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Singular boundary method for transient convection–diffusion problems with time-dependent fundamental solution

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ABSTRACT

This paper derives the time-dependent fundamental solution of the transient convection-diffusion problem by employing the exponential variable and Fourier transformations. A singular boundary method (SBM) formulation using this time-dependent fundamental solution is first applied in the simulation of the transient convection-diffusion problems. Accurate formulas are derived to evaluate the origin intensity factors in the SBM. The proposed method is mathematically simple, matrix-free and fully explicit. Furthermore, this scheme is computationally fast, stable, and requires low memory, since it does not need to solve any algebraic equations. Three benchmark examples, including three-dimensional cases, are presented to verify this time-dependent SBM strategy.

1. Introduction

The convection-diffusion equation describes physical phenomena where particles, energy, or other physical elements are transferred inside a physical system via two processes: diffusion and convection (advection). Solving the transient convection-diffusion equation remains a challenging task for most numerical methods because the model characterizes both wave and diffusion behaviors.

In recent decades, various numerical methods, such as the finite element methods (FEM) [1–3], the boundary element methods (BEM) [4–7], the method of fundamental solutions (MFS) [8–11] and alternating methods [12], have been developed and employed to solve physical problems of this kind. Compared with the domain-type techniques such as the FEM, the boundary-type methods [7,13,14] have certain advantages in terms of computational stability, boundary-only discretization, and semi-analytical approximation. However, if the steady-state fundamental solution is used, the boundary-type methods lose the boundary-only discretization merit. Consequently, the finite difference scheme is often used to handle the time derivative of the governing equation in combination with the dual reciprocity method (DRM) [15,16]. As far as numerical efficiency is concerned, the finite difference schemes can be quite time-consuming and can also cause instability if the time step is not carefully chosen.

The standard BEM, meanwhile, involves challenging mesh generation and costly numerical integration [7,17]. Compared with the BEM, the MFS is mathematically simple and very easy to program, since it does not require an elaborate discretization of the boundary and avoids computationally expensive and mathematically tricky singular integration. The MFS, however, requires a fictitious boundary for the placement of the source points to circumvent the singularity of the fundamental solution. The determination of the fictitious boundary is still a perplexing and tricky issue, especially for a complex three-dimensional geometric problem. On the other hand, great efforts have been made in recent years to overcome this barrier in the MFS, so that the source points can be placed directly on the real boundary [18–21].

As an alternative technique to the BEM and the MFS, the singular boundary method (SBM) [18,22] is a recently developed meshless boundary collocation method. It retains the merits of both the indirect BEM and the MFS. The main idea is to fully appropriate the dimensionality reduction and stability superiorities of the BEM and the meshless and integration-free merits of the MFS. In addition, the SBM can skillfully avoid the fictitious boundary issue in the MFS.

In recent years, the SBM has been successfully applied to elasticity [23], Stokes flow [24], and poroelastic wave [25] problems, just to mention a few. These applications show that the method

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Nomenclature

A_{ij}	matrix elements	q_{ii}	origin intensity factors on the Neumann boundary
C	concentration	u_{ii}	origin intensity factors on the Dirichlet boundary
D	diffusion coefficient	u^*	fundamental solution
H	Heaviside step function	$\boldsymbol{v}$	convective velocity
n	spatial dimension number	Δl	space increment
$\boldsymbol{n}$	unit outward normal vector	Δt	time increment
N_1	number of interior source points	$\mathcal{F}_x$	Fourier transform
N_2	number of boundary source points	$\mathcal{F}_\alpha^{-1}$	inverse Fourier transform
N	total number of source points	γ	Euler constant
Pe	Peclet number	ϑ	angle
q	flux	$\boldsymbol{\alpha}$	undetermined coefficient vector

is mathematically simple, easy-to-program, truly boundary-only, free of integration, mesh and fictitious boundary. Nevertheless, most studies involve the steady-state fundamental solutions rather than time-dependent fundamental solutions. When the steady-state fundamental solutions are used in the SBM to approximate the transient convection-diffusion problems, other techniques such as the finite difference scheme and the DRM should be employed to approximate the solution's functional dependence on the temporal variables.

This paper derives the time-dependent fundamental solution of transient convection-diffusion problems, and then develops an SBM formulation using that fundamental solution to solve the transient convection-diffusion problems. With the help of the integral average and surface fitting, the accurate calculation formulas are obtained to determine origin intensity factors (OIFs) in the SBM. Compared with the steady-state fundamental solution scheme, the present scheme is truly semi-analytical and boundary-only. Moreover, the proposed SBM formulation has clear physical meaning and does not need additional techniques such as the Laplace transform, the finite difference method, or the dual reciprocity method to handle the time-derivative term.

A brief outline of the rest of this paper is as follows. Section 2 derives the time-dependent fundamental solution of convection-diffusion equations, followed in Section 3 by a description of the SBM formulation using the time-dependent fundamental solutions. Section 4 compares and discusses the results of the present numerical scheme with the analytical results for the tested cases. Finally, some conclusions and remarks are provided in Section 5.

2. Time-dependent fundamental solution of convection-diffusion equations

Consider the following time-dependent convection-diffusion equation in a closed domain Ω bounded by $\partial\Omega = \Gamma$:

$$\frac{\partial C(\boldsymbol{x},t)}{\partial t} + \boldsymbol{v}\cdot\nabla C(\boldsymbol{x},t) = D\nabla^2 C(\boldsymbol{x},t), \quad \boldsymbol{x}\in\Omega, \tag{1}$$

where $\Omega \subset \boldsymbol{R}^n$, n denotes the spatial dimension number, $\boldsymbol{x}\in\boldsymbol{R}^n$ the general spatial coordinate, t the time, $\boldsymbol{v} = (v_1, v_2 \ldots, v_n)$ the convective velocity, and D the diffusion coefficient. The initial condition of the convection-diffusion problem is

$$C(\boldsymbol{x}, t=0) = \hat{C}_0(\boldsymbol{x}), \quad \boldsymbol{x}\in\Omega, \tag{2}$$

with the following Dirichlet and Neumann boundary conditions

$$\begin{aligned} &C(\boldsymbol{x},t) = \hat{C}(\boldsymbol{x},t), \quad \boldsymbol{x}\in\Gamma_D, \\ &\tfrac{\partial C(\boldsymbol{x},t)}{\partial \boldsymbol{n}} = \hat{q}(\boldsymbol{x},t), \quad \boldsymbol{x}\in\Gamma_N, \end{aligned} \tag{3}$$

where $\Gamma_D \cup \Gamma_N = \Gamma$, $\Gamma_D \cap \Gamma_N = \varnothing$, and $\boldsymbol{n}$ is the unit outward normal vector. $\hat{C}_0(\boldsymbol{x})$, $\hat{C}(\boldsymbol{x},t)$, and $\hat{q}(\boldsymbol{x},t)$ are specified functions.

Assuming that convective velocity $\boldsymbol{v}$ and diffusivity D are constant, we have an exponential variable transformation [26,27]:

$$C(\boldsymbol{x},t) = e^{\boldsymbol{v}\cdot\boldsymbol{r}/2D} w(\boldsymbol{x},t), \tag{4}$$

where $w(\boldsymbol{x}, t)$ is an intermediate field variable, and $\boldsymbol{r}$ represents the distance vector between the field point $\boldsymbol{x}$ and source point ξ. Using this transformation, Eq. (1) can be rewritten as:

$$D\nabla^2 w(\boldsymbol{x},t) - \beta w(\boldsymbol{x},t) = \frac{\partial w(\boldsymbol{x},t)}{\partial t}, \tag{5}$$

where $\beta = |\boldsymbol{v}|^2/4D$.

To determine the fundamental solution $w^*(\boldsymbol{x},t)$ for the above differential Eq. (5), we refer to Section 3.1 in Ref. [28], such that

$$\frac{\partial w^*}{\partial t} - D\nabla^2 w^* + \beta w^* = \delta(\boldsymbol{x},t). \tag{6}$$

Applying the Fourier transform $\mathcal{F}_x$ to both sides of Eq. (6), we have

$$\mathcal{F}_x\left(\frac{\partial w^*}{\partial t}\right) - D\mathcal{F}_x(\nabla^2 w^*) + \beta\mathcal{F}_x(w^*) = \mathcal{F}_x(\delta(\boldsymbol{x},t)). \tag{7}$$

According to the properties of Fourier transform, we have

$$\mathcal{F}_x(\delta(\boldsymbol{x},t)) = \mathcal{F}_x(\delta(\boldsymbol{x})\cdot\delta(t)) = \mathcal{F}_x[\delta](\alpha)\cdot\delta(t) = 1(\alpha)\cdot\delta(t), \tag{8}$$

$$\mathcal{F}_x\left(\frac{\partial w^*}{\partial t}\right) = \frac{\partial}{\partial t}\mathcal{F}_x(w^*), \tag{9}$$

$$\mathcal{F}_x(\nabla^2 w^*) = -|\alpha|^2\mathcal{F}_x(w^*). \tag{10}$$

If we denote $\mathcal{F}_x(w^*)(\alpha,t)$ by $\widehat{w}^*(\alpha,t)$, then

$$\frac{\partial \widehat{w}^*}{\partial t} + (D|\alpha|^2 + \beta)\widehat{w}^* = 1(\alpha)\cdot\delta(t), \tag{11}$$

which has the solution

$$\widehat{w}^*(\alpha,t) = H(t)e^{-(D|\alpha|^2+\beta)t}. \tag{12}$$

where $H(t)$ is the Heaviside step function [28]. Applying the inverse Fourier transform $\mathcal{F}_\alpha^1$, we can obtain the fundamental solution of Eq. (5)

$$\begin{aligned} w^*(\boldsymbol{x},t) = \mathcal{F}_\alpha^{-1}[\widehat{w}^*(\alpha,t)] &= \frac{H(t)\cdot e^{-\beta t}}{(2\pi)^n}\int_{R^n} e^{-D|\alpha|^2 t - i(\alpha\cdot\boldsymbol{x})}d\alpha \\ &= \frac{H(t)}{(4\pi Dt)^{n/2}}e^{-|\boldsymbol{x}|^2/4Dt-\beta t}. \end{aligned} \tag{13}$$

Then, we can easily get the time-dependent fundamental solution of the convection-diffusion equation via Eq. (4)

$$u^* = \frac{H(t)}{(4\pi Dt)^{n/2}}e^{-|\boldsymbol{r}|^2/4Dt+\boldsymbol{v}\cdot\boldsymbol{r}/2D-|\boldsymbol{v}|^2 t/4D}. \tag{14}$$