U.S. ARMY COMBAT CAPABILITIES DEVELOPMENT COMMAND – ARMAMENTS CENTER

Computational Energetic Material Cook-off Scenarios

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Equations for Heat Transfer

The generalized equation for conductive heat transfer (without mass transfer) with internal heat generation (Q) is given by:

$$-\lambda\nabla^2 T + \rho c\frac{dT}{dt} = Q$$

where:

λ = Material Thermal Conductivity
∇^2 = Lapace's Operator
T = Temperature
ρ = Density
c = Heat Capacity
Q = Internal Heat Generation

The Arrhenius equation is commonly used for the thermal decomposition of energetic materials:

$$Q = \rho \Delta H Z e^{\left(-\frac{E_a}{RT}\right)}$$

where:

E_a = Activation Energy
R = The Universal Gas Constant
H = Material Heat of Reaction
Z = A Material Time Constant

The generalized equation is then:

$$-\lambda\nabla^2 T + \rho c\frac{dT}{dt} = \rho\Delta H Z e^{\left(-\frac{E_a}{RT}\right)}$$

With one dimensional Heat Transfer:

$$\frac{dT}{dt} = \frac{1}{\rho c}\left(\rho\Delta H Z e^{\left(-\frac{E_a}{RT}\right)} + \lambda\frac{1}{r}\frac{\partial^2(ru)}{\partial r^2}\right)$$

At r=0

$$\frac{dT}{dt} = \frac{1}{\rho c}\left(\rho\Delta H Z e^{\left(-\frac{E_a}{RT}\right)} + \lambda 3\frac{\partial^2 T}{\partial r^2}\right)$$

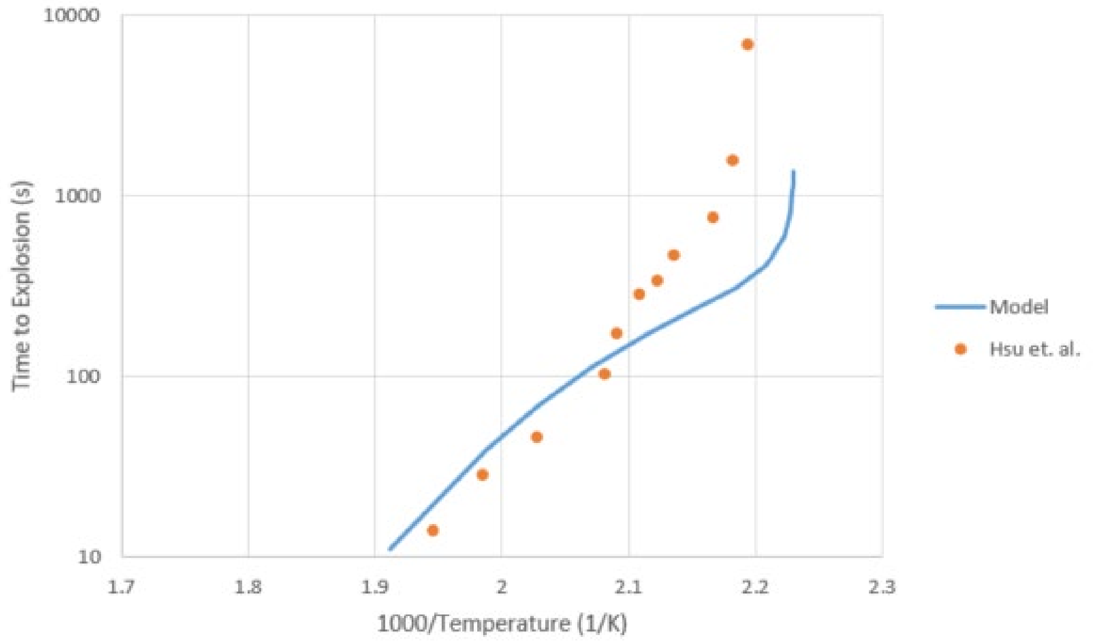
COMPARISON TO EXISTING DATA

The computer program stopped when a temperature in any of the intervals was high enough (550 to 600K (277-327 ° C)) that a run-away reaction could be assumed. As long as this cut-off temperature was suitably high, the results were not sensitive to this value as the temperature is rising very rapidly. The program was written in the python language, and could be easily modified for any particular problem. The variables used in the model are from Cooper.

Lawrence Livermore National Laboratory has conducted a One-Dimensional Time to Explosion test on RDX.

The test uses a spherical test sample at a diameter of 12:7x10_3 m (:5 inches) clamped between two aluminum anvils.

The approximation for the model was made such that the outer surface of the sample is constant at the test temperature. The model and the data were plotted in an Arrhenius plot.



Cooper, P. W. (2018). Explosives engineering. John Wiley & Sons.

Hsu, P. C., G. Hust, M. McClelland, and M. Gressholf. One-Dimensional Time to Explosion (Thermal Sensitivity) of DMDNP. No. LLNL-TR-667208. Lawrence Livermore National Lab.(LLNL), Livermore, CA (United States), 2014.

CRITICAL TEMPERATURES

Frank-Kamenetskii's solution determines the temperature at which a steady state solution cannot be determined, and a run-away reaction occurs. This method provides a critical temperature, however it does not predict the time to reaction. The time to reaction can be very long near the critical temperature. Additionally, the ignored decomposition of the material and its reduction in the available heat of reaction may have a significant influence on the cook-off.

$$\frac{E_a}{T_c} = R\ ln\left(\frac{r^2\ \rho\ H\ Z\ E_a}{3.32\ T_c^2\ \lambda\ R_g}\right)$$

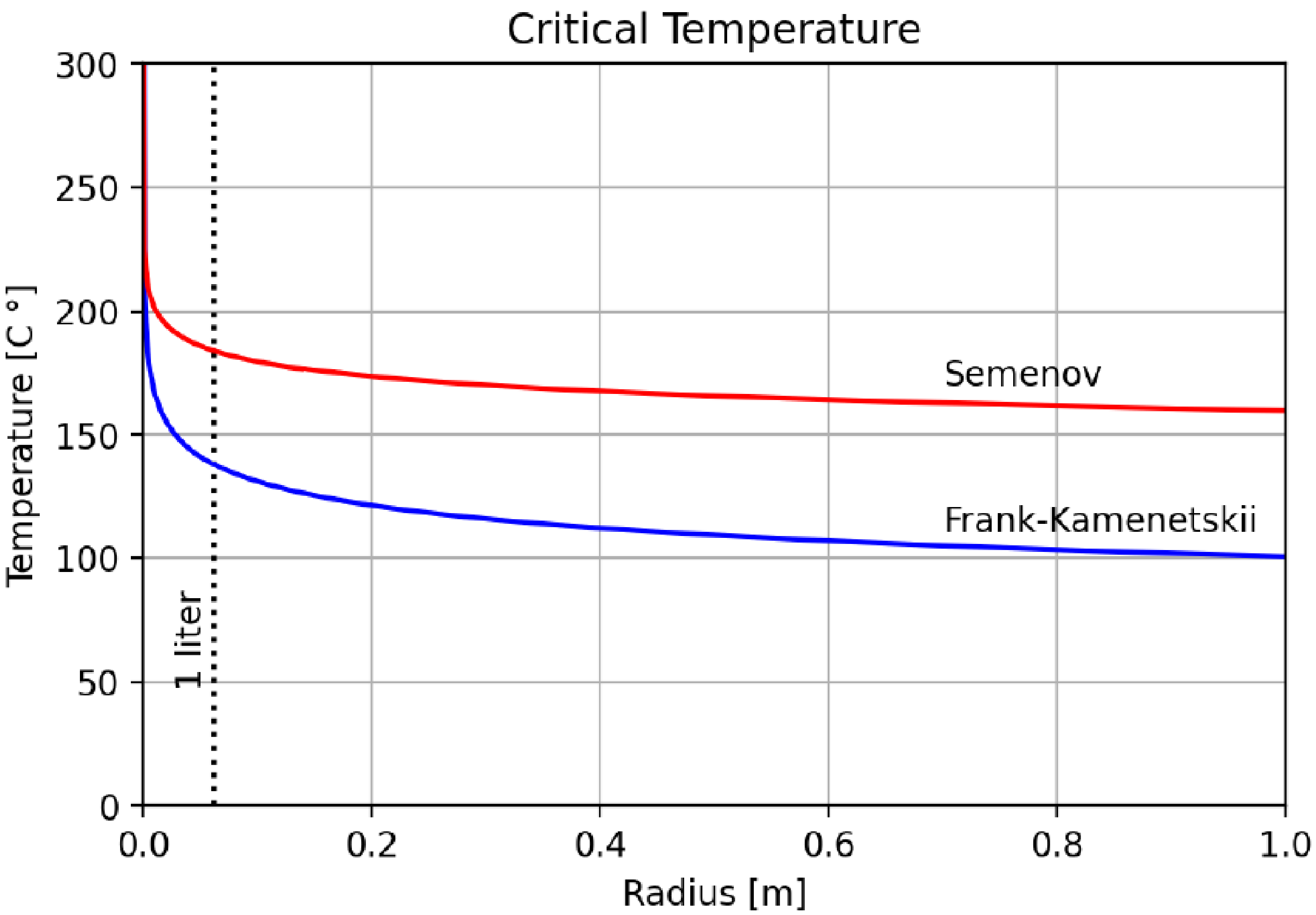
Semenov developed a critical temperature model for well stirred liquids.

$$T_c = \frac{E_a}{R}\frac{1}{ln\left(\frac{V\rho H Z E_a}{S\alpha R {T_c}^2}\right)}$$

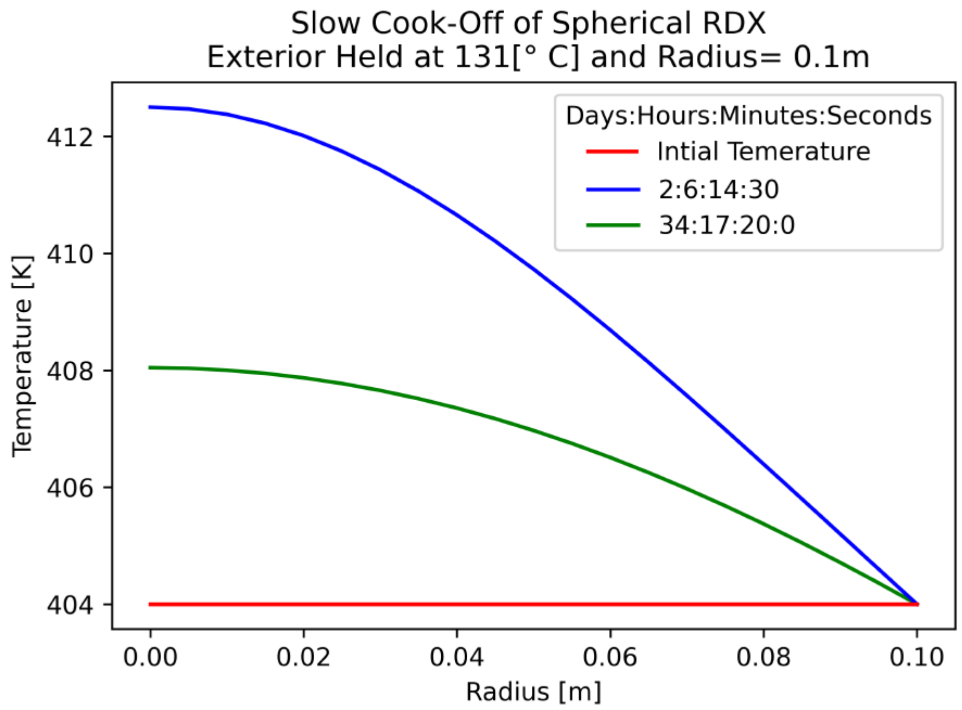
where:

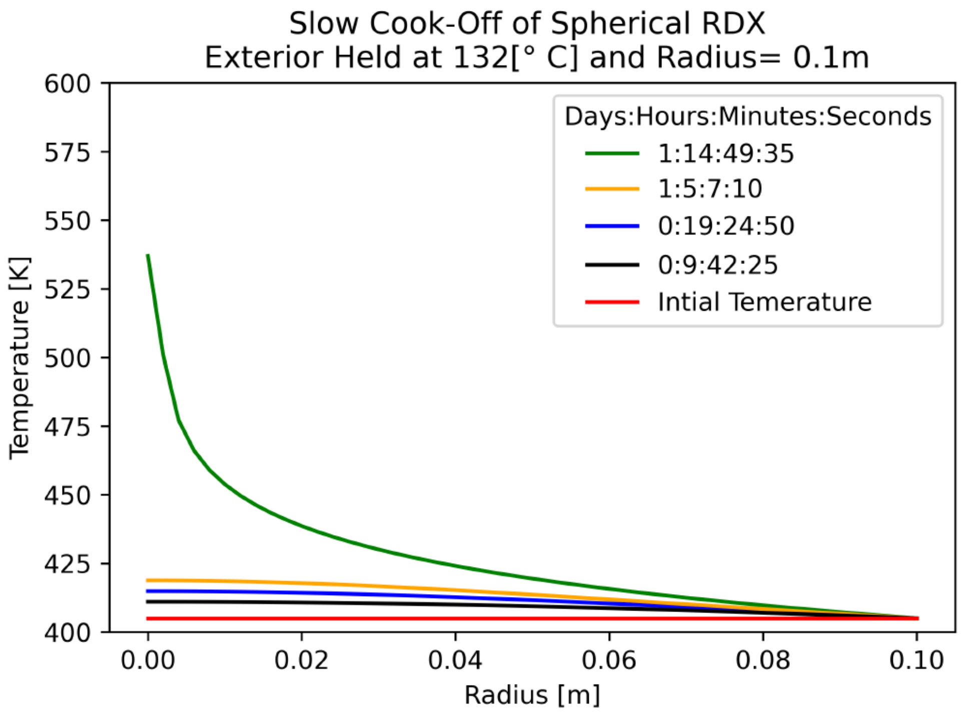
T_c = Critical Temperature
V = Volume
S = Surface Area
α = Convection coefficient

CRITICAL TEMPERATURE FOR RDX



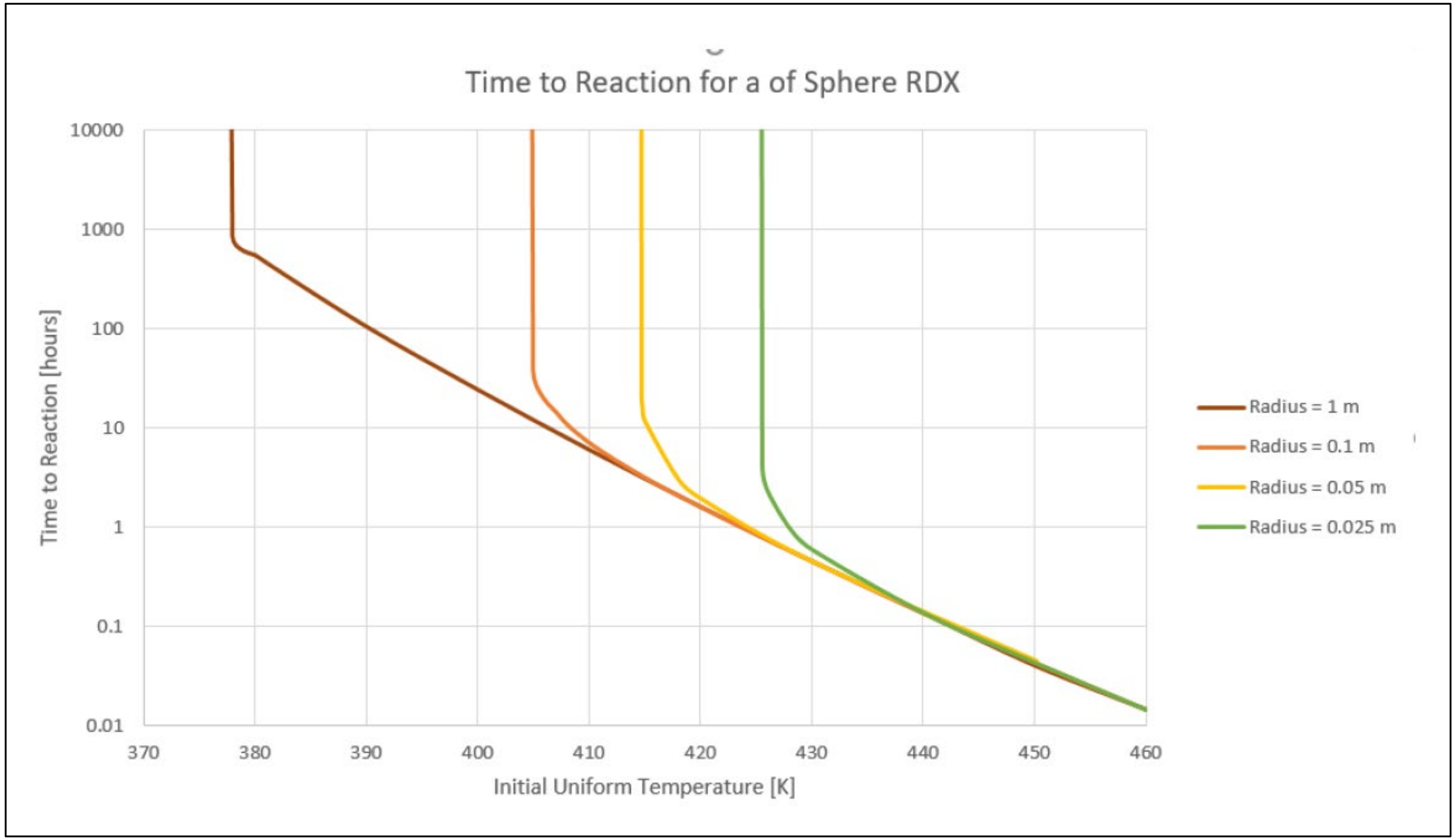
EFFECTS OF MATERIAL DEGRADATION



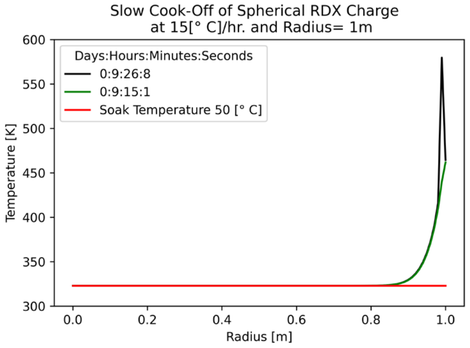


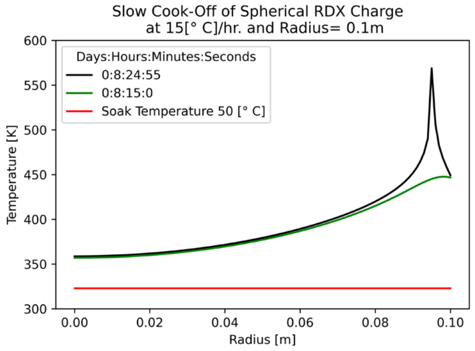
For a 0.1 m radius sphere, the Frank-Kamenetskii critical cook-off temperature is 403.96K (130.96˚C). A cook-off temperature of 404K (131˚C) resulted in the material reaching a maximum of 412.5K (139.5˚C) at 2 days and 6 hours, after which the degraded explosive produced less heat and the material started to cool.

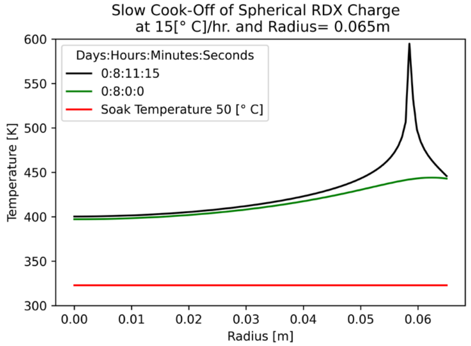
EFFECT OF SIZE

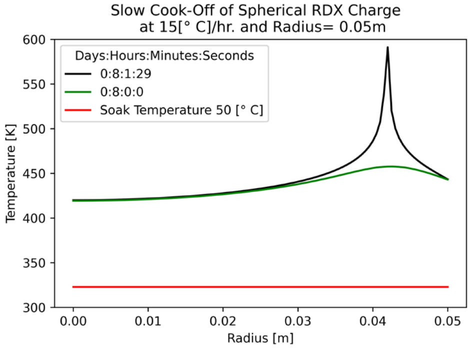


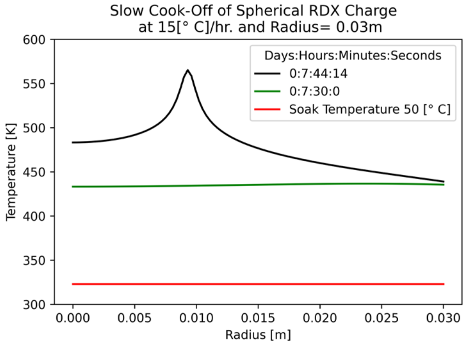
SLOW COOK-OFF OF VARIOUS DIAMETER SPHERES, 15˚C/HR. OLD RATE

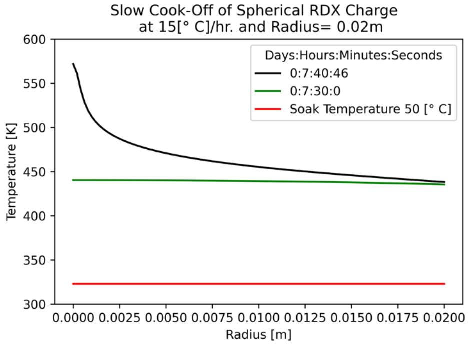


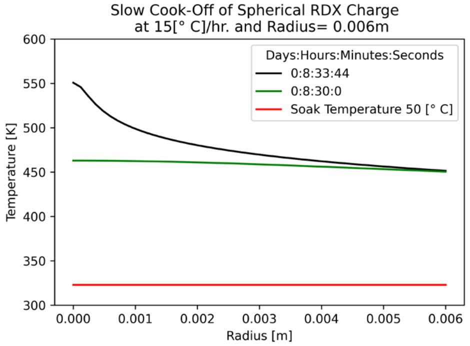






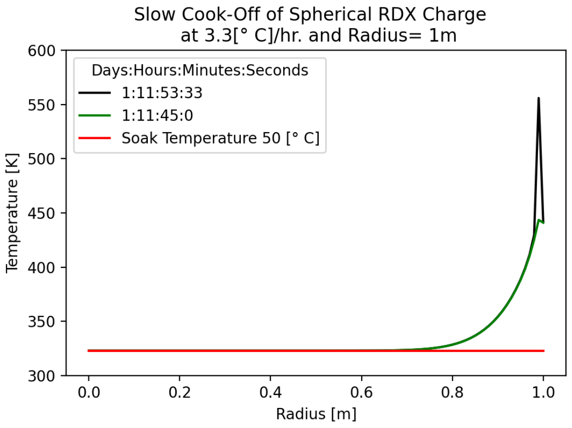


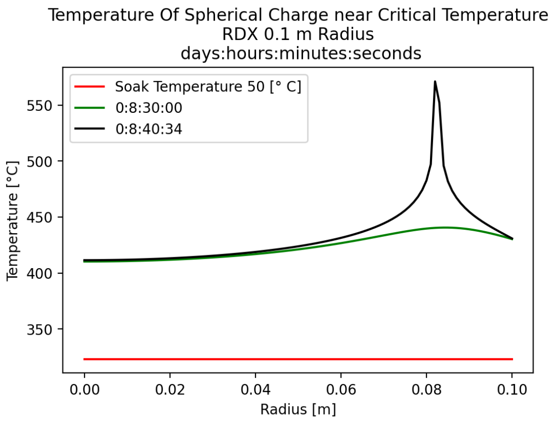


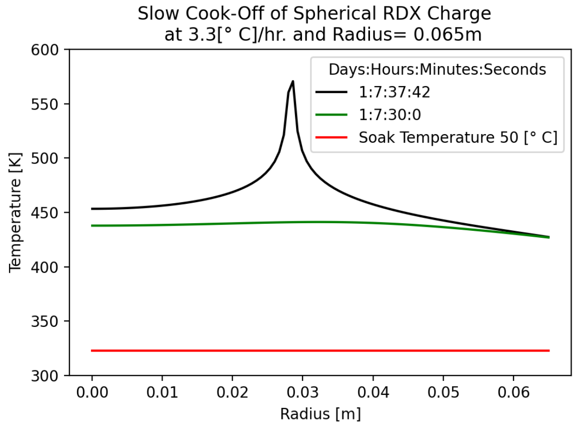


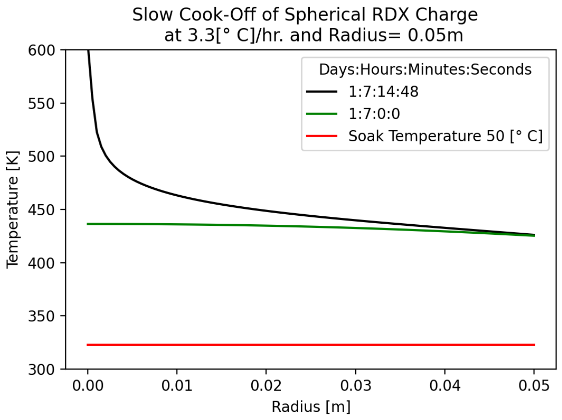
Old Rate 3.3˚C/hr.

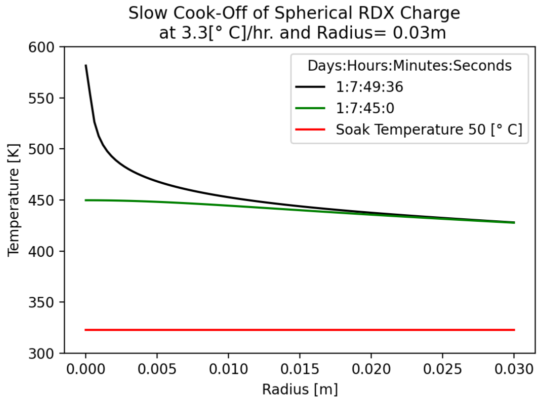
SLOW COOK-OFF OF VARIOUS DIAMETER SPHERES, 3.3˚C/HR. NEW RATE

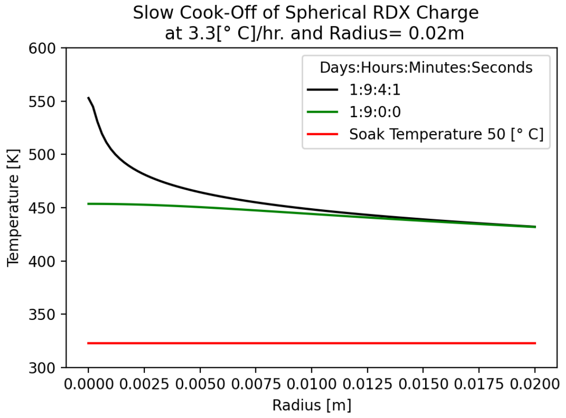




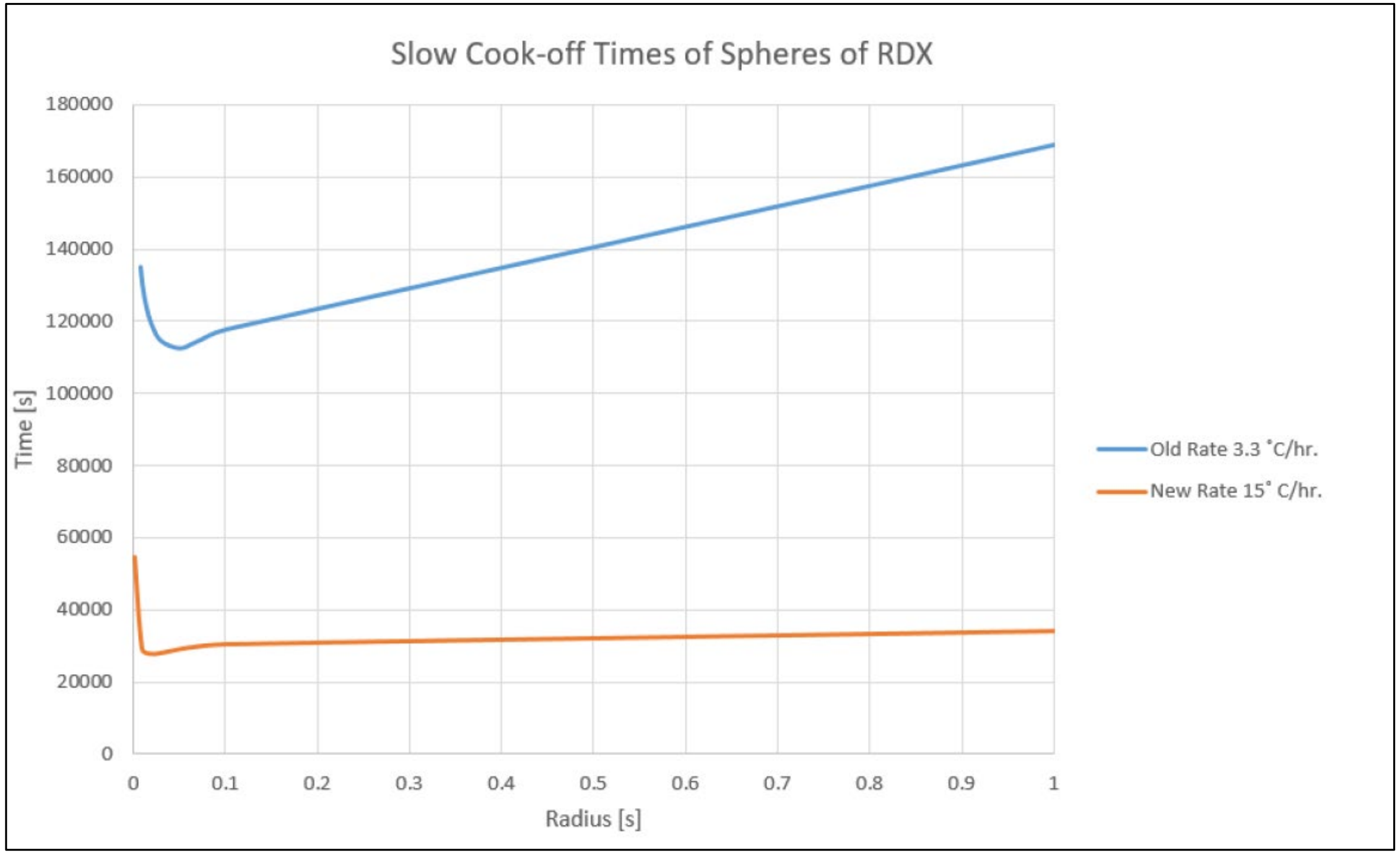








TIME TO REACTION WITH INCREASING SIZE, OLD AND NEW RATE



CONCLUSION

This study was conducted to find trends in the predicted values for cook-off using a simple Arrhenius equation for reaction. This should predict the following trends:

- Effects of degradation of the energetic materials in cook-off scenarios are more pronounced for slower rates and for smaller charges.
- Slower rates tend to move the ignition towards the center of the charge, but also allow for a greater degradation of the material and potentially less violent reactions.
- Faster cook-off rates not only decrease the time to ignition, they decrease the effects of size.
- It is possible to heat an item slowly enough such that no violent reaction occurs. This effect is more pronounced for smaller charges.
- Often impending violent reactions have no indication on the surface of the charge as there is no rapid increase in temperature on the surface.