

TRANSIENT ANALYSIS BY LAPLACE TRANSFORM AND COMBINED FINITE AND BOUNDARY ELEMENT METHODS FOR CONVECTIVE DIFFUSION PROBLEM

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SUMMARY

A numerical method for solving the problem of transient convective diffusion with a first-order chemical reaction is presented in this paper. The method is applicable over an infinite region. For steady problems the combined method of finite and boundary elements is recognized as a successful numerical technique for dealing with an infinite region. The present method is also useful in transient problems. In order to formulate the combined method for transient problems, we have developed a new method. In this paper the Laplace transform method incorporating the combined finite and boundary element methods will be considered. This transformation, holding complex values, transforms the transient problem into a steady state form. We also consider the present numerical solution which is obtained by using the numerical inverse Laplace transform as presented by Hosono. In numerical experiments the present method gives us an extremely accurate solution.

KEY WORDS: Laplace transform; combined method; transient problem; chemical reaction; convective diffusion; infinite region; finite element method; boundary element method; coupling method; unsteady problem

1. INTRODUCTION

A numerical method is presented for analysing the transient convective diffusion problem with a first-order chemical reaction defined on an infinite region. The present method for transient problems is based on the combined finite and boundary element methods¹ using the Laplace transform. For the time integration a numerical inverse Laplace transform presented by Hosono² has been successfully employed.

The finite element method is one of the useful numerical tools for analysing these problems. It is however, difficult to analyse a problem defined on an infinite region by use of the finite element method. The boundary element method satisfies unconditionally the infinite boundary condition by assuming that the problem is linear. However, the boundary element method has difficulties in solving problems involving non-homogeneous fields, because it is difficult to obtain the fundamental solution explicitly. If we appropriately combine the finite and boundary element methods, it is obvious that a method which avoids the difficulties of the two individual methods can be obtained. For steady problems the combined method is recognized as a successful numerical technique for dealing with infinite domains. This method is also useful in transient problems.

In the computation of a transient problem using the boundary element method, domain discretization must be employed to integrate over the infinite region. Furthermore, difficulties arise when the integral domain has to be expanded according to the expansion of the diffusion domain. The above-mentioned difficulties can be overcome by introducing the Laplace transform.³⁻⁹ The time dependency of the problem can be temporarily removed by this method.

Rizzo and Shippy³ first applied the direct formulation of the boundary element method in conjunction with the Laplace transform to solve the transient heat conduction problem. The transform inversion in their paper is essentially a curve-fitting process. It is important to have some knowledge of the expected behaviour of the solution in order to select values of the transform parameters, since the curve will not be represented correctly if the parameters are not selected suitably.

Hosono's numerical Laplace inversion² is very useful since it can be applied to general cases without any knowledge of the expected behaviour of the solution. Tazaki *et al.*⁸ presented the boundary element method in conjunction with this transform inversion to solve the problem of transient heat conduction. Okamoto and Kawahara⁹ applied this transform inversion to the boundary element method in order to solve the convective diffusion problem with a first-order chemical reaction. The effectiveness of the Hosono method has been shown in several numerical examples.^{8,9}

In this paper the approach of Hosono is applied to both the finite and boundary element regions and excellent results are obtained. The validity of the present method is shown via several numerical experiments.

2. BASIC EQUATION AND ITS LAPLACE TRANSFORM

The transient convective diffusion problem with a first-order chemical reaction in $\Omega \times I$, where Ω is a dimensional ($d = 1, 2$ or 3) infinite region and I is a time interval, is expressed as

$$\frac{\partial C_A}{\partial t} - D\nabla^2 C_A + v \cdot \nabla C_A + kC_A = 0 \quad \text{in } \Omega \times I, \quad (1)$$

where $C_A = C_A(P, t)$ represents the concentration of component A and is a function of the position $P = (X_1, X_2, X_3)$ in Cartesian co-ordinates x_1, x_2, x_3 and the time variable t . The symbols $\nabla, D, v = v(P)$ and k denote the gradient operator, the constant diffusivity, the velocity vector and the reaction rate constant respectively. Ω is constructed with the finite element region $\Omega^{(F)}$ and the boundary element region $\Omega^{(B)}$ (Figure 1). Suppose that the boundary Γ is split into two parts Γ_1 and Γ_2 . Then as the boundary conditions on (1), the following Dirichlet-type and Neumann-type conditions are considered:

$$C_A(P, t) = \bar{C}_A(P, t) \quad \text{on } \Gamma_1, \quad (2)$$

$$q_A(P, t) = \frac{C_A}{\partial n} = \bar{q}_A(P, t) \quad \text{on } \Gamma_2, \quad (3)$$

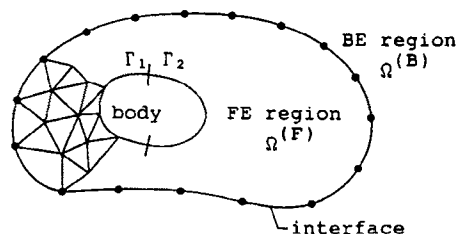


Figure 1. Internal (finite elements) and external regions

where the overbar denotes a prescribed function and n is the outer normal unit vector on the boundary. The initial condition is imposed as

$$C_A(P, 0) = C_{A0}(P) \quad \text{in } \Omega. \tag{4}$$

At infinity the boundary condition can be expressed as

$$C_A(P, t) = 0, \quad P \rightarrow \infty. \tag{5}$$

To remove the dependence of the time variable, the Laplace transform is applied to this problem. Employing the Laplace transform in (1), we obtain

$$-D\nabla^2 U + v \cdot \nabla U + (s + k)U - C_{A0} = 0, \tag{6}$$

where $U = U(P, s)$ is defined by

$$U(P, s) = \mathcal{L}[C_A(P, t)] = \int_0^\infty e^{-st} C_A dt. \tag{7}$$

In the Laplace transform space, equations (2) and (3) become respectively

$$U(P, s) = \mathcal{L}[\bar{C}_A] = \bar{U}(P, s) \quad \text{on } \Gamma_1, \tag{8}$$

$$Q(P, s) = \mathcal{L}[q_A] = \mathcal{L}[\bar{q}_A] = \bar{Q}(P, s) \quad \text{on } \Gamma_2. \tag{9}$$

Note that equation (6) is similar to the steady state convective diffusion problem with a first-order chemical reaction, except that the function is complex-valued; the boundary element method in Reference 10 can be used. The formulation satisfies the boundary condition at infinity in (5) because of the property of the fundamental solution. For simplicity it is assumed that $C_{A0} = 0$ throughout this paper.

3. BOUNDARY ELEMENT METHOD

Green's second identity over Ω for (6) can be expressed as

$$\int_\Omega (U_A^* L[U] - U L^*[U_A^*]) d\Omega = \int_{\Gamma_1} [(D\nabla U_A^*)U - U_A^*(D\nabla U) + vU_A^*U] \cdot nd\Gamma_1, \tag{10}$$

where $L^*[\cdot]$ and U_A^* are the adjoint operator and the adjoint potential field to U respectively and Γ_1 denotes the interface between the finite and boundary element regions. The d -dimensional fundamental solution U_d^* should satisfy

$$L^*[U_d^*] = -D\nabla^2 U_d^* - \nabla \cdot (vU_d^*) + kU_d^* = \delta(P_i - P), \tag{11}$$

in which P_i is an arbitrary source point and P is a reference point. The d -dimensional fundamental solutions $U_d^*(P_i, P)$ are given by¹⁰

$$U_1^* = \left(\frac{1}{2\mu D}\right) \exp\left(\frac{-v \cdot r}{2D} - |\mu r|\right), \tag{12}$$

$$U_2^* = \left(\frac{1}{2\pi D}\right) \exp\left(\frac{-v \cdot r}{2D}\right) K_0^{(2)}(|\mu r|), \tag{13}$$

$$U_3^* = \left(\frac{1}{4\pi D|r|}\right) \exp\left(-\frac{v \cdot r}{2D} - |\mu r|\right), \tag{14}$$

where

$$|r| = |P_i - P| = \left(\sum_{i=1}^d (x_i - \xi_i)^2 \right)^{1/2}, \tag{15}$$

$$v \cdot r = \sum_{i=1}^d v_i(x_i - \xi_i), \tag{16}$$

$$\mu^2 = \sum_{i=1}^d \left(\frac{|v_i|}{2D} \right)^2 + \frac{s+k}{D} \tag{17}$$

and $K_0^{(2)}$ denotes the complex modified Bessel function of the second kind of order zero. The fundamental solutions satisfy the boundary condition at infinity in (5). By choosing U_d^* instead of U_d^* in (10) and applying (6) and (11) to (10), the following integral equation is obtained:

$$a(P_i)U(P_i) + \int_{\Gamma_1} D \left(\frac{\partial U_d^*(P_i, P)}{\partial n} \right) U(P) d\Gamma_1 + \int_{\Gamma_1} U_d^*(P_i, P) \left[-D \left(\frac{\partial U(P)}{\partial n} \right) + v_n U(P) \right] d\Gamma_1 = 0. \tag{18}$$

For $d=2$, $\partial/\partial n = n_x(\partial/\partial x) + n_y(\partial/\partial y)$ and $a(P_i)$ is a weight depending on the solid angle of Ω , defined by

$$a(P_i) = \frac{\theta(P_i)}{2\pi}. \tag{19}$$

Here $\theta(P_i)$ is the external angle on the outer side of the internal region if the boundary element is used in the external region. Assume that the interface is divided into M linear boundary elements ($j = 1, 2, \dots, m$). Then the discretization of (18) gives

$$[H][U]_{\Gamma_1}^T = [G][Q]_{\Gamma_1}^T. \tag{20}$$

Since equation (6) includes the chemical reaction term $s + k$, the conservation law for the calculation of diagonal components of the matrix H cannot be satisfied. Namely, the diagonal component H_{ii} of the matrix H is

$$H_{ii} \neq - \sum_{j=1}^m H_{ij} \quad (i \neq j) \tag{21}$$

and the isoplethic concentration line and Γ_1 are not orthogonal to each other. Notice that H_{ii} must be calculated by

$$H_{ii} = a(P_i) + \bar{H}_{ii} \quad \bar{H}_{ii} = \int_{\Gamma_1} D \left(\frac{\partial C^*(P_i, P)}{\partial n} \right) \neq 0. \tag{22}$$

4. COMBINATION OF FINITE AND BOUNDARY ELEMENT METHODS

The combined method of the finite and boundary element methods will be described. The boundary elements are transformed into the equivalent finite elements.

For simplicity let Γ_1 of (20) be denoted as I. Multiplying both sides of (20) by $[G]^{-1}$, the following equation is obtained

$$[G]^{-1}[H][U^{(B)}]_I^T = [Q^{(B)}]_I^T, \tag{23}$$

where (B) denotes the boundary element region. In the internal region, equation (6) is discretized by the finite element method and then the following equation is obtained:

$$\begin{bmatrix} [Y]_{RR} & [Y]_{RI} \\ [Y]_{IR} & [Y]_{II} \end{bmatrix} \begin{bmatrix} [U^{(F)}]_R^T \\ [U^{(F)}]_I^T \end{bmatrix} = \begin{bmatrix} [\bar{Q}_V]_R^T \\ [Q_V]_I^T \end{bmatrix}, \tag{24}$$

where (F) denotes the finite element region. Here the matrix is expressed by separating the interface I and the internal region R which is not involved with the interface.

In combining (23) and (24), there is a slightly difficult problem, since Q is the flux at the node whereas Q_V is the volume flux crossing the element on the interface. Using the transformation matrix A , which can be considered as the continuity of the energy flow transmitted in the finite and boundary element regions, the following equation is obtained:

$$[Q_V]_I^T = [A][Q]_I^T. \tag{25}$$

Via the relation $[U^{(F)}]_I^T = [U^{(B)}]_I^T$ and from (23)–(25) the boundary elements can be transformed into the equivalent finite elements. Then the resulting global matrix is assembled as

$$\begin{bmatrix} [Y]_{RR} & [Y]_{RI} \\ [Y]_{IR} & [Y]_{II} - [A][G]^{-1}[H] \end{bmatrix} \begin{bmatrix} [U]_R^T \\ [U]_I^T \end{bmatrix} = \begin{bmatrix} [\bar{Q}_V]_R^T \\ [0]^T \end{bmatrix}. \tag{26}$$

The transformation matrix for the two-dimensional case is^{1,11}

$$[A] = \begin{bmatrix} a_2(l_m + l_1) & a_1 l_1 & & & & a_1 l_m \\ & a_1 l_1 & a_2(l_1 + l_2) & a_1 l_2 & & \\ & & \cdot & \cdot & & \\ & & a_1 l_{i-1} & a_2(l_{i-1} + l_i) & a_1 l_i & \\ & & & \cdot & \cdot & \\ & & & & a_1 l_{m-2} & a_2(l_{m-2} + l_{m-1}) & a_1 l_{m-1} \\ & a_1 l_m & & & & a_1 l_{m-1} & a_2(l_{m-1} + l_m) \end{bmatrix}, \tag{27}$$

where $a_1 = \frac{1}{6}$, $a_2 = \frac{1}{3}$ and l_i are the sizes of the combined finite and boundary elements.

5. INVERSE LAPLACE TRANSFORM

The inverse Laplace transform formula proposed by Hoson² is used in this paper. This formula has a great advantage since its applicable range is quite wide and its computational time is shorter than that for other formulae. The definition of the Laplace transform to $f(t)$ is

$$F(s) = \int_0^\infty e^{-st} f(t) dt \tag{28}$$

when $t > 0$. The inverse Laplace transform to $F(s)$ is given as

$$f(t) = \frac{1}{2\pi i} \int_{\alpha-i\infty}^{\alpha+i\infty} e^{st} F(s) ds, \tag{29}$$

where $f(t)$ is the function and $F(s)$ is the transformed function. The function e^s is approximated as

$$e^s \approx \frac{e^\sigma}{2 \cosh(\sigma - s)} \equiv E_{ec}(s, \sigma), \tag{30}$$

where σ is a positive number. When σ tends to infinity, then

$$e^s = \lim_{\sigma \rightarrow \infty} \frac{e^\sigma}{2 \cosh(\sigma - s)}. \tag{31}$$

The function $E_{ec}(s, \sigma)$ introduced in formulating the numerical inverse Laplace transform is written as

$$E_{ec}(s, \sigma) = \frac{e^\sigma}{2} \sum_{n=-\infty}^{\infty} \frac{-1}{s - [\sigma + i(n - 0.5)\pi]}. \tag{32}$$

Substituting (32) into (29), we have

$$f_{ec}(t, \sigma) = \frac{1}{2\pi i} \int_{\alpha-i\infty}^{\alpha+i\infty} F(s)E_{ec}(s, \sigma)ds. \tag{33}$$

The following conditions are assumed for a function $f(t)$:

- (a) $f(t) \in L^1(0, R)$ for any positive real number R
- (b) when $t \rightarrow \infty$ for any positive number γ , $f(t) = O(e^{-\gamma t})$
- (c) $f(t)$ is a real function for t .

Carrying out the complex integration, the following equation is obtained:

$$f_{ec}(t, \sigma) = \frac{e^\sigma}{t} \sum_{n=1}^{\infty} (-1)^n \text{Im} \left[F \left(\frac{\sigma + i(n - 0.5)\pi}{t} \right) \right], \tag{34}$$

where Im means imaginary part. An approximate value of the inverse Laplace transform is obtained from (34). Because (34) is an alternating series, the rate of convergence is not as fast. Thus it is not wise to calculate the numerical inverse Laplace transform with (34). It is well known that the Euler transform is an acceleration method for alternating series. If the Euler transform is applied to (34), we obtain

$$f_{ec}(t, \sigma) = \frac{e^\sigma}{t} \left(\sum_{n=1}^{\lambda-1} F_n + \frac{1}{2^{\mu+1}} \sum_{\nu=0}^{\mu} A_{\mu,\nu} F_{\lambda+\nu} \right), \tag{35}$$

where

$$F_n = (-1)^n \text{Im} \left[F \left(\frac{\sigma + i(n - 0.5)\pi}{t} \right) \right] = (-1)^n \text{Im}[F(s)] \tag{36}$$

and $A_{\mu,\nu}$ is determined recursively by the formulae

$$A_{\mu,\mu} = 1, \quad A_{\mu,\nu-1} = A_{\mu,\nu} + \binom{\mu+1}{\nu}. \tag{37}$$

Here $\binom{\mu}{\nu}$ denotes the binomial coefficient. Using (35), the numerical inverse Laplace transform of the numerical solution of (6) can be obtained. A numerical transform inverse procedure is then employed to compute the physical variables in the actual space.

6. COMPUTATIONAL PROCEDURE

The computational procedure is as follows.

1. Carry out the Laplace transform of the basic equation and the boundary conditions; then (6) can be rewritten as

$$L(U_n) = -D\nabla^2 U_n + v \cdot \nabla U_n + (s_n + k)U_n = 0, \tag{38}$$

where

$$s_n = \frac{\sigma + i(n - 0.5)\pi}{t}. \tag{39}$$

2. Discretize (38) by the combined method (here $s_n + k$ corresponds to k in Reference 1 and compute the field variables on the transformed space (the complex plane).
On implementation, set the time variable t in the actual space. Obtain the approximate value of U_n on the transformed plane using the parameters s_n corresponding to each n . Repeat this procedure for $n = 1, \dots, \lambda + \mu$.
3. Carry out the inverse Laplace transforms using (35). As a result, the approximate solution C_A^h on the physical plane can be derived. In the authors' numerical experiments, suitable values of the number of terms λ, μ and parameter σ are indicated as follows:
 - (a) $\lambda = 12, \mu = 7, \sigma = 5.5$ for calculation with single precision
 - (b) $\lambda = 15, \mu = 10, \sigma = 10.0$ for calculation with double precision.

7. NUMERICAL EXAMPLES

To examine the validity of the present method, three types of numerical experiments are carried out. The following non-dimensional parameters are used: the non-dimensional concentration of the reactant $\Phi = C_A/C_{A1}$, the non-dimensional time $T = Dt/b^2$, the non-dimensional co-ordinates $X = x_1/b$ and $Y = x_2/b$, the non-dimensional reaction rate constant $K = kb^2/D$ and the non-dimensional velocity (V_X, V_Y) becomes $V_X \equiv Pe = v_1b/D$ and $V_Y = v_2b/D$, in which Pe is the Peclet number, C_{A1} is the characteristic concentration of the reactant and b is the characteristic length. The initial condition is assumed as $\Phi(X, Y, 0) = 0$. The solution is characterized by K and Pe .

Example 1 (one-dimensional case)

Figure 2 shows the illustration of Example 1, where the finite element region (FE region in figures) is divided into 10 linear finite elements and the boundary element region (BE region) is combined at the point $X = 1$. The boundary conditions are prescribed as follows:

$$\text{BC1 } \Phi(0, T) = 1, \quad \text{BC2 } \Phi(\infty, T) = 0.$$

Figure 3 shows the computed results for Example 1, where the full curves are the exact solutions. It is seen that the transient numerical solutions of the combined method in conjunction with the Laplace transform are in good agreement with the exact solutions. Figure 4 shows the errors, which are less than 0.003 for $Pe = 10.0$ and $K = 10.0$.

Example 2 (two-dimensional case)

Figure 5 shows the geometry of Example 2, where the finite element region ($0 \leq X, Y \leq 1$) is discretized into 200 triangular elements, the boundary element region is combined at $X = 1$ and the

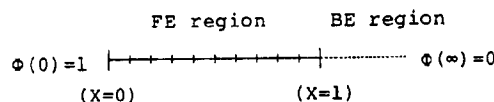


Figure 2. Numerical model for Example 1 (one-dimensional)

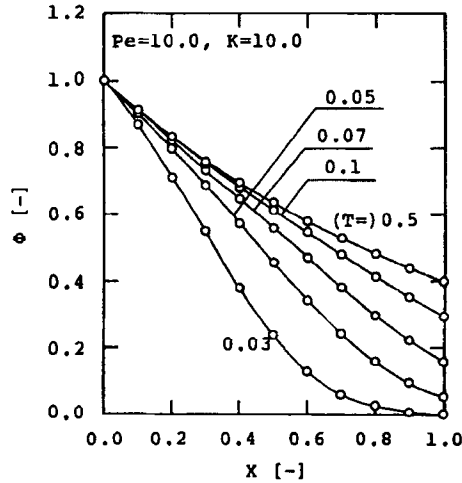


Figure 3. Numerical solutions for Example 1

flow direction is fixed parallel to the X -co-ordinate. Example 2 is treated as a duct problem. The analytical solution for this problem has not been obtained. Instead of the exact solution, the analytical solution obtained for the following boundary conditions is used for comparison:

$$BC1 \quad \Phi(0, Y, T) = 1, \quad BC2 \quad \partial\Phi(X, 0, T)\partial n = \partial\Phi(X, 1, T)/\partial n = 0, \quad BC3 \quad \Phi(\infty, Y, T) = 0.$$

The numerical results are approximately compared with the analytical solution at the central axis ($Y=0.5$). The boundary elements we used are linear elements, where the components H_{ij} and G_{ij} ($i \neq j$) are evaluated numerically with the eight-point Gaussian quadrature rule and the diagonal components H_{ii} and G_{ii} are evaluated with the 20-point Gaussian quadrature rule. The numerical solutions for Examples 1 and 2 are calculated with double precision. Figure 6 shows the results along $Y=0.5$ for Example 2. Figure 7 shows the errors, which are less than 0.012 for $Pe=30.0$ and $K=10.0$. Good results are obtained; hence it is shown that this method is applicable to the analysis of the duct problem with an open outlet.

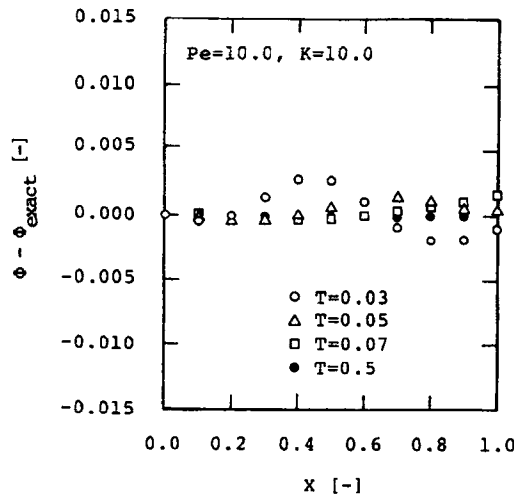


Figure 4. Errors in numerical solutions for Example 1

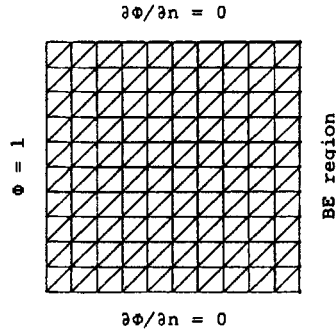


Figure 5. Numerical model for Example 2 (two-dimensional)

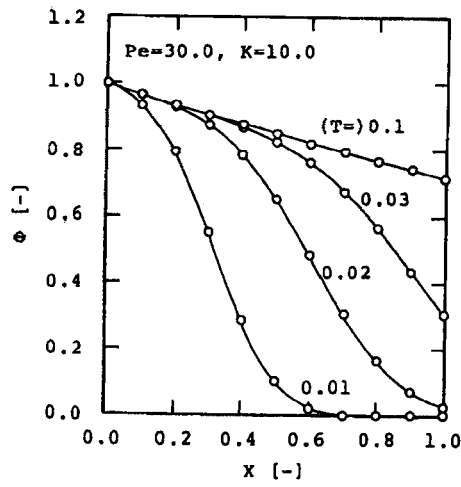


Figure 6. Numerical solutions for Example 2

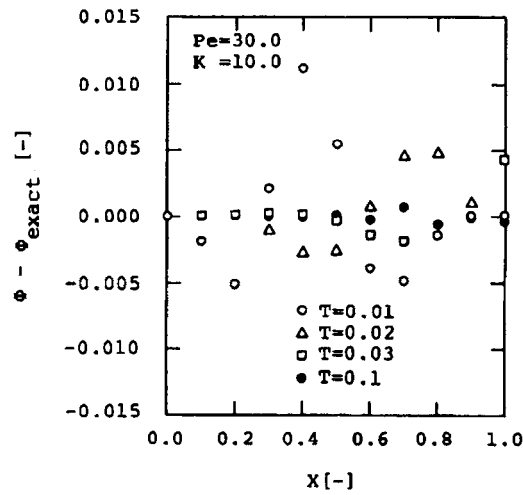


Figure 7. Errors in numerical solutions for Example 2

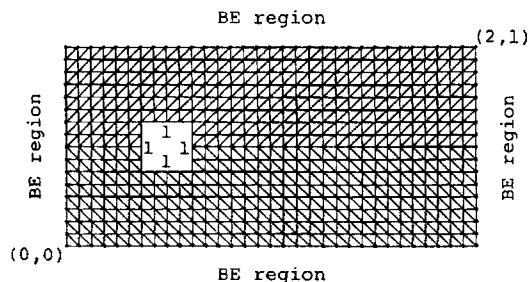


Figure 8. Numerical model for Example 3 (two-dimensional)

Example 3 (two-dimensional case)

Figure 8 illustrates the Example 3, where the finite element region is discretized into 992 triangular elements and the boundary element region is combined around the finite element region. The reactant diffuses from the small square body to the infinite space. Figure 9 shows the flow distribution which is calculated by the shallow water equation.¹² Figure 10 shows the results for Example 3. The quasi-steady state numerical solutions are in very good agreement with the steady state solutions obtained in Reference 1. It is concluded that excellent results can be obtained by the method presented in this paper. The numerical results using the conventional finite element method are shown in Figure 11 for comparison.

8. CONCLUSIONS

We have presented an efficient numerical method for solving the transient convective diffusion problem with a first-order chemical reaction defined on an infinite region. The present method is based on the Laplace transform and the finite element method combined with the boundary element method. Hosono's formula is applied to give the numerical solution in the physical space.

The results can be summarized as follows.

1. Using the present method, the time-dependent problem can be transformed into a time-dependent problem by means of the Laplace transform.
2. It is well known that the boundary element method with a time-marching scheme for the transient problem is not adaptable to an infinite region. However, using the Laplace transform procedure, the time-marching integration over the spatial domain which is usually necessary in the

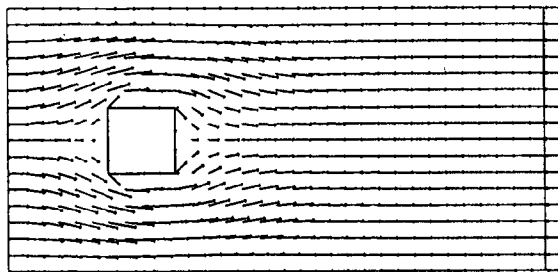


Figure 9. Flow distribution for Example 3

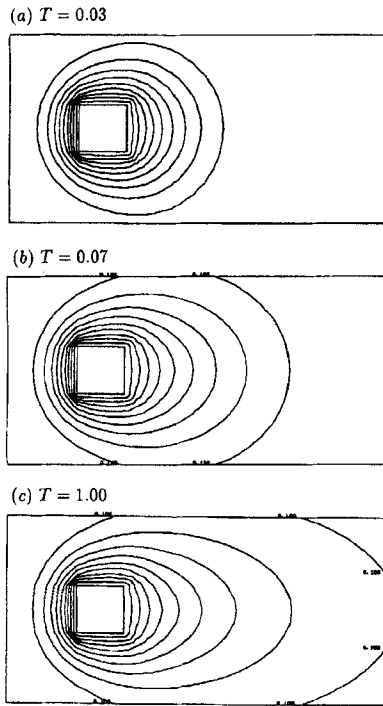


Figure 10. Equiconcentration contours for $Pe = 10$ and $K = 10$

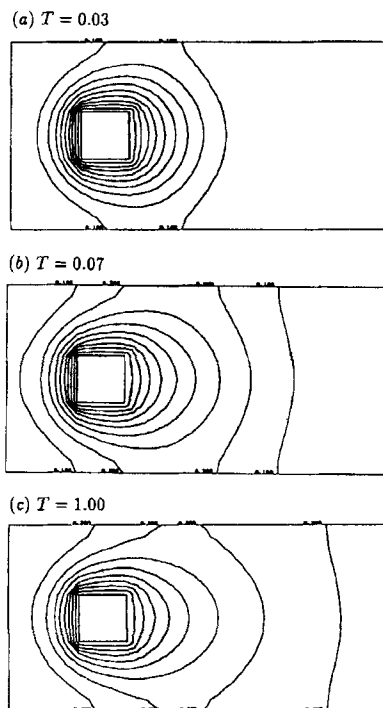


Figure 11. Equiconcentration contours using conventional FEM with Neumann boundary condition but without BEM

conventional boundary element analysis of transient problems is no longer necessary. The present transform procedure enables us to treat the problems of an infinite region by using the boundary element method.

3. It is shown that the application of Hosono's formula is an excellent procedure for both the finite boundary element regions.
4. In Examples 1 and 2 the numerical solutions by the proposed method are in good agreement with the exact solutions, while in Example 3 the quasi-steady state solution using the Laplace transform procedure and the steady state solution using only the combined method are in very good agreement. Thus the validity of the proposed method is demonstrated.

From these results it is concluded that the method presented in this paper is much superior to the conventional method.

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