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CALCULATION OF CRITICAL PARAMETERS FOR SPONTANEOUS COMBUSTION FOR SOME COMPLEX GEOMETRIES USING AN INDIRECT NUMERICAL METHOD

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Abstract

In the theory of spontaneous combustion, identifying the critical value of the Frank-Kamenetskii parameter corresponds to solving a bifurcation point problem. There are two different numerical methods used to solve this problem—the direct and indirect numerical methods. The latter finds the bifurcation point by solving a partial differential equation (PDE) problem. This is a better method to find the bifurcation point for complex geometries. This paper improves the indirect numerical method by combining the grid-domain extension method with the matrix equation computation method. We calculate the critical parameters of the Frank-Kamenetskii equation for some complex geometries using the indirect numerical method. Our results show that both the curve of the outer boundary and the height of the geometries have an effect on the values of the critical Frank-Kamenetskii parameter, however, they have little effect on the critical dimensionless temperature.

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1. Introduction

Frank-Kamenetskii theory [7] is the basic theory for spontaneous combustion. The dimensionless Frank-Kamenetskii equation and boundary condition are

$$\nabla^2\theta + \delta e^{\theta} = 0 \quad \text{and} \tag{1.1}$$

$$-\frac{\partial\theta}{\partial n} = Bi \cdot \theta. \tag{1.2}$$

In these equations, θ is the dimensionless temperature; δ is the Frank-Kamenetskii parameter; n is the direction perpendicular to the body surface; Bi is the Biot number, which is the ratio of the resistance to heat transfer within the body to that from the surface to the surroundings.

The original Frank-Kamenetskii theory considered the limiting case $Bi \to \infty$, as the values of Bi are very big in practice. In this case, the boundary conditions simplify to $\theta = 0$. Along an adiabatic or a symmetry boundary, the appropriate boundary conditions are $\partial\theta/\partial n = 0$.

For given boundary conditions, whether the Frank-Kamenetskii equation is solvable or not is determined by the value of the Frank-Kamenetskii parameter δ; the solution exists only when $\delta \leq \delta_{\text{cr}}$ [9]. This means that if the initial temperature is not too high and $\delta \leq \delta_{\text{cr}}$, then spontaneous ignition would not take place. The critical Frank-Kamenetskii parameter δ_{cr} and the critical dimensionless temperature θ_{cr} are the two critical parameters of spontaneous combustion. The problem of finding the critical Frank-Kamenetskii parameters is a bifurcation point (or branching point) problem. For most situations, it is difficult to obtain analytical solutions for δ_{cr} and θ_{cr}. Boddington et al. [4] and Bowes [5] have calculated the critical parameters of several problems using different methods. Table 1 shows the values of the critical Frank-Kamenetskii parameter for various geometries.

There are a variety of numerical methods which can be used to calculate the critical parameters for spontaneous combustion problems. Anderson and Zienkiewicz [1] studied the critical parameters of the Frank-Kamenetskii equation using a finite element method. Partridge and Wrobel [12] used the dual reciprocity formulation of the boundary element method. Sexton et al. [17] studied thermal ignition in rectangular and triangular regions using a finite difference method.

A direct numerical method to solve the bifurcation point problem is also widely used. Seydel [18], Moore and Spence [11] and Roose and Hlavacek [14, 15] introduced the direct numerical method to find bifurcation points of nonlinear equations. There are many papers about the calculation of the critical parameters of the Frank-Kamenetskii equation using the direct numerical method. Roose et al. [16] provided the direct numerical method for obtaining the bifurcation point of the Frank-Kamenetskii equation. Du and Feng [6] found the values of the critical parameters for some two-dimensional spontaneous combustion models using the direct numerical method.

There are several disadvantages when using the direct numerical method for the calculation of the critical parameters of the Frank-Kamenetskii equation.

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TABLE 1. Values of the critical Frank-Kamenetskii parameter for various geometries [9].

Geometry	Dimensions	δ_{cr}
Infinite plane slab	Width $2R$	0.878
Rectangular box	Sides $2L$, $2R$, $2M$ ($R < L, M$)	$0.873(1 + R^2/L^2 + R^2/M^2)$
Cube	Side $2R$	2.52
Infinite cylinder	Radius R	2.00
Equicylinder	Height $2R$, Radius R	2.76
Sphere	Radius R	3.32
Infinite square rod	Side $2R$	1.700

Luo et al. [10] discussed the disadvantages of the direct numerical method, and provide an indirect numerical method for calculating the critical parameters of the Frank-Kamenetskii equation. In their paper, the critical parameters of both two-dimensional (infinite rectangular rod) and three-dimensional (rectangular box) problems were determined.

The geometries of spontaneous combustion models can be very complex, for example, triangular prism and cone geometries. For these geometries, it is very hard to calculate the values of the critical Frank-Kamenetskii parameters using the direct numerical method. A major advantage of the indirect numerical method is its better adaptivity for complex geometries. This paper determines the critical parameters of the Frank-Kamenetskii equation for some complex geometries using the indirect numerical method.

2. The indirect numerical method

From the theory of bifurcation points, it is known that, if δ is too large, then there is no solution for the nonlinear equations (1.1) and (1.2). However, if the dimensionless temperature at the center of model θ_0 is given in advance, the situation is different. For any value of θ_0, there is a corresponding value for δ. Then we can modify the value of δ to solve the nonlinear equations. Luo et al. [10] provided an indirect numerical method which can calculate the critical parameters of the Frank-Kamenetskii equation. Figure 1 shows the flow chart of this indirect method. As shown on the flow chart, there are several important procedures.

(1) *Matrix equation.* Discretization of the PDE to build the matrix equation is very important. Building the matrix equation is more complicated when the model has a complex geometry.

(2) *δ correction.* For different values of δ, there may be no solution for the nonlinear equations (bifurcation point theory). If the dimensionless temperature at the centre of model θ_0 is given in advance, there is a value of δ which satisfies the nonlinear equations. However, there remains the problem of how to find the value of δ in complex geometries.

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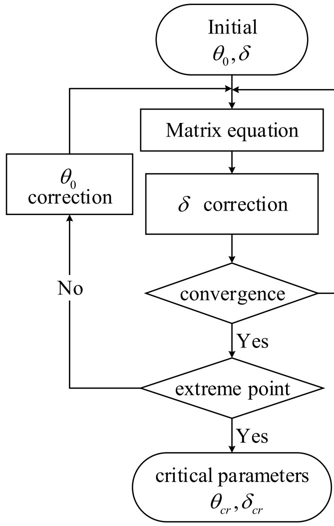

FIGURE 1. Flow chart for the indirect numerical method.

(3) θ_0 *correction.* From the $\delta - \theta_0$ curve, the peak point of these curves is the critical value δ_{cr}. It is not too hard to find the extreme point. MATLAB provides a function $x = fminbnd(\text{fun}, x1, x2)$ which can find the minimum of a single-variable function on a fixed interval, using the golden section search and parabolic interpolation algorithm.

3. Calculation of critical parameters

3.1. Mathematical model We calculate the critical parameters of the Frank-Kamenetskii equation for geometries in which the outer boundaries are irregular. In this section, we present our method for normal geometries. We provide details for the calculation of the critical parameters of the Frank-Kamenetskii equation for axisymmetrical geometries in Appendix A. The governing equation is

$$\frac{\partial^2\theta}{\partial x^2} + \frac{\partial^2\theta}{\partial y^2} + \delta e^{\theta} = 0.$$

Many complex geometry models can be simplified to two-dimensional problems. Figure 2 presents geometries with (a) linear outer boundary and (b) parabolic outer boundary and their corresponding grids. Considering the symmetry of the model, the left side of the two geometries is an adiabatic boundary. The bottom side of the two geometries can be regarded as an adiabatic boundary, as the ground prevents heat conduction. The boundary condition for the upright side of the two geometries is $\theta = 0$. Thus, the boundary conditions are

$$\left.\frac{\partial\theta}{\partial x}\right|_{x=0} = 0, \quad \left.\frac{\partial\theta}{\partial y}\right|_{y=0} = 0, \quad \theta|_l = 0.$$

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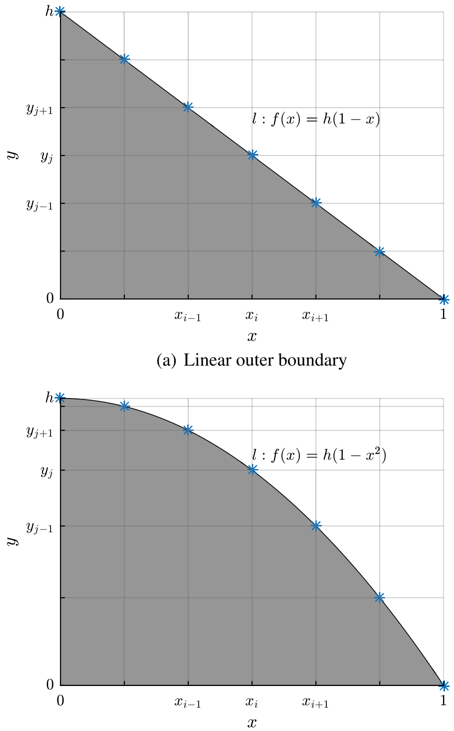

(a) Linear outer boundary

(b) Parabolic outer boundary

FIGURE 2. Geometries with (a) linear outer boundary and (b) parabolic outer boundary and their corresponding grids.

In these equations, x and y are dimensionless coordinates $(0 \leqslant x \leqslant 1, 0 \leqslant y \leqslant h)$. The parameter l indicates the upright boundary (l: $f(x) = h(1 - x)$ or l: $f(x) = h(1 - x^2)$). The length of the bottom boundary is regarded as a characteristic length $(0 \leqslant x \leqslant 1)$.

3.2. Grids with the domain extension method The body-fitted grids method is widely used in CFD (computational fluid dynamics) [2]. However, in order to combine the grid algorithm with the matrix equation, there is a better method, namely, the domain extension method. Tao [20, pp. 432–433] introduced some basics of this method. Prata and Sparrow [13] and Zhang [22] used this method for some CFD problems.

Figure 2 shows geometries with (a) linear outer boundary and (b) parabolic outer boundary and their corresponding grids. The actual grid is $I \times J$ (101 × 101). For convenience, the grids in x are equally spaced $(\Delta x = 1/(I - 1))$. There is a series of points at the original outer boundary (l: $f(x) = h(1 - x)$ or l: $f(x) = h(1 - x^2)$).

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There is an extension zone and the thermal conductivity of this zone is taken to be very high (far larger than the original zone). At the same time, the new boundary conditions are

$$\theta|_{x=1} = 0, \quad \theta|_{y=h} = 0.$$

3.3. Discretization and the matrix equation

3.3.1 *Discretization of the governing equation.* For the Frank-Kamenetskii equation, the result of discretization is

$$(a_i'\theta_{i-1,j} + a_i\theta_{i,j} + a_i''\theta_{i+1,j}) + (b_j'\theta_{i,j-1} + b_j\theta_{i,j} + b_j''\theta_{i,j+1}) = S_{i,j}, \tag{3.1}$$

where a_i', a_i, a_i'' and b_j', b_j, b_j'' are the relevant discretization parameters. Using a Taylor's series expansions method or the polynomial approach method [2, pp. 128–142], we obtain the second-order differences

$$\begin{cases} a'_i = \dfrac{1}{\Delta x^2}, & b'_j = \dfrac{2}{(y_j - y_{j-1})(y_{j+1} - y_{j-1})} \\ a_i = -\dfrac{2}{\Delta x^2}, & b_j = -\dfrac{2}{(y_j - y_{j-1})(y_{j+1} - y_j)} \\ a''_i = \dfrac{1}{\Delta x^2}, & b''_j = \dfrac{2}{(y_{j+1} - y_j)(y_{j+1} - y_{j-1})} \end{cases}.$$

In equation (3.1), $S_{i,j}$ is the source term which is different for different points (i, j).

$$S_{i,j} = \begin{cases} -\delta \exp(\theta_{i,j}), & y_{i,j} < f(x_{i,j}) \\ (a'_i\theta_{i-1,j} + a_i\theta_{i,j} + a''_i\theta_{i+1,j}) + (b'_j\theta_{i,j-1} & \\ \quad + b_j\theta_{i,j} + b''_j\theta_{i,j+1}) - \alpha(a_i + b_j)\theta_{i,j}, & y_{i,j} = f(x_{i,j}) \\ 0, & y_{i,j} > f(x_{i,j}). \end{cases}$$

3.3.2 *Discretization of the boundary conditions.* Considering the boundary conditions,

$$\begin{cases} \left.\dfrac{\partial\theta}{\partial x}\right|_{x=0} = 0 \Rightarrow (a_1\theta_{1,j} + a''_1\theta_{2,j}) + (b'_j\theta_{1,j-1} + b_j\theta_{1,j} + b''_j\theta_{1,j+1}) = S_{1,j}, \\ \left.\dfrac{\partial\theta}{\partial y}\right|_{y=0} = 0 \Rightarrow (a'_i\theta_{i-1,1} + a_i\theta_{i,1} + a''_i\theta_{i+1,1}) + (b_1\theta_{i,1} + b''_1\theta_{i,2}) = S_{i,1}, \\ \theta|_{x=1} = 0, \quad \theta|_{y=h} = 0 \Rightarrow \theta_{I,j} = 0, \quad \theta_{i,J} = 0, \end{cases}$$

where

$$\begin{cases} a_1 = -\dfrac{2}{\Delta x^2}, & a''_1 = \dfrac{2}{\Delta x^2}, \\ b_1 = -\dfrac{2}{(y_2 - y_1)^2}, & b''_1 = \dfrac{2}{(y_2 - y_1)^2}. \end{cases}$$

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3.3.3 *Matrix equation.* We build a matrix equation (Sylvester equation [21, p. 124]) from these nonlinear equations.

$$\mathbf{AX} + \mathbf{XB} = \mathbf{C} + \mathbf{D}. \tag{3.2}$$

Here, $\mathbf{A}$ and $\mathbf{B}$ are matrices of size $(I-1)\times(I-1)$ and $(J-1)\times(J-1)$, respectively, and $\mathbf{X}$, $\mathbf{C}$, $\mathbf{D}$ are matrices of size $(I-1)\times(J-1)$. Their expressions are

$$\mathbf{A} = \begin{pmatrix} a_1 & a''_1 & & & \\ a'_2 & a_2 & a''_2 & & \\ & \ddots & \ddots & \ddots & \\ & & a'_{I-2} & a_{I-2} & a''_{I-2} \\ & & & a'_{I-1} & a_{I-1} \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} b_1 & b'_2 & & & \\ b''_1 & b_2 & \ddots & & \\ & b''_2 & \ddots & b'_{J-2} & \\ & & \ddots & b_{J-2} & b'_{J-1} \\ & & & b''_{J-2} & b_{J-1} \end{pmatrix}$$

$$\mathbf{X} = \begin{pmatrix} \theta_{1,1} & \cdots & \theta_{1,J-1} \\ \vdots & \ddots & \vdots \\ \theta_{I-1,1} & \cdots & \theta_{I-1,J-1} \end{pmatrix}$$

$$\mathbf{C} = \begin{pmatrix} c_{1,1} & \cdots & c_{1,J-1} \\ \vdots & \ddots & \vdots \\ c_{I-1,1} & \cdots & c_{I-1,J-1} \end{pmatrix}, \quad \mathbf{D} = \begin{pmatrix} d_{1,1} & \cdots & d_{1,J-1} \\ \vdots & \ddots & \vdots \\ d_{I-1,1} & \cdots & d_{I-1,J-1} \end{pmatrix}.$$

For matrices $\mathbf{C}$ and $\mathbf{D}$, the expressions of $c_{i,j}$ and $d_{i,j}$ are

$$c_{i,j} = \begin{cases} S_{i,j}, & y_{i,j} < f(x_{i,j}), \\ 0 & \text{otherwise}, \end{cases} \qquad d_{i,j} = \begin{cases} S_{i,j}, & y_{i,j} = f(x_{i,j}), \\ 0 & \text{otherwise}. \end{cases}$$

There are many classical methods which can be used to solve the Sylvester equation [3, 8, 19]. MATLAB provides the function X= sylvester(A,B,C) to solve the Sylvester equation. For a nonlinear matrix equation, iteration is needed to obtain the solutions. However, in order to obtain convergence, relaxation techniques should be used, that is,

$$\mathbf{X} = \mathbf{X}^* + \alpha(\mathbf{X} - \mathbf{X}^*),$$

where α is the relaxation factor; the value $\alpha = 0.2$ was used for our problem.

3.4. Implementation of the indirect numerical method For the indirect numerical method, the equation at position (1,1) in equation (3.2) is replaced by a special equation $\theta_{1,1} = a$. We need to correct the value for δ after each loop of the iteration. We rewrite equation (3.2) as

$$\mathbf{AX} + \mathbf{XB} - \mathbf{D} = \mathbf{C}.$$

In this equation, only the matrix $\mathbf{C}$ has a close relationship with δ. Then, we correct the value of δ with the expression

$$\delta = \delta^* \frac{\sum_{i=1,j=1}^{I-1,J-1} (\mathbf{AX} + \mathbf{XB} - \mathbf{D})}{\sum_{i=1,j=1}^{I-1,J-1} \mathbf{C}}.$$

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TABLE 2. Critical parameters of the Frank-Kamenetskii equation for geometries with either a linear outer boundary or a parabolic outer boundary.

Outer boundary	Critical parameter	h 0.5	1	2	5
Linear	δ_{cr}	7.806	3.404	1.952	1.300
	θ_{cr}	1.393	1.391	1.393	1.391
Linear	δ_{cr}	11.383	5.692	3.658	2.676
(axisymmetrical)	θ_{cr}	1.619	1.615	1.613	1.606
Parabolic	δ_{cr}	5.556	2.339	1.495	1.121
	θ_{cr}	1.389	1.388	1.391	1.381
Parabolic	δ_{cr}	7.752	4.096	2.932	2.386
(axisymmetrical)	θ_{cr}	1.611	1.610	1.610	1.592

4. Results and discussion

We have introduced the indirect numerical method for complex geometries. The accuracy and efficiency of our approach is considered.

Accuracy. The grid of our problems is 101×101, which is finer than other direct methods. For obtaining a reliable value for δ in the internal loop of the flow chart, we consider that the iteration is convergent when the residual is very small (err $< 10^{-8}$). This ensures the accuracy of δ_{cr}. However, for the external loop, as the accuracy of θ_0 is limited by the accuracy of δ, the solution for θ_{cr} is less accurate than the solution for θ_{cr} (the termination tolerance is only 1×10^{-2} in the *fminbnd* function of MATLAB).

Efficiency. The efficiency of programs is greatly affected by the hardware and software system. We used the following hardware and software: (i) CPU: Intel(R) Core(TM) i5-4200U CPU @ 1.70GHz; (ii) RAM: 8.00 GB (1600 MHz); (iii) Operating System: Microsoft Windows 10 (64 bits); (iv) MATLAB R2015b. The computing time is 2–5 minutes for each problem.

The critical parameters of the Frank-Kamenetskii equation for geometries with a linear outer boundary and a parabolic outer boundary are shown in Table 2. The value of the critical parameters for different heights (h) and different outer boundaries is shown in Figure 3. In the calculation, "axisymmetrical" means the geometry is an axisymmetrical geometry according to the y-axis.

From the table, we see the following.

(1) The value of the critical parameter δ_{cr} decreases with increasing h. There is a higher risk of spontaneous combustion for geometries with a higher height h (the larger the value of δ_{cr}, the lower the risk of spontaneous combustion).
(2) If the height (h) is greater than 2, then the value of the critical parameter δ_{cr} decreases very slowly for all the geometries. This means that the risk of spontaneous combustion does not increase evidently when the height $h > 2$.

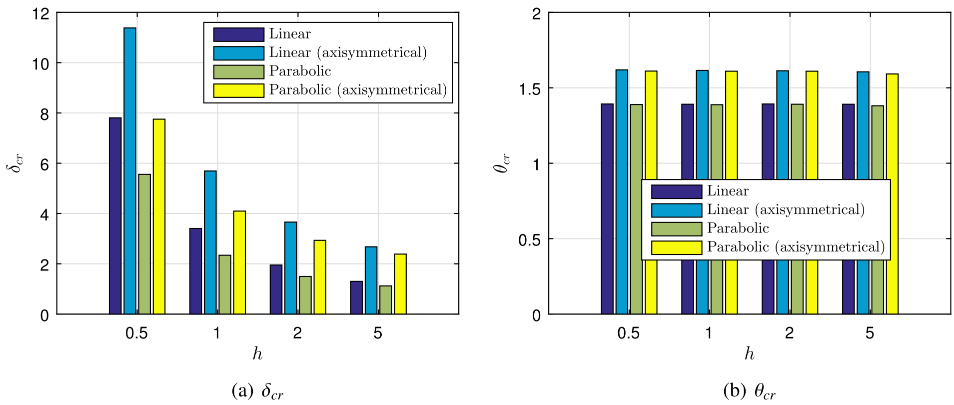

FIGURE 3. Bar graph of the critical parameters of the Frank-Kamenetskii equation for geometries with different heights (h) and different outer boundaries.

(3) The risk of spontaneous combustion for the geometry with the axisymmetrical linear outer boundary is the lowest of the four geometries, while the risk is largest for the geometry with the parabolic outer boundary. In general, the risk of spontaneous combustion for the geometry with the parabolic outer boundary is larger than the risk of the geometry with the linear outer boundary.

5. Conclusions

In this paper, we use an indirect numerical method to calculate the critical parameters of the Frank-Kamenetskii equation for some complex geometries, and we find the following.

(1) With the transformation introduced in the indirect numerical method, the bifurcation point problem of the Frank-Kamenetskii equation almost turns to a traditional PDE problem. Consequently, many traditional numerical methods for solving PDE can be used.
(2) For irregular geometries, we used the domain extension method for grid generation. This method is integrated with the matrix equation method for the calculation of the critical parameters of the Frank-Kamenetskii equation.
(3) We calculated the critical parameters of the Frank-Kamenetskii equation for some complex geometries. From the critical parameter δ_{cr}, we know that there is a close relationship between the geometries of the piles and the risk of spontaneous combustion. From the critical parameter θ_{cr}, the effect of the geometries on the critical dimensionless temperature θ_{cr} is relatively lower.

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Appendix A. Critical parameters for axisymmetrical geometries

Here, we calculate the critical parameters of the Frank-Kamenetskii equation problems with axisymmetrical geometries. As most parts are similar to previous sections, we only introduce some known differences in this section.

A.1. Mathematical models The governing equation for a cone is

$$\frac{\partial^2\theta}{\partial x^2} + \frac{1}{x}\frac{\partial\theta}{\partial x} + \frac{\partial^2\theta}{\partial y^2} + \delta e^{\theta} = 0,$$

where the y-axis is the axisymmetrical axis.

A.2. Matrix equation The grids method is the same as before. Here we discuss the discretization and matrix equation. The matrix equation is similar too, the differences come from matrices **A**, **B**, **C** and **D**.

$$\mathbf{AX} + \mathbf{XB} = \mathbf{C} + \mathbf{D}.$$

For the governing equation, the result of discretization is

$$(a'_i\theta_{i-1,j} - a_i\theta_{i,j} + a''_i\theta_{i+1,j}) + (b'_j\theta_{i,j-1} - b_j\theta_{i,j} + b''_j\theta_{i,j+1}) = S_{i,j},$$

where a'_i, a_i, a''_i and b'_j, b_j, b''_j are the relevant parameters of discretization

$$\begin{cases} a'_i = \left(1 - \dfrac{1}{2(i-1)}\right)\dfrac{1}{\Delta x^2}, & b'_j = \dfrac{2}{(y_j - y_{j-1})(y_{j+1} - y_{j-1})} \\ a_i = -\dfrac{2}{\Delta x^2}, & b_j = -\dfrac{2}{(y_j - y_{j-1})(y_{j+1} - y_j)} \\ a''_i = \left(1 + \dfrac{1}{2(i-1)}\right)\dfrac{1}{\Delta x^2}, & b''_j = \dfrac{2}{(y_{j+1} - y_j)(y_{j+1} - y_{j-1})}. \end{cases}$$

However, when $i = 1$, the situation is different. Considering that

$$\lim_{x\to 0}\frac{1}{x}\frac{\partial\theta}{\partial x} = \left.\frac{\partial^2\theta}{\partial x^2}\right|_{x=0} \quad \text{at } i = 1, \quad \text{then}$$

$$a_1 = -\frac{4}{\Delta x^2}, \quad a''_1 = \frac{4}{\Delta x^2}.$$

The other boundary conditions are the same as before. Hence, we obtain

$$b_1 = -\frac{2}{(y_2 - y_1)^2}, \quad b''_1 = \frac{2}{(y_2 - y_1)^2}.$$

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