

## Mathematical modelling of the calcination process

<sup>1</sup>R. O. Olayiwola, <sup>2</sup>A.T. Cole, <sup>3</sup>D. Hakimi and <sup>4</sup>R.O. Ayeni

<sup>1,2,3</sup>Department of Mathematics and Computer Science,  
Federal University of Technology, Minna, Nigeria.

<sup>4</sup>Department of Pure and Applied Mathematics,  
Ladoke Akintola University of Technology, Ogbomosho, Nigeria.

### Abstract

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High quality lime is an essential raw material for Electric Arc Furnaces and Basic Oxygen Furnaces, steelmaking, alumina production etc. Decrease in fuel consumption in metallurgical furnaces is a tremendous opportunity for reduction of greenhouse gas emissions into the atmosphere. In this paper, a mathematical model of calcination process was studied. An analytical solution is obtained for the model. From the numerical simulation, it is observed that the gas temperature increases as the activation energy and Frank-Kamenetskii parameter increases. It is also observed that the material temperature decreases with increase in activation energy while it increases with increase in Frank-Kamenetskii parameter.

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### Keywords

high quality lime, shaft furnace, fuel rate, fuel combustion, limestone calcination

## 1.0 Introduction

The thermo-chemical processes, occurring in shaft furnaces for high quality metallurgical lime production are highly energy intensive and very complicated. The furnaces design incorporate such major interdependent processes as fuel combustion, gas and material movement, heat and mass transfer and physico-chemical transformation of the burden materials. The temperature of the calcination zone of the shaft furnace for the production of high quality metallurgical lime is limited to the range 1200 – 1300<sup>o</sup>C [1].

Fuel combustion and limestone calcination are the major processes, which determine the amount of greenhouse gases CO<sub>2</sub>, NO<sub>x</sub>, SO<sub>2</sub> and toxic CO emitted from the shaft furnace into the atmosphere. Therefore decrease of the fuel rate is very important not only from economics point of view, but also for the protection of the environment.

The majority of shaft furnaces for limestone calcination operate with counter-current flows of burden materials and gases (Boynton [1], Terruzzi [5], Tabunshikov [4] and Monastirev and Aleksandrov [3]). The furnace incorporates three technological zones: preheating, calcination and cooling (from top to bottom).

Gordon et al [2] developed the multi-dimensional mathematical model to optimize the furnace design and the process parameters. The developed mathematical model belongs to the

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<sup>1</sup>Corresponding author:

e-mail: olayiwolarasaq@yahoo.co.uk

group of essentially non-linear models. According to them, it is not possible to develop an analytical solution of the problem. The finite element method was used to provide a solution. They showed that material and gas temperatures are almost constant along the height of the calcinations zone. These temperatures, they said, are favorable for formation of high quality quick lime.

In this paper we extend the problem posed by Gordon et al. [2] to Arrhenius heat generation and chemical reaction. We provide an analytical solution of the problem. We also investigate the effects of activation energy and Frank-Kamenetskii parameters on the gas and material temperatures.

**2.0 Mathematical model**

Following [2], the governing equations describing the calcination process is given by the following equation of heat exchange:

$$\text{For material: } \rho_m(1-\epsilon)C_m \frac{dT_m}{dt} = -\alpha_v(T_g - T_m) + q_m + QA \exp\left(-\frac{E}{RT_g}\right) \tag{2.1}$$

$$\text{For gas: } \rho_g \epsilon C_g \frac{dT_g}{dt} = \alpha_v(T_g - T_m) + q_g + QA \exp\left(-\frac{E}{RT_g}\right) \tag{2.2}$$

satisfying the initial conditions

$$T_m(0) = T_0, T_g(0) = T_0 \tag{2.3}$$

where  $\rho$  is the density,  $E$  is the activation energy,  $R$  is the gas constant,  $q$  is the heat source,  $\alpha_v$  is the heat transfer coefficient,  $C$  is the heat capacity,  $\epsilon$  is the porosity,  $T$  is the temperature,  $t$  is the time,  $Q$  is the heat of reaction and  $A$  is the pre-exponential factor,  $g$  is the gas and  $m$  is the material.

**2.1 Non-dimensionalisation analysis**

$$\text{Let } \theta = \frac{E}{RT_0^2}(T_g - T_0), \phi = \frac{E}{RT_0^2}(T_m - T_0), t' = \frac{t}{\tau}, \epsilon = \frac{RT_0}{E} \tag{2.4}$$

Using the dimensionless variables (2.4) in (2.1) and (2.2), we obtain the dimensionless equations (after dropping of prime) as

$$\frac{d\theta}{dt} = \alpha_1(\theta - \phi) + \beta_1 + \delta_1 \exp\left(\frac{\theta}{1+\epsilon\theta}\right) \tag{2.5}$$

$$\frac{d\phi}{dt} = -\alpha_2(\theta - \phi) + \beta_2 + \delta_2 \exp\left(\frac{\theta}{1+\epsilon\theta}\right) \tag{2.6}$$

$$\theta(0) = 0, \phi(0) = 0 \tag{2.7}$$

where,  $\alpha_1 = \frac{\alpha_v \tau}{\rho_g \epsilon C_g}$ ,

$$\beta_1 = \frac{q_g \tau}{\epsilon T_0 \rho_g \epsilon C_g}$$

$$\delta_1 = \frac{QA \exp\left(-\frac{E}{RT_0}\right)}{\epsilon T_0 \rho_g \epsilon C_g} \text{ is the Frank-Kamenetskii parameter, } \alpha_2 = \frac{\alpha_v \tau}{\rho_m(1-\epsilon)C_m}$$

$$\beta_1 = \frac{q_m T}{\varepsilon T_0 \rho_m (1 - \varepsilon) C_m}, \quad \beta_2 = \frac{Q \exp\left(-\frac{T}{T_0}\right)}{\varepsilon T_0 \rho_m (1 - \varepsilon) C_m}$$

*is the Frank-Kamenetskii parameter*

### 3.0 Method of solution

We consider the following asymptotic expansion of temperatures  $\theta$  and  $\phi$  in  $\varepsilon$ . Let

$$\left. \begin{aligned} \alpha_1 &= O(\varepsilon) \\ \alpha_2 &= O(\varepsilon) \\ \beta_1 &= O(\varepsilon) \\ \beta_2 &= O(\varepsilon) \\ \alpha_1 &= \varepsilon \alpha_1^* + \varepsilon^2 \alpha_1^{**} + \dots \\ \alpha_2 &= \varepsilon \alpha_2^* + \varepsilon^2 \alpha_2^{**} + \dots \\ \beta_1 &= \varepsilon \beta_1^* + \varepsilon^2 \beta_1^{**} + \dots \\ \beta_2 &= \varepsilon \beta_2^* + \varepsilon^2 \beta_2^{**} + \dots \\ \theta &= \theta_0 + \varepsilon \theta_1 + h.o.t \\ \phi &= \phi_0 + \varepsilon \phi_1 + h.o.t \end{aligned} \right\} \quad (3.1)$$

and equate the powers of  $\varepsilon$ , we have

$$\varepsilon^0: \frac{d\theta_0}{dt} = \delta_1 \exp(\theta_0) \quad (3.2)$$

$$\frac{d\phi_0}{dt} = \delta_2 \exp(\theta_0) \quad (3.3)$$

$$\varepsilon^1: \frac{d\theta_1}{dt} = \alpha_1^* (\theta_0 - \phi_0) + \beta_1^* + \delta_1 \theta_1 \exp(\theta_0) \quad (3.4)$$

$$\frac{d\phi_1}{dt} = -\alpha_2^* (\theta_0 - \phi_0) + \beta_2^* + \delta_2 \theta_1 \exp(\theta_0) \quad (3.5)$$

The solution of temperatures  $\theta$  and  $\phi$  is obtained as

$$\theta(t) = \ln \left( \frac{1}{\delta_1 \left( t - \frac{1}{\delta_1} \right)} \right) + \frac{1}{t\delta_1 - 1} \left( \epsilon \left( \frac{1}{2} \frac{\alpha_1 \ln \left( -\frac{1}{t\delta_1 - 1} \right)}{\delta_1} - \frac{1}{2} \alpha_1 t + \frac{1}{4} \frac{\alpha_1}{\delta_1} + \frac{1}{4} \delta_1 \alpha_1 t^2 + \frac{1}{2} \delta_1 \alpha_1 \ln \left( -\frac{1}{t\delta_1 - 1} \right) t^2 - \alpha_1 \ln \left( -\frac{1}{t\delta_1 - 1} \right) t + \frac{1}{2} \alpha_1 \delta_2 \ln(t\delta_1 - 1) t^2 + \frac{1}{2} \frac{\alpha_1 \delta_2 \ln(t\delta_1 - 1)}{\delta_1^2} - \frac{1}{4} \alpha_1 \delta_2 t^2 + \frac{1}{2} \frac{\alpha_1 \delta_2 t}{\delta_1} - \frac{1}{4} \frac{\alpha_1 \delta_2}{\delta_1^2} - \frac{\alpha_1 \delta_2 \ln(t\delta_1 - 1) t}{\delta_1} - \frac{1}{2} I \alpha_1 \delta_2 \pi t^2 + \frac{I \alpha_1 \delta_2 \pi t}{\delta_1} - \frac{1}{2} \delta_1 \beta_1 t^2 - \beta_1 t - \frac{1}{4} \frac{\alpha_1 (\delta_1 + 2I \delta_2 \pi - \delta_2)}{\delta_1^2} \right) \right) \quad (3.6)$$

$$\phi(t) = -\frac{\delta_2 \ln(t\delta_1 - 1)}{\delta_1} + \frac{I \delta_2 \pi}{\delta_1} + \epsilon \left( -\frac{\alpha_2 \delta_2}{\delta_1^2} - \frac{3 \alpha_1 \delta_2 t}{4 \delta_1} + \frac{3 \alpha_1 \delta_2^2 t}{4 \delta_1^2} + \frac{1}{4} \frac{\alpha_1 \delta_2^2}{\delta_1^3 (t\delta_1 - 1)} - \frac{1}{2} \frac{\alpha_1 \delta_2^2 \ln(t\delta_1 - 1) t}{\delta_1^2} + \frac{1}{2} \frac{\alpha_1 \delta_2^2 \ln(t\delta_1 - 1)}{\delta_1^3} - \frac{1}{2} \frac{\delta_2 \alpha_1 \ln \left( -\frac{1}{t\delta_1 - 1} \right) t}{\delta_1} + \frac{\alpha_2}{\delta_1} - \frac{1}{2} \frac{\alpha_1 \delta_2^2}{\delta_1^3} - \alpha_2 t - \alpha_2 \ln \left( -\frac{1}{t\delta_1 - 1} \right) t - \frac{1}{2} \frac{\delta_2 \beta_1 t}{\delta_1} - \frac{1}{2} \frac{\delta_2 \beta_1}{\delta_1^2 (t\delta_1 - 1)} + \frac{1}{2} \frac{\alpha_1 \delta_2}{\delta_1^2} + \frac{\alpha_2 \delta_2 \ln(t\delta_1 - 1)}{\delta_1^2} - \frac{1}{4} \frac{\delta_2 \alpha_1}{\delta_1^2 (t\delta_1 - 1)} + \frac{\alpha_2 \ln \left( -\frac{1}{t\delta_1 - 1} \right)}{\delta_1} + \frac{\alpha_2 \delta_2}{\delta_1} - \frac{\alpha_2 \delta_2 \ln(t\delta_1 - 1) t}{\delta_1} + \frac{I \alpha_2 \delta_2 \pi t}{\delta_1} - \frac{1}{2} \frac{I \alpha_1 \delta_2^2 \pi t}{\delta_1^2} + \frac{1}{2} \frac{\delta_2 \alpha_1 \ln \left( -\frac{1}{t\delta_1 - 1} \right)}{\delta_1^2} + \beta_2 t - \frac{1}{4} \frac{1}{\delta_1^3} \left( -4 \alpha_2 \delta_2 \delta_1 - 3 \alpha_1 \delta_2^2 + 2I \alpha_1 \delta_2^2 \pi + 4 \alpha_2 \delta_1^2 + 2 \delta_2 \beta_1 \delta_1 + 3 \alpha_1 \delta_2 \delta_1 + 4I \alpha_2 \delta_2 \pi \delta_1 \right) \right)$$

The results presented in figures 4.1 to 4.6 demonstrate the effect of activation energy and Frank-Kamenetskii parameters on the gas temperature and material temperature profile.

#### 4.0 Result and discussion

Figures 4.1-4.3 show the gas temperature profiles against time  $t$  for different values of activation energy  $\epsilon$  and Frank-Kamenetskii parameters  $\delta_1$  and  $\delta_2$ . Figures 4.4-4.6 show the material temperature profiles against time  $t$  for different values of activation energy  $\epsilon$  and Frank-Kamenetskii parameters  $\delta_1$  and  $\delta_2$ .

Figure 4.1 displays the gas temperature profile for the different values of  $\epsilon$  at  $\delta_1 = 0.4$ ,  $\delta_2 = 0.3$ . It is shown that the gas temperature increases as the activation energy increases.

From the practical point of view, maintaining a high temperature of calcinations increases the furnace productivity. This temperature is favorable for formation of high quality quick lime.

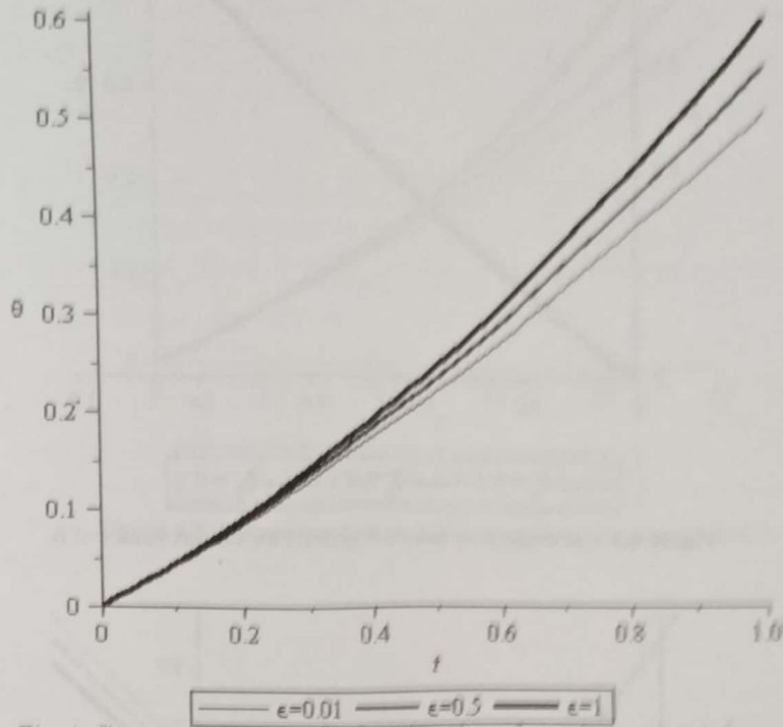


Figure 4.1: Gas temperature profile  $\theta$  against  $t$  for various values of  $\epsilon$

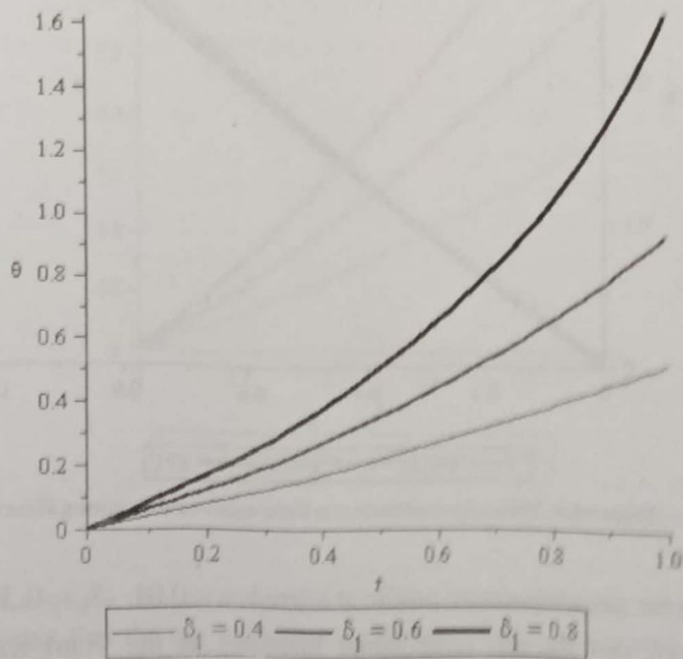


Figure 4.2: Gas temperature profile  $\theta$  against  $t$  for various values of  $\delta_1$

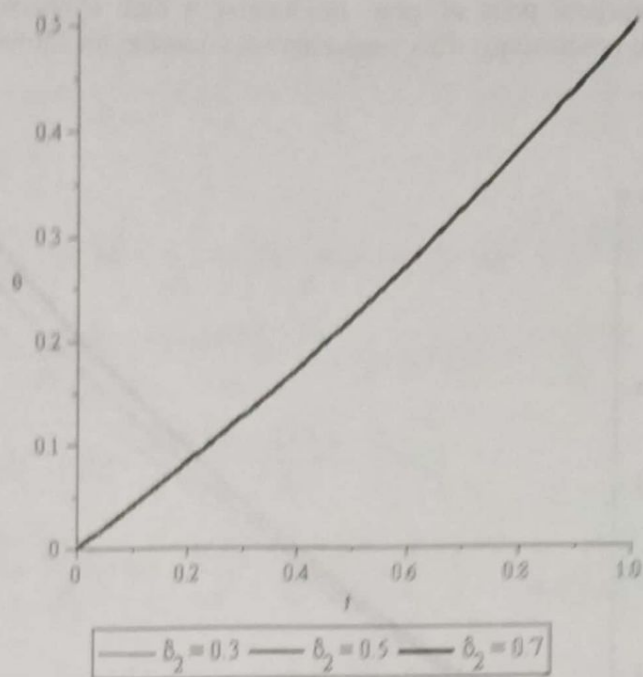


Figure 4.3: Gas temperature profile  $\theta$  against  $t$  for various values of  $\delta_2$

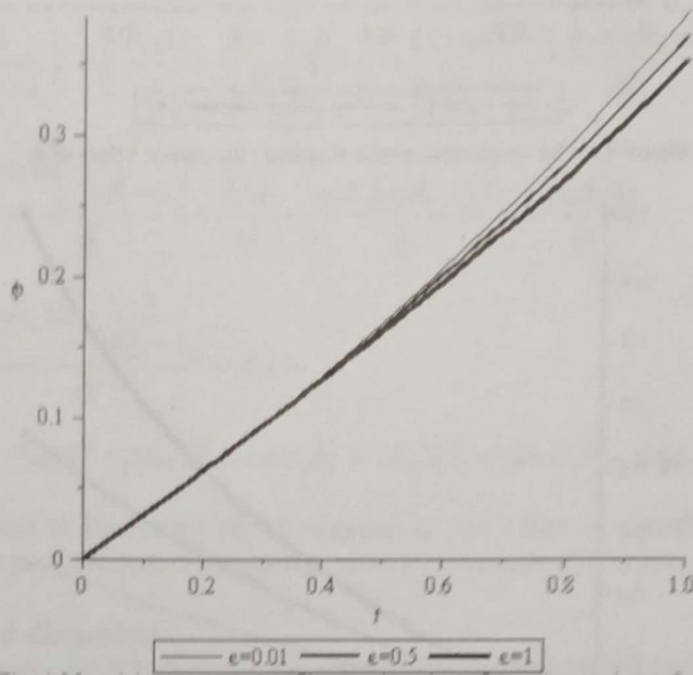


Figure 4.4: Material temperature profile  $\phi$  against  $t$  for various values of  $\epsilon$

Figure 4.2 reveals the gas temperature profile at a fixed  $\epsilon = 0.01$ ,  $\delta_2 = 0.3$  for varying values of  $\delta_1$ . It is shown that the gas temperature increases as the Frank-Kamenetskii number increases. This is as result of increase in heat of reaction.

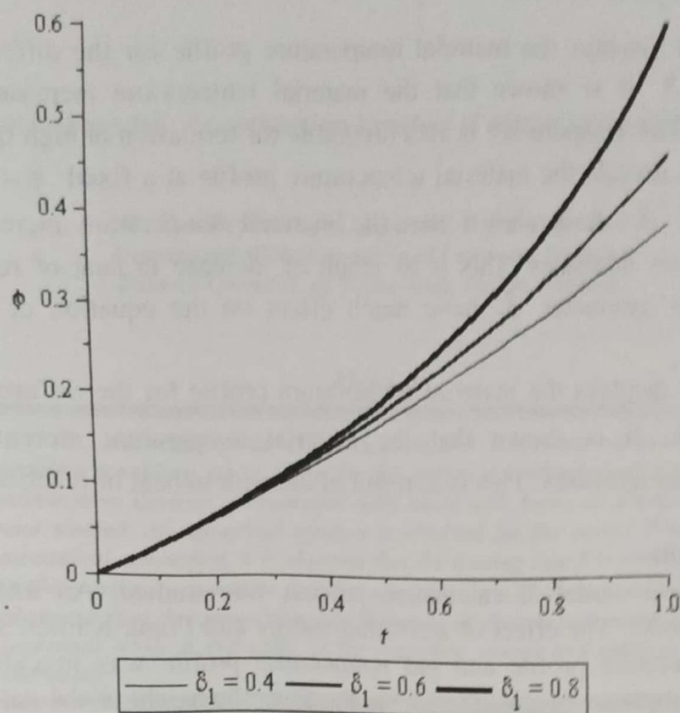


Figure 4.5: Material temperature profile  $\phi$  against  $t$  for various values of  $\delta_1$

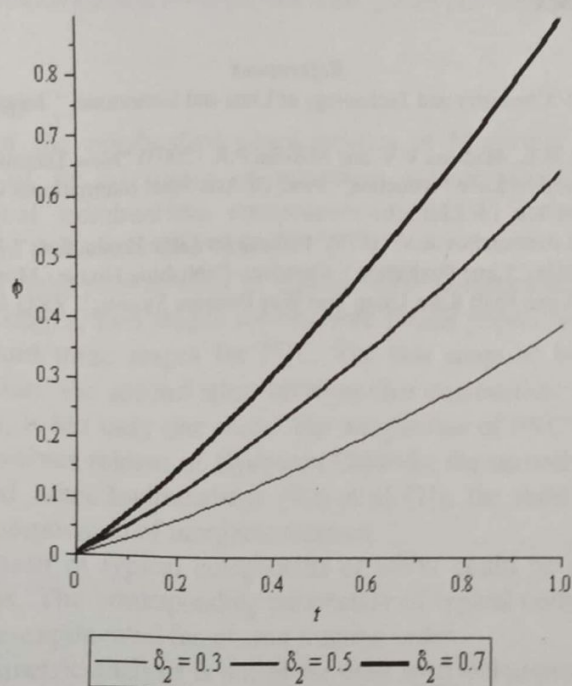


Figure 4.6: Material temperature profile  $\phi$  against  $t$  for various values of  $\delta_2$

Figure 4.3 displays the gas temperature profile for the different values of  $\delta_2$  at  $\delta_1 = 0.4$ ,  $\epsilon = 0.01$ . It is shown that the gas temperature does not change much with increase in Frank-Kamenetskii number. This shows that the Frank-Kamenetskii parameter  $\delta_2$  does not have much effect on the equation of heat exchange for gas.

Figure 4.4 displays the material temperature profile for the different values of  $\epsilon$  at  $\delta_1 = 0.4$ ,  $\delta_2 = 0.3$ . It is shown that the material temperature increases as the activation energy decreases. This temperature is also favorable for formation of high quality quick lime.

Figure 4.5 reveals the material temperature profile at a fixed  $\epsilon = 0.01$ ,  $\delta_2 = 0.3$  for varying values of  $\delta_1$ . It is shown that the material temperature increases as the Frank-Kamenetskii number increases. This is as result of increase in heat of reaction and that the Frank-Kamenetskii parameter  $\delta_1$  have much effect on the equation of heat exchange for material.

Figure 4.6 displays the material temperature profile for the different values of  $\delta_2$  at  $\delta_1 = 0.4$ ,  $\epsilon = 0.01$ . It is shown that the material temperature increases as the Frank-Kamenetskii number increases. This is as result of increase in heat of reaction.

### 5.0 Conclusion

Mathematical model of calcination process was studied. An analytical solution is obtained for the model. The effect of activation energy and Frank-Kamenetskii parameters on the material temperature profile and gas temperature profile was investigated. In [2], the material and gas temperatures are almost constant along the height of the calcination zone. But, in our study, the material and gas temperatures increase as the Frank-Kamenetskii number increases. Also as the activation energy increases the material temperature decreases and the gas temperature increases.

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