Non-Adiabatic Explosion: A Numerical Analysis

University of Colorado at Boulder

APPM 4650

Intermediate Numerical Analysis 1

Authors:	*Affiliations:*
Nathan Biesterfeld	Applied Mathematics
Cooper Simpson	Applied Mathematics
Jaden Wang	Applied Mathematics

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1 Introduction:

We consider a box constructed of an unspecified material that contains a mixture of fuel and oxidizer. Spontaneously or due to an ignition, the contents begin to react exothermically. We investigate this reaction numerically, specifically looking at the cases when the reaction parameters facilitate an explosion or a "fizzle". The latter term in our numerical investigation indicates that the box does not explode but instead reaches some heat equilibrium. Importantly, we are considering a non-adiabatic scenario meaning that there is a possible loss of heat to the environment which allows for the fizzle case. We define a mathematical model in the form of ordinary differential equations (ODE's) that describe the reaction dynamics inside the box and then non-dimensionalize these to study the scenarios in a general sense. In addition, we will investigate long and short time approximations to solutions of the explosion and fizzle cases. We then discuss the results of our numerical findings with respect to the physical problem.

2 Mathematical Model:

The reactants (unspecified fuel and oxidizer) are initially at temperature T_0 inside a box where the temperature is a function of time $T(t)$. The chemical reaction that takes place in the box is assumed to have an activation energy E. The heat released by the reaction of individual molecules brings more and more of the remaining reactants above this activation energy threshold – causing the reaction to progress at a faster rate. For an amount of fuel A, the ODE that describes this rate of change is given by

$$\frac{dA}{dt} = -cAe^{-E/RT}, \qquad A(0) = A_0 \tag{1}$$

where R is the universal gas constant and c is a positive constant of proportionality. We note that the minus sign indicates that the fuel A is being consumed. This brings up an important assumption that we will make throughout our analysis. Namely, we do not consider the actual amounts of fuel and oxidizer. Instead we assume that there are infinite amounts of both to drive the reaction forever. In reality this is not the case and the relative amounts can have a large impact on the reaction dynamics. We are more concerned with the dynamics specifically related to an explosion or a fizzle, so it is beneficial to assume that in either case the quantities of reactants are negligible.

In the beginning, the thermal energy of the gas, RT, is small compared to the activation energy E. As time progresses, small quantities of the gas reach the activation energy and small quantities of heat are released, increasing the temperature. This increases the magnitude of the exponential term in (1), speeding up the reaction.

Additionally, considering the box to be made of an imperfect insulating material, there is energy lost in proportion to the temperature difference between the inside and outside of the box. Conservation of energy leads to the following relation describing the rate of change of the temperature inside the box:

$$c_v \frac{dT}{dt} = -c \frac{dA}{dt} - h\left(T - T_0\right), \qquad T(0) = T_0 \tag{2}$$

where c_v is the specific heat capacity of the fuel-oxidizer mixture and h is a convective heat transfer coefficient describing how much energy is lost across the boundary of the box. A small value for h reflects a good insulator while a large value indicates a poor insulator. The left-hand side of (2) represents the change in the internal energy within of the box, and the terms on the right-hand side represent the release of energy due to the chemical reaction and the heat loss across the boundary of the container, respectively.

We can simplify (2) further by non-dimensionalizing the variables. Letting $\epsilon = \frac{T_0 R}{E}$, $\bar{T} = \frac{T}{T_0} = 1 + \epsilon\theta$, and $\sigma = \frac{t}{\delta t_{ref}}$ where t_{ref} is a reference time and $\delta \frac{1}{h}$, we obtain the non-dimensional temperature variable θ and non-dimensional time variable σ. We can rewrite (2) in terms of these two variables and obtain an autonomous first-order ODE:

$$\frac{d\theta}{d\sigma} = \delta e^{\theta} - \theta \tag{3}$$

Considering (3), we can see that for some values of δ (such as $\delta = \frac{1}{2}$) our derivative will always be positive (i.e. $\delta e^{\theta} > \theta \, \forall \theta$). For smaller values of δ (such as $\delta = \frac{1}{3}$), the exponential is scaled down so that the line $y = \theta$ intersects the line $y = \delta e^{\theta}$. These two different scenarios define two very different solutions to the initial value problem.

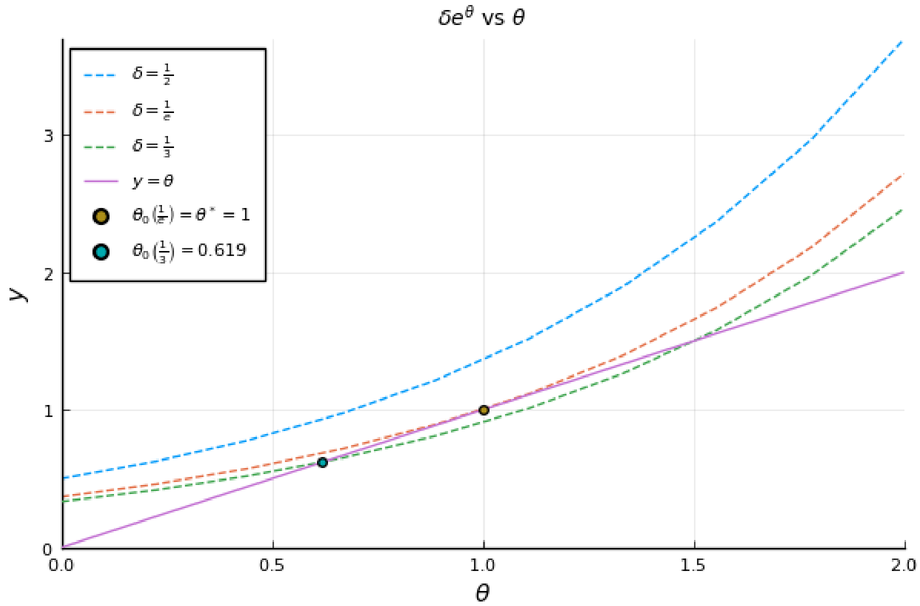

Figure 1: The "power dynamics" between δe^{θ} and θ at different values of δ. At $\delta = \frac{1}{e}$, $y = \delta e^{\theta}$ represented by the dashed orange curve touches $y = \theta$ at exactly one point with $\theta^* = 1$.

When δ is large enough so that $\delta e^\theta > \theta$ for all θ (like the $\delta = \frac{1}{2}$ case in Figure 1), the solution is increasing at all values of θ as the derivative is always positive. Furthermore, since the exponential term e^θ grows much more quickly than the linear term θ, the slope is also growing very quickly. This amounts to the solution $\theta(\sigma)$ growing very quickly and without bound in time. We call this the "explosion" case.

On the other hand, consider the case where δ is small enough so that (3) exhibits fixed points (where the derivative is zero). This follows because a small enough δ will cause the graphs of δe^θ and θ to intersect (like the case of $\delta = \frac{1}{3}$ case in Figure 1). To determine the long term behaviour of the solution for this case one must examine the stability of the fixed points.

The observations above motivate us to find the critical value δ^* that divide the two distinct behaviors of $\theta(\sigma)$. Based on Figure 1, we can see that the critical value occurs when $y = \delta e^\theta$ touches $y = \theta$ at exactly one point. Because $y = \delta e^\theta$ is monotonically increasing with a positive derivative and $y = \theta$ has a constant derivative, this means we are looking for where $y = \theta$ is tangent to $y = \delta e^\theta$. To find the tangent point, we require that the function values and their slopes equal to each other, yielding a system of two equations:

$$\begin{cases} \delta^* e^{\theta^*} = \theta^* \\ \delta^* e^{\theta^*} = 1 \end{cases} \tag{4}$$

Solving this gives us $\delta^* = \frac{1}{e}$ and $\theta^* = 1$. Using δ^* as the border value, we can supply a full mathematical description of the fizzle and explosion scenarios.

2.1 Fizzle

In the case when $\delta \leq \frac{1}{e}$, as Figure 1 shows, the curve and the line have the first intersection point at $\theta = \theta_0(\delta)$. This intersection is the fixed point for the ODE (3). We note that there are actually two fixed points for $\delta < \frac{1}{e}$, but we will only consider the smaller value. This is because our initial condition is $\theta(0) = 0$ and a continuous solution will always encounter the first fixed point before the second. To analyze the stability of θ_0 we must look at the value of the derivative around the fixed point. As shown in Figure 1 we can see that the slope is is always positive when $\theta < \theta_0$ as the curve $y = \theta$ is below $y = \delta e^\theta$. Beyond this fixed point the opposite is true and so the slope is always negative. This tells us that fixed point is attracting as solutions are drawn into the point from below and above. Although the function has positive slope and increases rapidly at first, it eventually approaches the attracting fixed point at $\theta = \theta_0$. The function value will approach θ_0 from below as $\sigma \to \infty$. Thus, we see that for any $\delta \leq \frac{1}{e}$ we have a fizzle. Next, we derive the short and long time approximations for the fizzle case to better understand the solution.

Long-time behavior

As $\sigma \to \infty$ we have just seen that $\theta(\sigma)$ will converge and the slope will approach zero. That is,

$$\lim_{\sigma \to \infty} \frac{d\theta}{d\sigma} = 0 \tag{5}$$

$$\delta e^{\theta} = \theta \tag{6}$$

Recall that θ_0 solves (6) so it follows that $\theta(\sigma)$ converges to θ_0. This result matches the expectation that the function would approach its attracting fixed point which is $\theta = \theta_0$.

Short-time behavior

In the case when σ is small, since $\theta(0) = 0$, θ must also be small. Therefore, we can simplify (3) using 1st-order Taylor approximation and solve it analytically:

$$\begin{aligned} \frac{d\theta}{d\sigma} &= \delta e^{\theta} - \theta \\ &\approx \delta(1+\theta) - \theta \\ &= \delta + (\delta - 1)\theta \end{aligned} \tag{7}$$

Note that the higher-order terms are $\mathcal{O}(\theta^n),\ n > 1$ and are negligible because θ is small. Hence, 1st-order Taylor approximation gives us good short-time result and greatly simplifies the ODE. This allows us to solve it analytically by a simple separation of variables:

$$\begin{aligned} \frac{d\theta}{\delta + (\delta - 1)\theta} &= d\sigma \\ \frac{d\theta}{\theta + \frac{\delta}{\delta - 1}} &= (\delta - 1)d\sigma \\ \ln\left(\theta + \frac{\delta}{\delta - 1}\right) &= (\delta - 1)\sigma + C \end{aligned} \tag{8}$$

Using $\theta(0) = 0$, we can solve the IVP and obtain our short-time approximation of the function $\theta(\sigma)$.

$$\theta = \left(\frac{\delta}{\delta - 1}\right)\left(e^{(\delta-1)\sigma} - 1\right) \tag{9}$$

2.2 Explosion

The explosion case is a result of unbounded growth in θ. This requires $\delta > \frac{1}{e}$ so that the slope is always positive and $\theta(\sigma)$ grows indefinitely, triggering an explosion. As for the fizzle case we will next investigate the short and long time approximations to the true solution.

Long-time behavior

We already know that an explosion implies that θ approaches ∞. Thus, in addition to the solution trajectory, we are interested in finding the time of explosion, σ_{exp}, for the case $\delta > \frac{1}{e}$. The explosion time as we define it is the asymptotic time approached as the heat grows to infinity. We note that in a physical situation the real explosion time may be much earlier and is determined by the pressure that the box can withstand. It is tricky to find this time with the way the problem is currently defined, so we will swap the independent variable θ for the dependent variable σ. We can do this because the function is monotonically increasing, and it allows us to take the limit as $\theta \to \infty$. The resulting ODE is given as follows:

$$\frac{d\sigma}{d\theta} = \frac{1}{\delta e^{\theta} - \theta} \tag{10}$$

We can cleverly apply the Fundamental Theorem of Calculus to evaluate $\sigma(\infty)$ using the fact the $\sigma(0) = 0$.

$$\begin{aligned} \sigma(\theta) &= \sigma(\theta) - 0 \\ &= \int_0^{\theta} d\sigma \\ &= \int_0^{\theta} \frac{d\sigma}{d\theta} d\theta \\ &= \int_0^{\theta} \frac{1}{\delta e^{\theta} - \theta} d\theta \\ &= \int_0^{\theta} \frac{1}{\delta e^{x} - x} dx \end{aligned} \tag{11}$$

Note that in the last step, we replaced the dummy variable inside the integral with x to avoid confusion. Now this function allows us to find σ_{exp} by evaluating the following improper integral:

$$\sigma_{exp} = \lim_{\theta \to \infty} \int_0^{\theta} \frac{1}{\delta e^{x} - x} dx \tag{12}$$

We note that this cannot be accomplished analytically as there is no known anti-derivative. After obtaining σ_{exp}, we can once again simplify (3) and solve the approximated equation analytically:

$$\begin{aligned} \frac{d\theta}{d\sigma} &= \delta e^{\theta} - \theta \\ &\approx \delta e^{\theta} \\ \frac{d\theta}{e^{\theta}} &= \delta d\sigma \\ -e^{-\theta} &= \delta\sigma + C \end{aligned} \tag{13}$$

Using the fact that $\lim_{\theta \to \infty} \sigma = \sigma_{exp}$, we have

$$\begin{aligned} \lim_{\theta \to \infty} -e^{-\theta} &= \lim_{\theta \to \infty} \delta\sigma + C \\ 0 &= \delta\sigma_{exp} + C \\ C &= -\delta\sigma_{exp} \end{aligned} \tag{14}$$

Hence, the solution to the IVP is

$$\sigma = \sigma_{exp} - \frac{1}{\delta e^{\theta}} \tag{15}$$

Notice that we again swap the independent and dependent variables here and obtain the closed-form version of the function $\sigma(\theta)$ that fully describes the long term trajectory of the explosion.

Short-time behavior

The assumptions for the short-time solution from the fizzle case remain the same here, so we can still use (9) as our approximation. However, a major difference results from the fact that because $\delta > \frac{1}{e}$, it can now take the value of $\delta = 1$ – making (9) undefined. In this isolated case, we can further simplify the approximation using Taylor expansion:

$$\begin{aligned} \theta &= \frac{\delta}{\delta - 1}\left(e^{(\delta-1)\sigma} - 1\right) \\ \theta &= \frac{\delta}{\delta - 1}\left(1 + (\delta - 1)\sigma + \frac{(\delta-1)^2\sigma^2}{2} + \ldots - 1\right) \\ \theta &= \delta\left(\sigma + \frac{(\delta - 1)\sigma^2}{2} + \ldots\right) \end{aligned} \tag{16}$$

Plugging in $\delta = 1$ yields

$$\theta = \sigma \tag{17}$$

This allows us to plot the short-time approximation of the solution when $\delta = 1$. Next, we present our numerical results.

3 Numerical Results:

As thoroughly discussed in section 2 there are two specific cases to consider for our non-adiabatic problem: a fizzle or an explosion. These cases are differentiated by the parameter δ and its relation to the critical value e^{-1}. We numerically investigate the heat dynamics of our box for a specific δ from either case. In solving the necessary ODE's ((3) and (10)), we employ a standard fourth-order Runge-Kutta integration scheme using the analysis from section 2 to guide our approach. In each case we also examine the long and short time approximations to the solution.

We begin by considering $\delta = \frac{1}{3} < \frac{1}{e}$ which should facilitate a fizzle instead of an explosion. The ODE is easily solved, but we need to determine our long time approximation that our solution should asymptote to. This requires us to solve (6) which is equivalent to finding our fixed point $\theta_0(\frac{1}{3}) = \theta_{fiz}$. Posing this as a simple root finding problem $\delta e^{\theta_{fiz}} - \theta_{fiz} = 0$, we employ the Newton-Raphson method and get the following result accurate to six significant figures:

$$\theta_{fiz} = 0.619061 \tag{18}$$

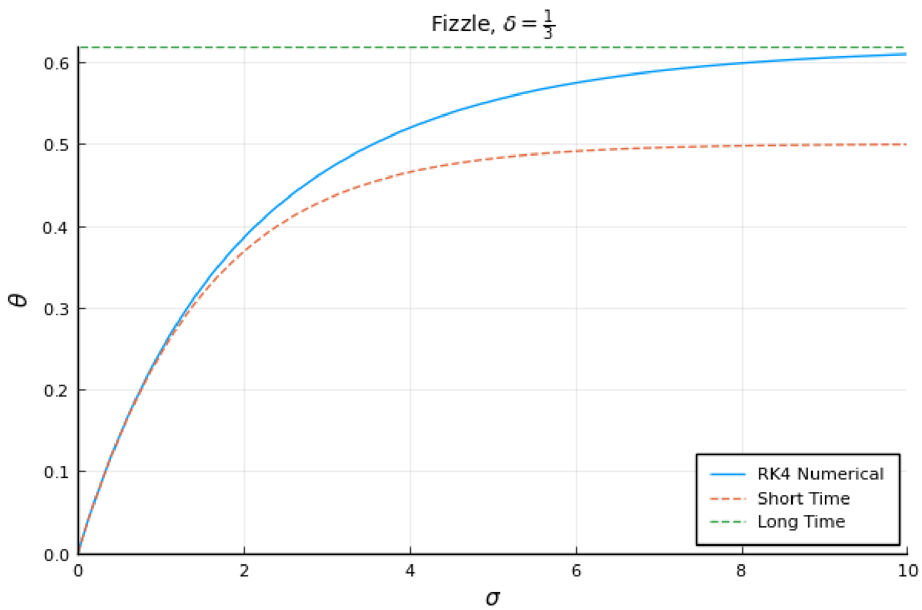

Figure 2: Trajectories of the RK4 solution, short-time approximation, and long-time approximation.

In the plot above we see the numerical solution given in blue with our long and short time approximations in green and orange respectively. The long time approximation θ_{fiz} is clearly constant and is the asymptotic non-dimensional heat in the box. It is clear to see that the short time approximation is very accurate for smaller σ, while the long time approximation is very accurate for large σ.

The next case we consider is for $\delta = 1 > \frac{1}{e}$ where this time we predict an explosion as opposed to a fizzle. We note that as described in subsection 2.2 we have swapped our independent and dependent variables to facilitate the numerical solution of the ODE. This means we have σ as a function of θ which we will maintain for the numerical analysis of the explosion. After solving the ODE, the only remaining step is to determine the asymptotic value σ_{exp} that denotes non-dimensionalized time at which the heat in the box goes to infinity. We just need to evaluate the integral in (12) for which we must resort to numerical methods. The method we have employed first uses a high-order numerical integration scheme to integrate on the domain $[0, c]$ where c is an arbitrary constant. Then the transformation $x = \frac{1}{t}$ transforms our integral to one on the domain $[0, 1/c]$ with a singularity at zero. Standard techniques for left-hand singularities (setting $f(0) = 0$) with a high-order integration scheme are then used to evaluate this integral. The sum of the two gives us our asymptotic value to six significant figures:

$$\sigma_{exp} = 1.359098 \tag{19}$$

We note that one might have also integrated the function directly on a very large domain with a high-order method, and because the function decays rapidly this will also provide an accurate answer.

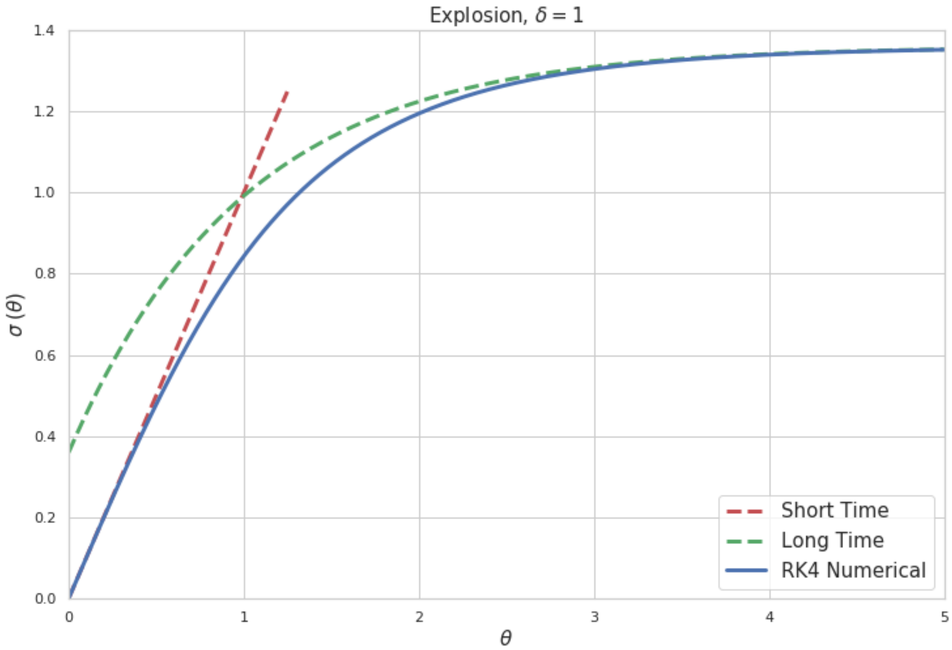

Figure 3: Numerical solution with short and long time approximations.

In the plot above we see the numerical solution given in blue with our long and short time approximations in green and red respectively. Like before it is clear that our long and short time approximations are very accurate for their respective time ranges.

In the next plot we have reverted our explosion case back to θ as a function of σ. This shows the more accurate dynamics of the problem where for $\delta = 1$ an explosion occurs, and for $\delta = \frac{1}{3}$ a fizzle occurs.

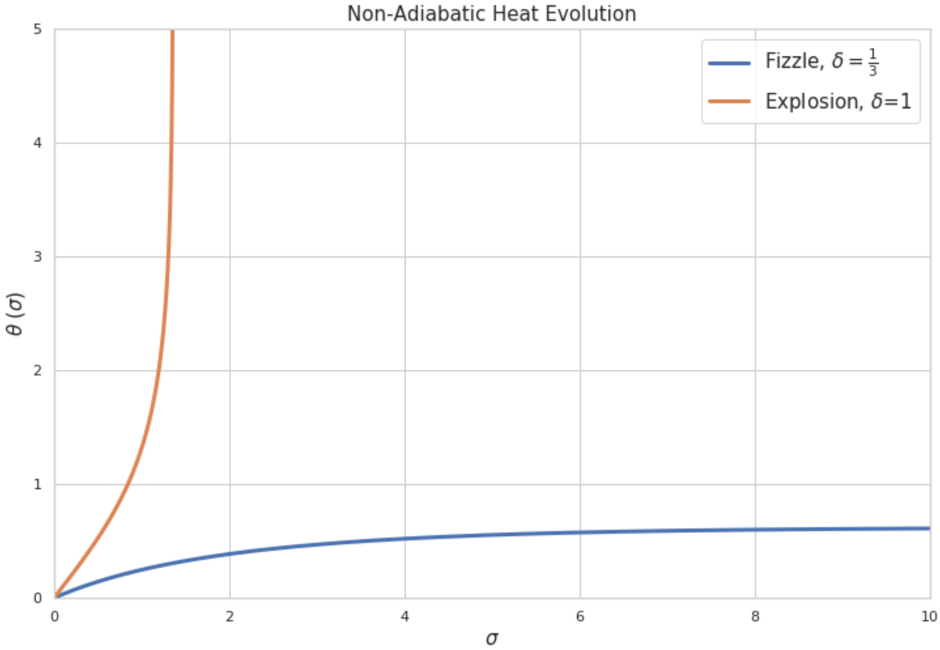

Figure 4: Numerical solutions for a fizzle and an explosion.

We can clearly see that in the explosion case the non-dimensionalized heat blows up to infinity. For the fizzle case this non-dimensionalized heat asymptotes to a stable value.

4 Discussion:

We have presented an investigation into the non-adiabatic evolution of heat inside a box. Inside the box, which contains a mixture of fuel and oxidizer, a chemical reaction causes the temperature to increase, potentially resulting in an explosion. We discussed a mathematical model of ODE's that describes the temperature dynamics, and non-dimensionalized this model to study it in a general sense. Importantly, during a non-adiabatic process, heat is transferred from the box to its surrounding environment. Because of this, there is a possibility the box will not explode – which we call a fizzle. We analytically determined the critical value of δ (the governing parameter) that differentiates an explosion and a fizzle. Furthermore, we also determined (analytically) short and long time approximations to the true ODE solution for both cases to verify our numerical solutions. With this we considered a specific δ from either case and investigated numerically. The ODE's were solved with a fourth order Runge-Kutta, and the asymptotic values θ_{fiz} and σ_{exp} were determined using numerical root finding and integration techniques respectively.

An important assumption made throughout our analysis is that of an infinite amount of reactants. We assume that inside the box there is enough fuel and oxidizer to perpetuate the reaction for infinite time. Notably, this is what allows for the nice constant asymptotes that appear in Figures 2 to 4. In a real physical situation, the reaction would end once the limiting reactant had been entirely consumed. This can result in some interesting variations on the explosion and fizzle scenarios. In all cases the temperature in the box would eventually fall into equilibrium with the surrounding environment. This follows because the reactants would eventually run out, halting the reaction, but heat would continue to leak out of the box until the temperature of the systems was equivalent. If the quantity of reactants were small enough, then even in the case of a δ that should lead to an explosion, there would be a fizzle. This further brings up the question: why do the asymptotes occur in either case? In the explosion case, there is an intuitive answer. Because of the exponential form of the ODE that describes the heat change, the more the temperature increases, the more the rate of temperature change does so as well. This results in a point where the temperature asymptotes to infinity because it grows at such an increasing rate. In the fizzle case, we see that the asymptote is a result of the equilibrium between heat growth due to the reaction and heat loss to the environment. As discussed in section 2 this asymptote is a stable fixed point which means the derivative is zero. The heat is neither increasing nor decreasing, exactly as much heat that is created is also lost.

In Figure 3 and elsewhere we have referred to the σ value at which the heat asymptotes as σ_{exp}. This seems to imply that this is the (non-dimensionalized) time at which the box explodes. However, the reality is somewhat more complicated than this. If we define "explosion time" as the time where the temperature in the box approaches infinity, then σ_{exp} is indeed an apt name. However, if, as in a physical situation, we define "explosion time" as the time at which the box structure dramatically fails, then this name is somewhat misleading. The temperature itself is not what would cause the box to explode, but it is instead the pressure inside. These two values are directly related in the $pv = nRT$ equation, but because of this, it is the specific properties of the box that determine when it would explode. Depending on the materials and method of construction, one box might be able to withstand far more pressure than another. Take, for example, an iron box and a plastic box. The iron box will survive a higher pressure (and thus a higher temperature) than the plastic box, and both might explode far earlier than the labeled σ_{exp}.

Our mathematical model reveals the significance of the parameter δ in dictating the outcome of the exothermic reaction. Specifically, even if δ is only slightly larger than $\frac{1}{e}$, our model predicts that a mild reaction in the beginning can turn into a disastrous explosion. In a real life scenario this can be a matter of life and death. Recall that δ is proportional to $\frac{1}{h}$, where h is the coefficient affecting the rate of heat loss from the box to the environment. Therefore, the larger h is (indicating that the box dissipates the heat faster), the more likely that δ would be less than $\frac{1}{e}$ and prevent an explosion from occurring. An immediate consequence from this analysis is that in situations where explosive exothermic chemical reactions are a concern, one would want to use materials and techniques that dissipate heat quickly. Counter-intuitively, according to our model, keeping the environment at a low temperature cannot reduce the risk of explosion as δ is the only parameter that determines the outcome and doesn't depend on T_0. The only effect T_0 has on the situation is in how quickly molecules begin to achieve activation energy and the reaction begins – the outcome will always be the same.

One assumption present in our mathematical model is that both the heat and chemical reactants are homogeneously spread through the volume of the box. This assumption may lead our model to give inaccurate predictions. For example, consider the region in the center of a cubic box. When an exothermic reaction occurs in the center, heat is released locally and spreads outwards toward the boundary. There is a period of time over which the heat must diffuse outwards before it can diffuse across the boundary. During this period of time, the center of the box is at a slightly higher temperature than the rest of the box, so the chemical reaction proceeds at a faster rate, further increasing the local heat. This process can continue and eventually cause the whole box to explode. Note that this locality argument is largely dependent on the thermal diffusivity of the fuel inside the box. If the thermal diffusivity is high, heat will diffuse to the boundary quickly and local heat spots will be less frequent. Conversely, if the thermal diffusivity is low, local heat spots will diffuse much more slowly and be more frequent. It's also important to consider the locality of fuel within the box. If an exothermic reaction occurs in some area of the box, that area of the box will be locally hot but will also have less fuel for further exothermic reaction. Since the increase in temperature and decrease in amount of fuel compete in the rate of exothermic reaction, it is unclear whether considering locality will either increase or decrease the critical value of δ, (δ^*). However, it is clear that a model considering the shape of the box, thermal and molecular diffusivity, and locality could be more complete for approaching this problem.

We have seen that there are many complicated interactions, considerations, and parameters in the study of confined exothermic chemical reactions. Our investigations have given a good general overview of the two basic outcomes of such a process, but there is always more that can be taken into account. We have made several simplifying assumptions that in reality may not be accurate. These deviations could result in many more complex situations arising out of a simple fuel oxidizer chemical reaction. Overall, regardless of the specific dynamics at play in a physical situation, either an explosion or a fizzle will take place – the variance lies in the trajectory of the solution.

References:

[BFB19] Richard L Burden, Douglas J Faires, and Annette M Burden. *Numerical Analysis*. 10th ed. Cengage, 2019.

Appendix:

4.1 Code:

```
def rk4(funcs, t, y0):
    num_funcs = y0.shape[0]
    if num_funcs != len(funcs):
        raise ValueError('Number of functions dont match number of initial conditions!')

    h = t[1]-t[0] #Assuming everything is evenly spaced
    K = np.zeros((4, num_funcs)) #K's

    #Make a solution array
    y = np.zeros((len(t), num_funcs))
    y[0,:] = y0

    for i in range(len(t)-1):
        #Iterate and evaluate
        #K's
        for j in range(num_funcs):
            K[0,j] = h*funcs[j](t[i], y[i,:])
        for j in range(num_funcs):
            K[1,j] = h*funcs[j](t[i]+(h/2), y[i,:]+(K[0,:]/2))
        for j in range(num_funcs):
            K[2,j] = h*funcs[j](t[i]+(h/2), y[i,:]+(K[1,:]/2))
        for j in range(num_funcs):
            K[3,j] = h*funcs[j](t[i]+h, y[i,:]+K[2,:])

        #Next point
        y[i+1,:] = y[i,:] + (1/6)*(K[0,:]+2*K[1,:]+2*K[2,:]+K[3,:])

    return y

#Legendre polynomial roots (i.e. eval locations)
gqLoc = np.array([-np.sqrt(15)/5, 0, np.sqrt(15)/5])
gqCoeff = np.array([5/9, 8/9, 5/9])

#Gaussian Quadrature integration n=3
def gaussQuad(f, a, b):
    #Need to convert to [-1,1]
```

```
    factor = (b-a)/2
    def transform(x):
        return (x*(b-a)+a+b)/2

    #Using lookup table
    t = transform(gqLoc)
    c = gqCoeff

    I = factor*(np.dot(c,f(t)))

    return I

#Integrate with singularity on left
def leftSingular(f, a, b):
    def func(t):
        y = np.zeros(len(t))
        for i in range(len(t)):
            if t[i]==0:
                y[i]=0
            else:
                y[i]=f(t[i])

        return y

#     return gaussQuad(func, a, b)
    return simpson_13(func, a, b, h=0.01)

#Integrate with infinite endpoint
#Assuming right endpoint is infinity
def intImproper(f, a, c):
    I1 = 0

    #Calculate first bit if need be
    if a==0:
        I1 = gaussQuad(f, a, c)
        a = c

    #Transform first
    a = 1/a
```

```
    def func(t):
        return (1/t**2)*f(1/t)

    I2 = leftSingular(func, 0, a)

    return I1+I2
```

```
using Printf,DataFrames, Plots, StatsPlots, LaTeXStrings
pyplot()
theme(:default)
function RK4(f,fiv,a,b,N::Int64)
    T = zeros(N+1,2)
    eta = LinRange(a,b,N+1)
    w = zeros(N+1,1)
    k = zeros(4,1)
    h=(b-a)/N
    w[1] = fiv
    for i in 1:N
        wi=w[i]
        k[1]=h*f(eta[i],wi)
        k[2]=h*f(eta[i]+h/2,wi+0.5*k[1])
        k[3]=h*f(eta[i]+h/2,wi+0.5*k[2])
        k[4]=h*f(eta[i]+h,wi+k[3])
        w[i+1]=wi+1/6*(k[1]+2*k[2]+2*k[3]+k[4])
    end
    return [eta w]
end

function Newton_Raphson(f,grad,p0,tol::Float64=1e-6,maxIter::Float64=1e5)
    i = 1
    while i <= maxIter
        p = p0 - f(p0)/grad(p0)
        if abs((p-p0)/p0) < tol
            @printf "Newton-Raphson: root is found after %d iterations.\n" i
            return p
        end
        i += 1
        p0 = p
    end
```

```
    @printf "Method failed after reaching %d iterations.\n" maxIter
end
#RK4
delta=1/3;
f(sigma,theta)=delta*exp(theta)-theta;
fiv=0.0;
a=0.0;
b=10.0;
N=100;
T = RK4(f,fiv,a,b,N)
#Newton-Ralphson
f1(theta)=exp(theta)/theta-1/delta;
g1(theta)=exp(theta)/theta-exp(theta)/theta^2;
p0=0.8;
theta_fiz = Newton_Raphson(f1,g1,p0,1e-4)
#short-time fizzle
ST(sigma) = -1/2 *(exp((delta-1)*sigma)-1)
sigma = LinRange(a,b,N+1)
STsigma = ST.(sigma)
#plotting
df=DataFrame(sigma=T[:,1],RK4=T[:,2],shortTime=STsigma)
@df df plot(:sigma, [:RK4,:shortTime],label=["RK4 Numerical" "Short Time"],
    legend=:bottomright,linestyle=[:solid :dash :dash],widen=:false)
hline!([theta_fiz],label=("Long Time"),linestyle=:dash)
xlabel!(L"$\sigma$")
ylabel!(L"$ \theta $")
title!(L"Fizzle, $\delta=\frac{1}{3}$",titlefontsize=10)
#Figure 1
y1(delta,theta)=delta*exp(theta);
y2(theta)=theta;
theta=LinRange(0,2,10);
y1o=y1.(1/2,theta);
y1e=y1.(1/exp(1),theta);
y1u=y1.(1/3,theta);
y2e=y2.(theta);
df1=DataFrame(theta=theta,y0=y1o,y1=y1e,y2=y1u,y=y2e)
@df df1 plot(:theta, [:y0,:y1,:y2,:y],label=[L"$\delta=\frac{1}{2}$"
    L"$\delta=\frac{1}{e}$" L"$\delta=\frac{1}{3}$" L"$y=\theta$"],
    legend=:topleft,linestyle=[:dash :dash :dash :solid],widen=:false)
```

```
xlabel!(L"$\theta$")
ylabel!(L"$ y $")
title!(L"$\delta e^{\theta}$ vs $\theta$",titlefontsize=10)
scatter!([1 0.6190612865418521],[1
    0.6190612865418521],label=[L"$\theta_0\left(\frac{1}{e}\right)=\theta^*=1$"
    L"$\theta_0\left(\frac{1}{3}\right)=0.619$"])
```