

## Thermal Explosion with Arrhenius Kinetics in Parallel Plates Subject to Various Boundary Conditions

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### Introduction

It was demonstrated that the original formulation of the problem by Semenov (1928) correctly characterizes the phenomena and explains the cause of the explosion after a review and analysis of the historical evolution of the thermal-explosion theory. Semenov demonstrated that an explosion happens when a solid's internal heat creation surpasses its external heat dissipation. According to Frank-Kamenetskii's (1969) critique of Semenov's reasoning, the explosion was caused by a temperature differential between the solid's surface and center. But his well-known and clever small-temperature model and the resulting differential equation solution warped the issue and slowed down the process of fully comprehending it.

Frank-Kamenetskii came to the conclusion that an explosion happens when there is no way to solve the issue. The validity of Semenov's formulation was confirmed by Donaldson and Tsao's (2006) precise solution to the problem. The problem's physics was fully understood after more research on how reactant use affected the issue.

Thermal Explosion may be due to a violent reaction between the overcharged anode and the high temperatures of the electrolytes that results in an exothermic reaction between the delithiated cathode and electrolyte by Ohsaki (2005).

When a chemical system goes through an exothermic reaction, insufficient heat is extracted from the system, causing the reaction process to become self-heating. This results in a thermal explosion.

However, thermal explosion theory is based on the idea that progressive heating raises the rate at which heat is released by the reaction until it exceeds the rate of heat loss from the area. At a given composition of the mixture and a given pressure, explosion will occur at a specific ignition temperature that can be determined from the calculation of heat loss and heat gain.

The transition from Combustion to Explosion is caused by an acceleration of the reaction induced either by a raise in temperature or by increasing length of the reaction Chain. The first is called thermal explosion, and the second is called Chain explosion.

If the heat released by the exothermic chemical reaction exceeds the rate at which heat is lost from the body to its surroundings, then an unstable build-up of heat inside a body can occur. This is because the increase in the internal temperature causes the reaction rate to increase, so more heat is generated, leading to a further increase in temperature. If the increase in the reaction rate outweighs the increase in the rate at which heat is lost to the surroundings, an unstable thermal runaway /explosion can occur (Brain, 2019).

**Objectives of the Study**

The specific objectives of the study are to;

- i. Formulate an energy balance equation for the thermal explosion with Arrhenius kinetics in parallel plates;
- ii. Solve the formulated energy equation using standard techniques; and
- iii. Examine the effects of various boundary conditions on the thermal explosion with Arrhenius kinetics.

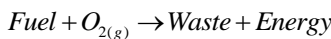
**Conceptualization/Definition of Terms**

For a better understanding of later discussions, the following definitions of important terms used in this study are given below.

**Definition 1.1: (Combustion)**

Combustion: is a chemical process or a reaction between fuel and oxygen which releases heat and light energy.

**General Equation:**



**Definition 1.2: (Chemical Kinetics)**

Chemical Kinetics: is the study of the rates of chemical reactions.

**Definition 1.3: (Steady state)**

A system is said to be steady when variables (such as velocity, temperature, density etc.)

Constant with time (that is  $\frac{\partial}{\partial x} = 0$ ) (Schlichting & Gersten, 2017).

**Definition 1.4: (Arrhenius Equation)**

An Arrhenius Equation: gives the dependence of the rate constant of a chemical reaction on

the absolute temperature, a pre-exponential factor and other constants of the reaction.

**Definition 1.5: (Boundary Conditions)**

Boundary conditions: this condition specifies the value that a solution must take in some

region of space and it is independent of time.

**Definition 1.6: (Thermal Explosion)**

Thermal Explosion: An explosion is a rapid increase in volume and release of energy in an

extreme manner, usually with the generation of high temperatures and the release of gases. It's

an event that once initiated grows rapidly and initially unbounded.

**Definition 1.8: (Self-Heating)**

Self-Heating: is a process where a material increases in temperature due to the release of heat

from ongoing chemical reactions and without drawing heat from its surroundings.

**Definition 1.9: (Criticality)**

The critical point of a function of a single real variable,  $f(x)$  is a value in the domain of  $f$

where its derivative is 0 (i.e.  $f'(x) = 0$ ).

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This is the conversion of one form of energy (such as nuclear, electrical, chemical energy) into

heat energy in a medium. A lot of heat transfer applications involve heat generation and this heat

generation according to (Azim and Chowdhury, 2013) modifies the temperature distribution.

Heat transfer by natural convection significantly influences temperatures of power generating systems (Theodore et al., 2011).

**Statement of Problem**

The study of thermal explosion with Arrhenius kinetics has attracted a great deal of interest

from researchers in the past few decades because of its occurrence, as seen in volcanic eruption and nuclear plants. However, relatively little is known about the combined mixture of symmetric and asymmetric conditions on thermal explosion with Arrhenius kinetics for a slab; hence, this study.

**Methodology**

The study presents the fundamental energy equation for the thermal explosion with Arrhenius kinetics in parallel plates under varied boundary conditions. First, the fundamental equation of energy is presented, followed by a discussion of the model assumptions that were used to create the governing equations. The dimensionless Heat transport properties are covered and variables utilized in non-dimensionalizing the constructed equation are defined. A demonstration and discussion of the integration technique used to solve the given problem are provided.

**Basic Equations**

**Equation of Conservation of Energy**

The law of conservation of energy states that the amount of work done on a system and the amount of heat it receives cause the system's internal energy to rise proportionately. The energy equation controls heat transport in a medium when chemical reactions and insignificant radiant energy are present;

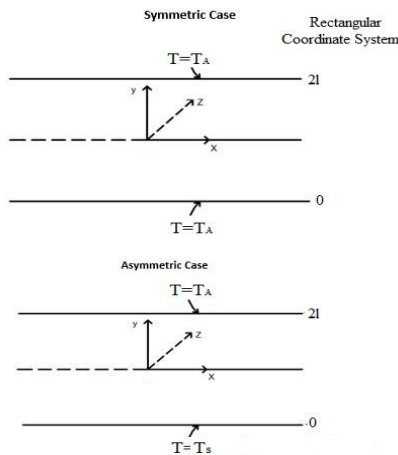
$$\rho Cp \frac{DT}{Dt} = K \nabla^2 T + \phi + e_g \quad (1)$$

Where the specific heat at constant pressure,  $T$  is the temperature,  $\phi$  is the viscous dissipation function,  $k$  is the thermal conductivity,  $e_g$  is the heat generation term.

**Problem Formulation**

A stationary one-dimensional parallel plate of a reacting material having thickness  $2L$  with its plane surfaces maintained at different boundary conditions is being considered.

Figures 1 and 2 show the geometry and co-ordinates system of our problem.



### Results and Discussion

The energy equation in (3.1) above was reduced with some assumptions to give

$$k \frac{d^2T}{dx^2} + A\Delta R\rho \exp(-E/RT) = 0 \quad (3.2)$$

An equation (3.2) is the energy equation subject to some assumptions used.

The temperature T and distance y are rescaled so as to compare terms in the equations without reference to units. The temperature equations are non-dimensionalized with the variables;

$$\begin{cases} z = \frac{x}{l} \\ \theta = \frac{E}{RT_A}(T - T_A) = \frac{1}{\beta T_A}(T - T_A) \end{cases} \quad (3.4)$$

The equation (3.2) is reduced to give a dimensionless temperature equation

$$\frac{d^2\theta}{dz^2} = -A\Delta H_{R\rho} \left(\frac{r^2}{k}\right) \left(\frac{E}{RT_A^2}\right) \exp\left(-\frac{E}{RT_A}\right) \exp\left(\frac{\theta}{1+\beta\theta}\right) \quad (3.5)$$

Where

$$\delta = A\Delta H_{R\rho} \left(\frac{r^2}{k}\right) \left(\frac{E}{RT_A^2}\right) \exp\left(-\frac{E}{RT_A}\right) \exp\left(\frac{\theta}{1+\beta\theta}\right) \quad (3.6)$$

is the Frank-Kamenetskii number.

$$\frac{d^2\theta}{dz^2} = -\delta \exp\left(\frac{\theta}{1+\beta\theta}\right) \quad (3.7)$$

When  $\beta \rightarrow 0$ , equation (3.7) reduced becomes;

$$\frac{d^2\theta}{dz^2} = -\delta \exp(\theta) \quad (3.8)$$

The linear ordinary differential equation (3.8) can be solved by multiplying both of its sides by

$$\begin{aligned} &2 \frac{d\theta}{dz} \\ &2 \frac{d\theta}{dz} \frac{d^2\theta}{dz^2} + 2\delta \exp(\theta) \frac{d\theta}{dz} = 0 \quad (3.9) \end{aligned}$$

By integrating both sides of Equation (3.9), we have;

$$\left(\frac{d\theta}{dz}\right)^2 + 2\delta \exp(\theta) = A_0 \quad (4.0)$$

NOTE:  $A_0$  is the constant of integration.

By separating the variables in Equation (4.0) above gives,

$$\frac{d\theta}{\sqrt{A_0 - 2\delta \exp(\theta)}} = dz \quad (4.1)$$

Integrating both sides, we have;

$$\int \frac{d\theta}{\sqrt{A_0 - 2\delta \exp(\theta)}} = dz \quad (4.2)$$

Note that the left hand side is integrated by replacing  $A_0$  with  $2\delta A$ .

$$\int \frac{d\theta}{\sqrt{2\delta A - 2\delta \exp(\theta)}} = z + A_1 \quad (4.3)$$

By factoring out  $\sqrt{2\delta A}$  and multiplying both sides by  $\sqrt{2\delta A}$ , we have,

$$\int \frac{d\theta}{\sqrt{1 - A^{-1} \exp(\theta)}} = \pm \sqrt{2\delta A} z + B \quad (4.4)$$

Where  $B = (\sqrt{2\delta A}) A_1$

By letting  $\theta = -2 \ln P = -2 \frac{dp}{p}$  L.H.S of Equation (4.4) above becomes;

$$-2 \int \frac{dp}{\sqrt{(1 - A^{-1} P^{-2})}} = -2 \int \frac{dp}{P \sqrt{(1 - A^{-1} P^{-2})}} \quad (4.5)$$

Equation (4.5) becomes,

$$-2 \int \frac{dp}{P \sqrt{(1 - A^{-1} P^{-2})}} = \pm \sqrt{2\delta A} z + B \quad (4.6)$$

Dividing both sides by -2 gives,

$$\int \frac{dp}{\sqrt{(P^2 - A^{-1})}} = \sqrt{\frac{\delta A}{2}} z - B \quad (4.7)$$

Letting,

$P = \sqrt{A^{-1}} \cosh q$ , the L.H.S of the Equation becomes;

$$\int \frac{(\sqrt{A^{-1}} \sinh q) dq}{\sqrt{A^{-1} (\cosh^2 q - 1)}} = \int dq = q \quad (4.8)$$

From the above,

$$\theta = -2 \ln P \text{ and } \sqrt{A^{-1}} \cosh q \Rightarrow q = \cosh^{-1}(\sqrt{A} \exp(-\theta/2))$$

Hence, Equation (4.8) becomes,

$$\sqrt{A} \exp(-\theta/2) = \cosh\left(\sqrt{\frac{\delta A}{2}} z - B\right) \quad (4.9)$$

Divide both sides by  $\sqrt{A}$

$$\exp(-\theta/2) = \cosh\left(\frac{\sqrt{\delta A}}{\sqrt{2}} z - B\right) \quad (5.0)$$

Squaring both sides, and taking the reciprocal, we have;

$$\exp(\theta) = \frac{A}{\cosh^2\left(\sqrt{\frac{\delta A}{2}}z - B\right)} \quad (5.1)$$

Taking ln of both sides, we have;

$$\theta(z) = \ln\left(\frac{A}{\cosh^2\left(\sqrt{\frac{\delta A}{2}}z - B\right)}\right) \quad (5.2)$$

Equation (5.2) represents the temperature equation of the parallel plates with Arrhenius kinetics which will be analyzed for four (4) different boundary conditions.

Here, A and B are integration constants, z is the dimensionless distance and  $\delta$  is the Frank-Kamenetskii parameter.

**Case 1: Symmetric Boundary Condition**

The symmetric boundary condition given as;

$$\begin{cases} T = T_A \text{ at } x = 0 \\ T = T_A \text{ at } x = 2l \end{cases} \quad (5.3)$$

is non-dimensionalized with the variables in Equation (3.4) to give,

$$\begin{cases} \theta = 0 \text{ at } z = 0 \\ \theta = 0 \text{ at } z = 2 \end{cases} \quad (5.4)$$

Substituting the boundary condition  $\theta(0) = 0$  into Equation (5.2) above gives,

$$0 = \ln\left[\frac{A}{\cosh^2(-B)}\right] \quad (5.5)$$

Equation (5.5) reduced to;

$$A = \cosh^2(-B)$$

$$\Rightarrow A = \cosh^2 B$$

(5.6)

By substituting the boundary condition  $\theta(2) = 0$  into Equation (5.2) above gives,

$$0 = \ln\left[\frac{\cosh^2 B}{\cosh^2\left(\sqrt{2\delta} \cos B - B\right)}\right] \Rightarrow \sqrt{2\delta} = \frac{2B}{\cosh B} \quad (5.7)$$

Taking exponential of both sides gives,

$$\cosh^2 B = \cosh^2(\sqrt{2\delta} \cosh B - B) \quad (5.8)$$

$$B = \sqrt{2\delta} \cosh B - B \quad (5.9)$$

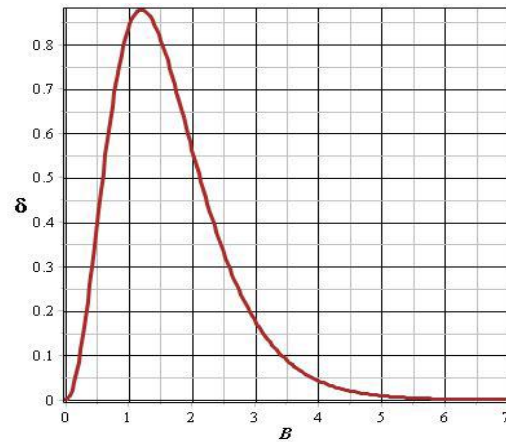
$$\sqrt{2\delta} = \frac{2B}{\cosh B} \quad (6.0)$$

Squaring both sides and dividing by 2

$$\delta = \frac{2B^2}{\cosh^2 B} \quad (6.1)$$

Since  $\delta = \delta(B)$ ,  $\delta$  is plotted against  $B$  to obtain  $\delta_{cr}$  and the value of  $B$  (6.2)

A graph of  $\delta$  against  $B$  for symmetric boundary condition.



From the graph above  $\delta_{cr} = 0.878$  and the value of

$$B = 1.193 \text{ from equation (5.6), } A = \cosh^2(1.193) = 3.240 \quad (6.3)$$

Substituting the values of  $A, B, A, B$  and  $\delta_{cr}$  into equation (5.2) gives,

$$\theta(z) = \ln\left(\frac{3.240}{\cosh^2\left(\sqrt{\frac{(0.878)3.240}{2}}z - 1.193\right)}\right) \quad (6.4)$$

$$\theta(z) = \ln\left(\frac{3.240}{\cosh^2(1.193z - 1.193)}\right) \quad (6.5)$$

The graph of  $\theta_{max}$  against z is plotted and discussed.

**Case 2: Asymmetric Boundary Condition**

The asymmetric boundary condition

$$\begin{cases} T = T_A \text{ at } X = 0 \\ T = T_S \text{ at } X = 2l \end{cases} \quad (6.6)$$

is non-dimensionalized with the variables in Equation (3.4) to give

$$\begin{cases} \theta = 0 \text{ at } z = 0 \\ \theta = \theta_s \text{ at } z = 2 \end{cases} \quad (6.7)$$

Substituting the boundary condition  $\theta(0) = 0$  into equation (5.2) gives,

$$0 = \ln\left[\frac{A}{\cosh^2(-B)}\right] \quad (6.8)$$

$$\Rightarrow A = \cosh^2 B \quad (6.9)$$

By substituting the boundary condition  $\theta(2) = \theta_s$  into equation (5.2) gives,

$$\theta_s = \ln\left[\frac{\cosh^2 B}{\cosh^2(\sqrt{2\delta} \cosh B - B)}\right] \quad (7.0)$$

By taking exp of both sides gives,

$$\text{Exp}(\theta_s) = \frac{\cosh^2 B}{\cosh^2(\sqrt{2\delta} \cosh B - B)} \quad (7.1)$$

Again, taking square root of both sides,

$$\pm\sqrt{\exp(\theta_s)} = \frac{\cosh B}{\cosh(\sqrt{2\delta} \cosh B - B)} \quad (7.2)$$

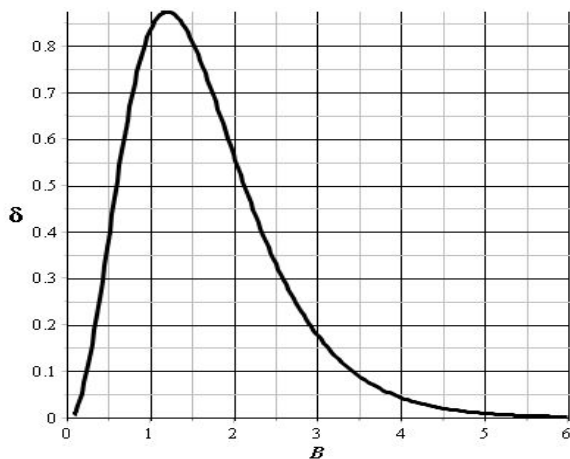
$$\cosh(\sqrt{2\delta} \cosh B - B) = \pm \exp(-\theta_s/2) \cosh B \quad (7.3)$$

$$\sqrt{2\delta} \cosh B = B + \cosh^{-1}\{\pm \exp(-\theta_s/2) \cosh B\} \quad (7.4)$$

Squaring both sides and dividing through by  $2 \cosh^2 B$

$$\delta = \frac{1}{2} \left[ \frac{B + \cosh^{-1}\{\pm \exp(-\theta_s/2) \cosh B\}}{\cosh B} \right]^2 \quad (7.5)$$

Here,  $\delta_{cr}$  is obtained by plotting  $\delta$  against  $B$ , while the surface is assumed to be at temperature  $\theta_s = 0.01$ .



Plot of  $\delta$  against  $B$  for asymmetric boundary condition.

From the graph above  $\delta_{cr} = 0.874$  and the value of  $B = 1.197$

From equation (6.9),

$$A = \cosh^2(1.197) = 3.262 \quad (7.6)$$

Substituting  $A, B$  and  $\delta_{cr}$  into equation (5.2) gives,

$$\theta(Z) = \ln \left( \frac{3.262}{\cosh^2 \left( \sqrt{\frac{(0.874)3.262}{2}} Z - 1.197 \right)} \right) \quad (7.7)$$

$$\theta(Z) = \ln \left( \frac{3.262}{\cosh^2(1.194Z - 1.197)} \right) \quad (7.8)$$

The graph of  $\theta_{max}$  and  $Z$  is plotted, and therefore discussed below.

### Results Discussion and Findings

In this section, effect of the various boundary conditions are presented graphically and their effects on the temperature profiles are discussed. Except in cases where they are indicated as variable parameters, the following constant values are assumed for the relevant parameters: and.

Figure 4.1 represents the plots of  $\delta$  against  $B$  and  $\theta$  against  $z$ . The plots in figure 4.1a, shows that moving along  $B$ , the Frank Kamenetskii parameter  $\delta$ , start increasing from zero to the maximum value of  $\delta = 0.878$  at  $B = 1.193$ . The maximum point  $\delta = 0.878$  beyond which the curve of  $\theta$  starts decreasing is the critical Frank Kamenetskii  $\delta_{cr}$ . Beyond  $\delta_{cr}$ , the curve decreases monotonically to zero and maintains zero value for  $B > 5.5$ .

Figure 4.1b; depict a parabolic curve bounded above for the plot of  $\theta_{max}$  against the dimensionless distance  $z$ .

It is seen that,  $\theta_{max}$  increases uniformly to a peak value of 1.176.

Also, along  $z$ ,  $\theta_{max}$  increases uniformly for to a zero for  $Z > 1$

Figure 4.1 therefore reveal that a parallel plate of dimensionless thickness of 2 with Arrhenius Kinetic will have a critical Frank Kamenetskii value of  $\delta_{cr} = 0.878$  and a critical maximum temperature of  $\theta_{maxcr} = 1.176$  when the walls are subjected to symmetric dimensionless temperature ( $\theta = 0$ ).

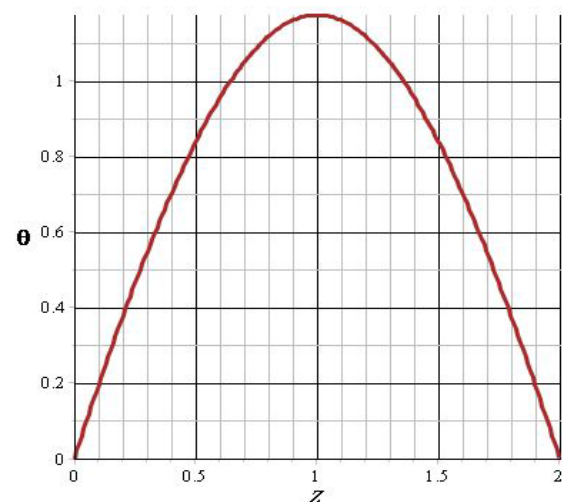
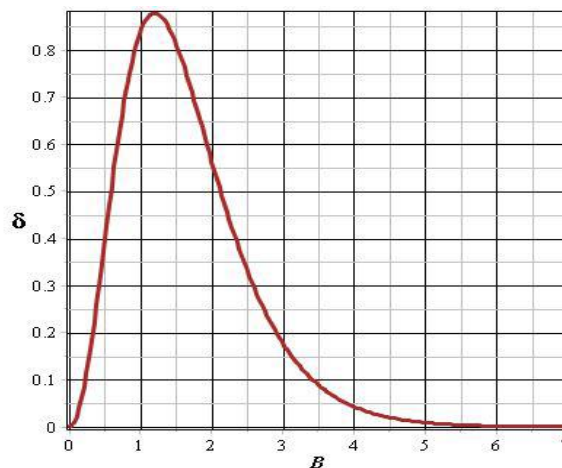


Figure 4.1: Graphs of (a)  $\delta$  against  $B$  and (b)  $\theta$  against  $Z$  for symmetric boundary condition.



However, figure 4.2 represents the graphs of  $\delta$  and  $B$  and  $\theta$  and  $z$ . The plots in figures 4.2a, shows that, moving along  $B$ , the Frank Kamenetskii parameter  $\delta$  increases from zero to a maximum value of  $\delta = 0.874$  at the point where  $B = 1.197$ . The maximum point  $\delta = 0.874$  where the value of  $\theta$  starts decreasing is the critical Frank Kamenetskii  $\delta_{cr}$ . Beyond  $\delta_{cr}$  the curve decreases monotonically to zero and maintain zero value for  $B > 5.5$

Figures 4.2b, shows a parabolic curve of  $\theta_{max}$  against the dimensionless distance  $z$ . it is seen that,  $\theta_{max}$  increases uniformly to a peak value of 1.176. Also, along  $z$ ,  $\theta_{max}$  increases uniformly for  $z < 1$  and decreases uniformly to zero for  $z > 1$

Figure 4.2 therefore reveals that the parallel plates will have a critical Frank Kamenetskii value of  $\delta_{cr} = 0.874$  and a critical maximum temperature ( $\theta = 0$ ) at  $z = 0$  and ( $\theta = \theta_s = 0.01$ ) at  $z = 2$ .

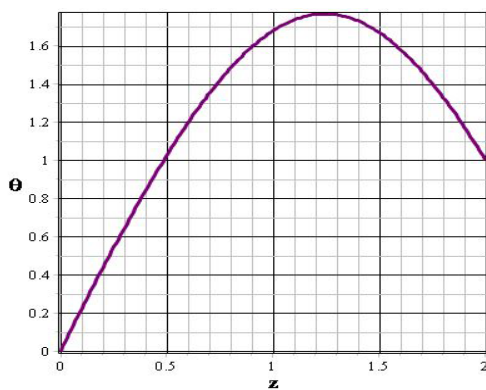
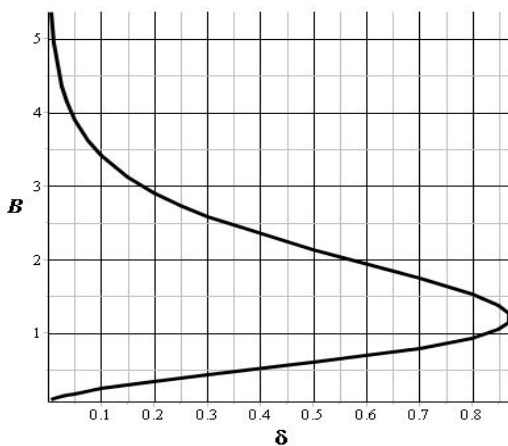


Figure 4.2: plots (a)  $\delta$  against  $B$  and (b)  $\theta$  against  $z$  for asymmetric boundary condition

### Conclusion

From this paper, the following significant conclusions were drawn:

- i. The maximum critical temperature  $\theta_{max cr}$  increases with increasing  $\theta_s$  and decreasing  $\delta_{cr}$  for the asymmetric boundary condition model.

- ii. The symmetric boundary condition model serves a limiting case to the asymmetric boundary condition model.
- iii. The maximum critical temperature  $\theta_{max cr}$  and the critical Frank-Kamenetskii parameter  $\delta_{cr}$  of the parallel plates changes significantly as the boundary conditions changes.

### Recommendation

Based on the findings, it is therefore recommended that, the right and accurate information about the maximum critical temperature  $\theta_{max cr}$  and the critical Frank-Kamenetskii parameter  $\delta_{cr}$  of materials should be known and taken into consideration in industries and working environments. This is to ensure safety of both workers and the environment.

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