	159.5	165.1	3.5
3 inch	151.5	158.0	4.3

Diameter	F-K Model (T_c °C) Predicted	F-K Model (T_c °C) Predicted via Measured values	% Error from Predicted
20 inch	117.5	133.0	13.2

Comparison of SCO Testing to Predictive Models: CXM-7



Diameter	F-K Model (T_c °C) Predicted	F-K Model (T_c °C) Measured	% Error from Predicted
1 inch	185.2	169.8	8.3
2 inch	173.9	163.2	6.2
3 inch	167.6	158.1	5.7

Diameter	F-K Model (T_c °C) Predicted	F-K Model (T_c °C) Predicted via Measured values	% Error from Predicted
20 inch	140.2	140.4	0.1

Summary

- Semenov and Frank-Kamenteskii Models were used to estimate critical temperatures of increasing diameter vessels
- Slow Cook-Off Testing was performed to validate the predicted results from the models
- The SCO test setup performed well throughout the testing. For future testing, it is suggested that the data collection rate be slowed from two data points per second to a data point every 5 seconds to reduce the amount of data collected and to potentially reduce noise in the data due to oversampling.
- The measured Tc values for all RDX based samples were within 15% of the theoretical Tc calculated from the F-K equation.
- The measured Tc values for HMX based samples were within 16% of the theoretical Tc calculated from the F-K equation.
- The general agreement between these two methods supports the screening of the Tc of future products via determination of the Arrhenius equation kinetic parameters using Differential Scanning Calorimetry (DSC) and application of the F-K equation.

Acknowledgements – to be updated

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