

## Article

# Fully Transient Analytical Solutions for Organic Contaminant Transport Through GMB/CCL and GMB/GCL Composite Liners Considering Advection, Degradation and Thermodiffusion for Sustainable Mitigation

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## Abstract

This paper presents fully transient analytical solutions for organic contaminant transport through composite liner systems consisting of a geomembrane (GMB) underlain by either a compacted clay liner (CCL) or a geosynthetic clay liner (GCL). The proposed solutions simultaneously account for three key mechanisms, namely advection due to GMB defects and wrinkles, first-order degradation, and thermodiffusion induced by temperature gradients. The solutions provide steady-state temperature distribution, transient contaminant concentration profiles, mass flux, and cumulative mass outflow at the base of the liner. The analytical solutions are rigorously verified against experimental thermodiffusion data from the literature, an existing analytical solution, and a numerical model using COMSOL Multiphysics 5.4. A parametric study is conducted to investigate the effects of thermodiffusion, Soret coefficient, and thermal conductivity on benzene transport. Results show that thermodiffusion substantially increases benzene outflow; neglecting it may lead to unconservative liner design. The benzene transport rate increases almost linearly with the Soret coefficient. The thermal conductivity of the GMB and GCL significantly affects benzene transport in the GMB/GCL system, while the thermal conductivities of the GMB and CCL have negligible effects on the GMB/CCL system. The proposed analytical solutions enable rapid parametric analysis, preliminary liner design, environmental risk assessment, and early warning. By enabling rapid comparison of GMB/CCL versus GMB/GCL systems (material selection), optimization of clay layer thickness for required breakthrough time (thickness optimization), and quantification of thermal effects on contaminant flux (temperature control), the solutions serve as an efficient tool for sustainable liner design.

**Keywords:** composite liners; geomembrane; geosynthetic clay liner; thermodiffusion; analytical solutions; sustainable design

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## 1. Introduction

Bottom liner systems consisting of a geomembrane (GMB) underlain by either a compacted clay liner (CCL) or a geosynthetic clay liner (GCL) are widely used in modern municipal solid waste landfills to isolate waste and leachate from the surrounding environment [1–3]. Although such GMB-based composite liners are effective, organic contaminants can still diffuse through intact GMBs [4,5]. Moreover, defects and wrinkles are commonly present in GMBs even under strict construction quality assurance programs [6,7]. Advection through these defects can significantly enhance contaminant migration, especially when a high leachate head and many defects exist [8–11]. In addition, degradation has been recognized as a key attenuation process for organic contaminants in clay liners [12–14].

Numerous analytical and numerical models have been developed to predict organic contaminant transport in liner systems considering molecular diffusion, advection, and degradation [9–11,15–17]. However, most of these studies have been conducted under isothermal conditions, neglecting the fact that landfills often experience elevated temperatures due to waste degradation or hydration of incinerated ash. Temperatures in landfill liners can reach 50–70 °C [18–20] and even up to 80 °C in mining applications [21]. Such thermal gradients induce thermodiffusion (Soret effect), which can drive additional contaminant mass flux comparable to molecular diffusion [22–23]. Experimental evidence has confirmed that thermodiffusion enhances solute transport in compacted clays [23]. Therefore, a reliable assessment of liner performance must account for the combined effects of advection through GMB defects, degradation, and thermodiffusion.

In recent years, several studies have incorporated thermodiffusion into analytical models for liner systems. Xie et al. [24] presented an analytical model for chemical diffusion under thermal effects in semi-infinite porous media. Yan et al. [25] derived analytical solutions for thermally induced diffusion under steady-state heat transfer. Peng et al. [26] developed an analytical model for organic contaminant transport through a GMB/CCL composite liner, including thermodiffusion but without considering GMB defects or degradation. More recently, Qiu et al. [27] proposed analytical solutions for a GMB/GCL/CCL triple-layer liner under non-isothermal conditions, accounting for temperature-dependent diffusion and partition coefficients; nevertheless, advection due to GMB defects was neglected. Qiu et al. [28] provided analytical solutions for a GMB/CCL composite liner that incorporated GMB defects, effective porosity, and thermodiffusion, but degradation was not included. Meanwhile, numerical solutions capable of handling transient heat transfer and temperature-dependent properties (e.g., [29,30]) have been developed, but they are not as convenient for rapid parametric studies or for use as benchmarking tools.

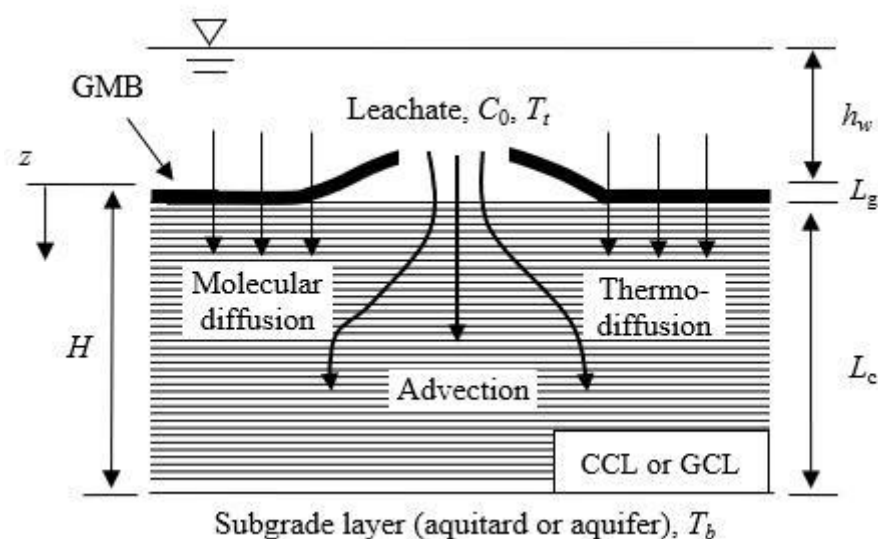
However, no analytical solution has been reported that simultaneously considers (i) advection due to GMB defects/wrinkles, (ii) first-order degradation, and (iii) thermodiffusion in a unified framework covering both GMB/CCL and GMB/GCL composite liners. Furthermore, most existing analytical solutions are limited to steady-state approximations, which cannot capture the transient evolution of contaminant concentration, mass flux, and cumulative outflow. These transient characteristics are key information for liner design and breakthrough time assessment.

This paper fills the above gap by presenting fully transient analytical solutions for organic contaminant transport through GMB-based composite liners (GMB/CCL and GMB/GCL), considering the combined effects of advection, degradation, and thermodiffusion. The proposed solutions account for the presence of GMB defects and wrinkles, and they provide both temperature distribution (steady-state heat conduction) and transient contaminant concentration profiles, mass flux, and cumulative mass outflow at the base of the liner. Two common bottom boundary conditions (zero-concentration and zero-concentration-gradient) are considered, which bracket the realistic range of subgrade

conditions. The analytical solutions are rigorously verified against experimental thermodiffusion data, an existing analytical solution, and a numerical model using COMSOL Multiphysics. Using the verified solutions, a parametric study is performed to investigate the effects of thermodiffusion, Soret coefficient, and thermal conductivity on benzene transport. The results highlight the importance of including thermodiffusion in performance assessments. Furthermore, the solutions enable rapid evaluation of alternative liner configurations, supporting the selection of eco-friendly designs that minimize material consumption while maintaining containment performance. This capability contributes to environmental risk assessment and sustainable mitigation of pollution caused by contaminant leakage from landfills.

## 2. Mathematical Model

Figure 1 presents the configuration of the composite liner system consisting of two individual layers, i.e., from top to bottom, a geomembrane (GMB) and a clay layer (denoted as CL, which can be either a CCL or a GCL), with an aquitard or aquifer underlying the CL. The CL is assumed to be non-deformable, homogeneous, and fully saturated. The thicknesses of the GMB and CL are  $L_g$  and  $L_c$ , respectively, and the total thickness  $H = L_g + L_c$ , with the vertical coordinate  $z$  directed downward from the top of the GMB. The hydraulic leachate head is  $h_w$ . The concentration of organic contaminant contained in the leachate is  $C_0$ , which is assumed to be sufficiently dilute and could not change the properties of CL [31,32]. Because defects and wrinkles are commonly found in GMBs used for landfill liners, the GMB is assumed to contain wrinkles and defects in this study; consequently, advection plays a role in driving organic contaminant transport in the liner system. The temperature on the top and bottom of the GMB/CL liner system are  $T_t$  and  $T_b$ , respectively, which will produce a temperature gradient and generate contaminant thermodiffusion.



**Figure 1.** Configuration of GMB/CL composite liner system. (Solid Horizontal Lines: Denote physical boundaries and material interfaces. Triangular Symbol (▽): Indicates the free leachate surface (upper hydraulic boundary). Double-Headed Vertical Arrows: Indicate dimensional measurements. Vertical/Curved Flux Arrows: Represent mass and heat transport pathways.).

The governing equation for organic contaminant transport through the GMB, considering advection, molecular diffusion, and thermodiffusion, can be expressed as [10,11,24]

$$\frac{\partial C_g(z,t)}{\partial t} = D_g \frac{\partial^2 C_g(z,t)}{\partial z^2} - v_a \frac{\partial C_g^{\text{hole}}(z,t)}{\partial z} + \frac{\partial}{\partial z} \left( D_{Tg} \frac{\partial T}{\partial z} \right) \quad (1)$$

where  $C_g(z,t)$  is the concentration of organic contaminant in the GMB;  $D_g$  is the effective diffusion coefficient of organic contaminant in the GMB;  $v_a$  is Darcy velocity of the leakage flow through the composite liner;  $T$  is the temperature;  $D_{Tg}$  is the thermodiffusion coefficient of organic contaminant in the GMB, and  $D_{Tg} = C_g(z,t) S_T D_g$ ;  $S_T$  is the Sorret coefficient, which is defined as the ratio of the thermodiffusion coefficient to the molecular diffusion coefficient [24];  $D_g$  is the effective diffusion coefficient of organic contaminant in the GMB;  $C_g^{\text{hole}}(z,t)$  is the concentration of organic contaminant in the flow through the holes in GMB, and  $C_g^{\text{hole}}(z,t) = C_g(z,t) / K_g$  [10]; and  $K_g$  is the partition coefficient for the organic contaminant and GMB. According to Park and Nibras [33], the sorption between organic contaminant and GMB can be assumed to follow a linear, equilibrium sorption isotherm for low concentrations (<100 mg/L). According to Rowe et al. [34], the  $D_g$  and  $K_g$  are changed with different temperatures, and can be obtained by

$$D_g = D_g(T_r) \theta_{dg}^{(T-T_r)} \quad (2)$$

$$K_g = K_g(T_r) \theta_{kg}^{(T-T_r)} \quad (3)$$

where  $D_g(T_r)$  and  $K_g(T_r)$  are the effective diffusion coefficient and partition coefficient at a reference temperature  $T_r$ , respectively;  $\theta_{dg}$  and  $\theta_{kg}$  are the constant temperature coefficients for  $D_g$  and  $K_g$ , respectively. The explicit solution to Equation (1) is difficult to obtain because of the variable coefficients. In this study, the  $D_g$  and  $K_g$  are assumed to be the average value in the GMB for simplified.

Similarly, organic contaminant transport in the CL, considering molecular diffusion, advection, degradation, and thermodiffusion, can be expressed as [10,11,24]

$$\frac{\partial C_c(z,t)}{\partial t} = \frac{D_c}{R_{dc}} \frac{\partial^2 C_c(z,t)}{\partial z^2} - \frac{v_c}{R_{dc}} \frac{\partial C_c(z,t)}{\partial z} + \frac{1}{R_{dc}} \frac{\partial}{\partial z} \left( D_{Tc} \frac{\partial T}{\partial z} \right) - \lambda C_c(z,t) \quad (4)$$

where  $C_c(z,t)$  is the contaminant concentration in the CL;  $D_c$  is the effective diffusion coefficient of the organic contaminant in the CL;  $v_c$  is the seepage velocity in CL and is calculated as  $v_c = v_a / n_c$ ,  $n_c$  is the porosity of the CCL;  $D_{Tc}$  is the thermodiffusion coefficient of the organic contaminant in the CCL, and  $D_{Tc} = C_c(z,t) S_T D_c$ ;  $\lambda$  is the first-order degradation constant for dissolved organic contaminant masses in the pore water of CL and is assumed to be calculated as  $\lambda = \ln(2) / t_{1/2}$ ,  $t_{1/2}$  is the organic contaminant half-life in CL; and  $R_{dc}$  is the retardation factor and can be obtained by

$$R_{dc} = 1 + \frac{\rho_{dc} K_{dc}}{n_c} \quad (5)$$

where  $\rho_{dc}$  and  $K_{dc}$  are, respectively, the dry density and distribution coefficient of the CL. The effective diffusion coefficient  $D_c$  and distribution coefficient  $K_{dc}$  are reported

to change with different temperatures [7,35], which are neglected in this study for simplicity, and this is the limitation of the proposed analytical model.

One-dimensional heat conduction in the GMB/CL is assumed to be at steady state. Under this assumption, the general solution to the governing equation of one-dimensional heat conduction is

$$T_g = A_g z + B_g \quad (6)$$

$$T_c = A_c z + B_c \quad (7)$$

where  $T_g$  and  $T_c$  are the temperature in the GMB and CL, respectively;  $A_g$  and  $A_c$  are proportionality constants about the temperature distribution of GMB and CL, respectively; and  $B_g$  and  $B_c$  are coefficients to be determined by the temperature boundary conditions.

According to Bouazza et al. [36], the heat flux,  $Q_T$ , in the GMB/CCL composite liner can be expressed as

$$Q_T = -\kappa \nabla T + C_p v_a \rho_w (T - T_r) \quad (8)$$

where  $\kappa$  is the thermal conductivity;  $\Delta T$  is the temperature gradient;  $C_p$  is the specific heat capacity of liquid;  $\rho_w$  is the density of liquid; and  $T_r$  is the reference temperature.

Substituting Equations (6) and (7) into Equations (1) and (4), the governing equation of  $C_g(z, t)$  and  $C_c(z, t)$  can be reformulated as

$$\frac{\partial C_g(z, t)}{\partial t} = D_g \frac{\partial^2 C_g(z, t)}{\partial z^2} - \left( \frac{v_a}{K_g} - A_g S_T D_g \right) \frac{\partial C_g(z, t)}{\partial z} \quad (9)$$

$$\frac{\partial C_c(z, t)}{\partial t} = \frac{D_c}{R_{dc}} \frac{\partial^2 C_c(z, t)}{\partial z^2} - \left( \frac{v_c}{R_{dc}} - \frac{A_c S_T D_c}{R_{dc}} \right) \frac{\partial C_c(z, t)}{\partial z} - \lambda C_c(z, t) \quad (10)$$

The Darcy velocity of the leakage flow through the composite liner  $v_a$  can be determined from the leakage rate through the GMB defects. The leakage rate through a single hole in the composite liner is given by [1,37]

$$Q = \frac{2h_w L_w}{H} (kb + \sqrt{kl\theta}) \quad (11)$$

where  $L_w$  is the length of wrinkle;  $2b$  is the width of wrinkle;  $\theta$  is the transmissivity of the interface between GMB and CL; and  $k$  is the hydraulic conductivity of CL.  $v_a$  can then be obtained by [8,16,38]

$$v_a = m_h Q / A_0 \quad (12)$$

where  $m_h$  is the number of the defects in GMB per unit area;  $A_0$  is the cross-sectional area of the flow.

The leakage rate  $Q$  in Equation (11) adopts the analytical solution developed by Rowe [1] to predict the leakage rate of leachate flow through a single hole of GMB coincident with a wrinkle. This leakage solution agrees well with the results of numerical analysis [37], and has been widely used by researchers to evaluate contaminant transport in liner systems [10,28,29]. According to El-Zein and Rowe [39], one-dimensional predictions of leakage and transport can provide reasonable estimates of contamination in most cases.

It should be noted that the effect of wrinkles is accounted for through the geometric parameters  $L_w$  and  $2b$  in Equation (11), rather than by artificially increasing the number of defects  $m_h$  in Equation (12).

The initial concentrations of the contaminant in GMB and CL are assumed to be  $h_g(z)$  and  $h_c(z)$ , respectively, and therefore, the initial condition of the GMB and CL can be given as

$$C_g(z, t = 0) = h_g(z) \quad (13)$$

$$C_c(z, t = 0) = h_c(z) \quad (14)$$

The top boundary condition for the GMB/CCL composite liner system is [40]:

$$C_g(z, t) \Big|_{z=0} = K_g C_0 \quad (15)$$

The continuity conditions in terms of the contaminant concentration and mass flux at the interface between GMB and CL are

$$C_g(z, t) \Big|_{z=L_g} = K_c C_c(z, t) \Big|_{z=L_g} \quad (16)$$

$$\begin{aligned} & \left( v_a / K_g - A_g S_T D_g \right) C_g(z, t) \Big|_{z=L_g} - D_g \frac{\partial C_g(z, t)}{\partial z} \Big|_{z=L_g} = \\ & \left( v_c n_c - A_c S_T D_c n_c \right) C_c(z, t) \Big|_{z=L_g} - n_c D_c \frac{\partial C_c(z, t)}{\partial z} \Big|_{z=L_g} \end{aligned} \quad (17)$$

where  $K_c$  is the partition coefficient between GMB and CCL.

Two different bottom boundary conditions are considered: (1) a zero-concentration boundary (ZC), and (2) a zero-concentration-gradient (ZCG) boundary, expressed, respectively, as

$$C_c(z, t) \Big|_{z=H} = 0 \quad (18)$$

$$\frac{\partial C_c(z, t)}{\partial z} \Big|_{z=H} = 0 \quad (19)$$

The ZC and ZCG conditions bracket the range of possible subgrade conditions [10,11]. The ZC condition corresponds to a highly permeable subgrade (e.g., an active aquifer), providing an upper-bound estimate of contaminant flux, while the ZCG condition corresponds to a low-permeability subgrade (e.g., bedrock or an aquitard), providing a lower-bound estimate. The choice between them for practical applications should be guided by site-specific hydrogeological conditions. Mixed or transition boundaries, though potentially more refined, are not considered, as they would significantly complicate the analytical solution.

### 3. Analytical Solutions

#### 3.1. Steady-State Analytical Solutions

Separating  $C_g(z, t)$  and  $C_c(z, t)$  into two parts:

$$C_g(z, t) = w_g(z, t) + u_g(z) \quad (20)$$

$$C_c(z, t) = w_c(z, t) + u_c(z) \quad (21)$$

Substituting Equations (20) and (21) into Equations (9) and (10), respectively, leads to the governing equation and boundary conditions of  $u_g(z)$  and  $u_c(z)$ . The  $u_g(z)$  and  $u_c(z)$  are the steady-state concentrations for GMB and CL, respectively, and are determined by the following equation:

$$D_g \frac{\partial^2 u_g(z)}{\partial z^2} - \left( \frac{v_a}{K_g} - A_g S_T D_g \right) \frac{\partial u_g(z)}{\partial z} = 0 \quad (22)$$

$$\frac{D_c}{R_{dc}} \frac{\partial^2 u_c(z)}{\partial z^2} - \left( \frac{v_c}{R_{dc}} - \frac{A_c S_T D_c}{R_{dc}} \right) \frac{\partial u_c(z)}{\partial z} - \lambda u_c(z) = 0 \quad (23)$$

The top boundary condition for Equations (22) and (23) is

$$u_g(z) \Big|_{z=0} = K_g C_0 \quad (24)$$

The continuity conditions at the interface between GMB and CL are

$$u_g(z) \Big|_{z=L_g} = K_c u_c(z) \Big|_{z=L_g} \quad (25)$$

$$\begin{aligned} & \left( v_a / K_g - A_g S_T D_g \right) u_g(z) \Big|_{z=L_g} - D_g \frac{\partial u_g(z)}{\partial z} \Big|_{z=L_g} \\ &= \left( v_c n_c - A_c S_T n_c D_c \right) u_c(z) \Big|_{z=L_g} - n_c D_c \frac{\partial u_c(z)}{\partial z} \Big|_{z=L_g} \end{aligned} \quad (26)$$

The bottom boundary conditions for Equations (22) and (23) are

$$u_c(z) \Big|_{z=H} = 0 \quad (27)$$

$$\frac{\partial u_c(z)}{\partial z} \Big|_{z=H} = 0 \quad (28)$$

The general solution to Equations (22) and (23) are

$$u_g(z) = E_1 \exp \left[ \frac{v_a - A_g S_T D_g K_g}{D_g K_g} z \right] + F_1 \quad (29)$$

$$u_c(z) = E_2 \exp(r_1 z) + F_2 \exp(r_2 z) \quad (30)$$

where  $E_1$  to  $F_2$  are coefficients that can be obtained by substituting Equations (29) and (30) into Equations (24) to (26) and Equation (27) or Equation (28);  $r_1$  and  $r_2$  are determined by

$$r_{1,2} = \frac{(v_c - A_c S_T D_c) \pm \sqrt{(v_c - A_c S_T D_c)^2 + 4 \lambda_c D_c R_{dc}}}{2 D_c} \quad (31)$$

The steady-state mass flux,  $J_{ss}$ , at the bottom boundary can be obtained as follows:

$$J_{ss} = \begin{cases} -n_c D_c (E_2 r_1 \exp(r_1 H) + F_2 r_2 \exp(r_2 H)) & \text{for ZC boundary condition} \\ (v_a - A_g S_T n_c D_c) (E_2 \exp(r_1 H) + F_2 \exp(r_2 H)) & \text{for ZCG boundary condition} \end{cases} \quad (32)$$

where “ZC” and “ZCG” represent the zero-concentration bottom boundary and zero-concentration-gradient bottom boundary, respectively.

### 3.2. Fully Transient Analytical Solutions

Substituting Equations (20) and (21) into Equations (9) and (10), respectively, leads to the governing equation of  $w_g(z, t)$  and  $w_c(z, t)$ :

$$\frac{\partial w_g(z, t)}{\partial t} = D_g \frac{\partial^2 w_g(z, t)}{\partial z^2} - \left( \frac{v_a}{K_g} - A_g S_T D_g \right) \frac{\partial w_g(z, t)}{\partial z} \quad (33)$$

$$\frac{\partial w_c(z, t)}{\partial t} = \frac{D_c}{R_{dc}} \frac{\partial^2 w_c(z, t)}{\partial z^2} - \left( \frac{v_c}{R_{dc}} - \frac{A_c S_T D_c}{R_{dc}} \right) \frac{\partial w_c(z, t)}{\partial z} - \lambda w_c \quad (34)$$

Similarly, substituting Equations (24) to (28) into Equations (15) to (19), respectively, leads to the boundary conditions and continuity conditions of  $w_g(z, t)$  and  $w_c(z, t)$ :

$$w_g(z, t)|_{z=0} = 0 \quad (35)$$

$$w_g(z, t)|_{z=L_g} = K_c w_c(z, t)|_{z=L_g} \quad (36)$$

$$\begin{aligned} & \left( v_a / K_g - A_g S_T D_g \right) w_g(z, t)|_{z=L_g} - D_g \frac{\partial w_g(z, t)}{\partial z} \bigg|_{z=L_g} \\ &= \left( v_c n_c - A_c S_T n_c D_c \right) w_c(z, t)|_{z=L_g} - n_c D_c \frac{\partial w_c(z, t)}{\partial z} \bigg|_{z=L_g} \end{aligned} \quad (37)$$

$$w_c(z, t)|_{z=H} = 0 \quad (38)$$

and

$$\frac{\partial w_c(z, t)}{\partial z} \bigg|_{z=H} = 0 \quad (39)$$

The initial conditions of Equations (33) and (34) can be obtained by substituting Equations (20) and (21) into Equations (13) and (14), respectively, and can be expressed as follows:

$$w_g(z, 0) = h_g(z) - u_g(z) \quad (40)$$

$$w_c(z, 0) = h_c(z) - u_c(z) \quad (41)$$

Based on the conditions and assumptions discussed above, the analytical solutions are derived to solve Equations (33) and (34) (see Appendix A). The analytical solutions to the governing Equations (33) and (34) are given as follows:

$$w_g(z, t) = \sum_{k=1}^{\infty} S_k f_{k,g}(z) \exp(a_g z - \delta_k t) \quad (42)$$

$$w_c(z, t) = \sum_{k=1}^{\infty} S_k f_{k,c}(z) \exp(a_c z - \delta_k t) \quad (43)$$

where

$$a_g = \frac{v_a - A_g S_T D_g K_g}{2 D_g K_g}, \quad a_c = \frac{v_c - A_c S_T D_c}{2 D_c} \quad (44)$$

$$f_{k,g}(z) = \begin{cases} H_k \sin(\xi_{k,g} z) & \text{when } \delta_k \geq \frac{(v_a - A_g S_T D_g K_g)^2}{4 D_g K_g^2} \\ H_k \sinh(\xi_{k,g} z) & \text{when } \delta_k < \frac{(v_a - A_g S_T D_g K_g)^2}{4 D_g K_g^2} \end{cases} \quad (45)$$

$$f_{k,c}(z) = \begin{cases} G_k \sin(\xi_{k,c} z) + Q_k \cos(\xi_{k,c} z) & \text{when } \delta_k \geq \frac{(v_c - A_c S_T D_c)^2}{4 D_c R_{dc}} + \lambda \\ G_k \sinh(\xi_{k,c} z) + Q_k \cosh(\xi_{k,c} z) & \text{when } \delta_k < \frac{(v_c - A_c S_T D_c)^2}{4 D_c R_{dc}} + \lambda \end{cases} \quad (46)$$

$$\xi_{k,g} = \sqrt{\left| \frac{\delta_k}{D_g} - a_g^2 \right|}, \quad \xi_{k,c} = \sqrt{\left| \frac{R_{dc} \delta_k}{D_c} - a_c^2 - \frac{R_{dc} \lambda}{D_c} \right|} \quad (47)$$

$$H_k = \frac{N_{3k} N_{7k} - N_{8k} N_{2k}}{N_{1k} N_{7k}} Q_k \quad (48)$$

$$G_k = -\frac{N_{8k}}{N_{7k}} Q_k \quad (49)$$

$$S_k = \frac{\int_0^{L_g} [h_g(z) - u_g(z)] f_{k,g}(z) \exp(-a_g z) dz + n_c R_{dc} \eta K_c \int_{L_g}^H [h_c(z) - u_c(z)] f_{k,c}(z) \exp(-a_c z) dz}{\int_0^{L_g} f_{k,g}^2(z) dz + n_c R_{dc} \eta K_c \int_{L_g}^H f_{k,c}^2(z) dz} \quad (50)$$

The values of  $\delta_k$  can be obtained by the following equation:

$$N_{7k} (N_{1k} N_{6k} - N_{3k} N_{4k}) + N_{8k} (N_{2k} N_{4k} - N_{1k} N_{5k}) = 0 \quad (51)$$

where the expressions of  $N_{1k}$  to  $N_{8k}$  are given in Appendix A.

The fully transient analytical solution to the governing Equation (1) can be obtained by substituting Equations (30) and (43) into Equation (21) as follows:

$$C_g(z, t) = E_1 \exp\left[\frac{v_a - A_g S_T D_g K_g}{D_g K_g} z\right] + F_1 + \sum_{k=1}^{\infty} S_k f_{k,g}(z) \exp(a_g z - \delta_k t) \quad (52)$$

Similarly, the fully transient analytical solution to the governing Equation (4) can be obtained by substituting Equations (30) and (43) into Equation (21) as follows:

$$C_c(z, t) = E_2 \exp(r_1 z) + F_2 \exp(r_2 z) + \sum_{k=1}^{\infty} S_k f_{k,c}(z) \exp(a_c z - \delta_k t) \quad (53)$$

The contaminant mass flux,  $J$ , at the base of the liner can be obtained as

$$J(z, t)|_{z=H} = (v_a - A_c S_T n_c D_c) C_c(z, t)|_{z=H} - n_c D_c \left. \frac{\partial C_c(z, t)}{\partial z} \right|_{z=H} \quad (54)$$

The cumulative mass outflow,  $M$ , at the base of the liner can be obtained as

$$M(z, t)|_{z=H} = (v_a - A_c S_T n_c D_c) \int_0^t C_c(z, \tau)|_{z=H} d\tau - n_c D_c \int_0^t \left. \frac{\partial C_c(z, \tau)}{\partial z} \right|_{z=H} d\tau \quad (55)$$

The infinite series in Equations (53) and (54) converges quickly, with errors smaller than 1%, 0.1%, and 0.01% when summing 5 terms, 10 terms, and 15 terms, respectively.

## 4. Model Verification

### 4.1. Comparisons with Experimental Results

Two thermodiffusion experiments in compact clays reported by Rosanne et al. [23] are used to validate the proposed analytical solution. Both experiments describe the transport of NaCl solution in a 2 mm thick compact clay with porosity  $n = 0.6$ . Although the present study focuses on organic contaminants, the proposed solution can also be used to analyze the transport of inorganic compounds. For experiment 1, the concentrations of NaCl solution on the top and bottom boundaries were  $1.01 \text{ mol/m}^3$  ( $C_t$ ) and  $9.14 \text{ mol/m}^3$  ( $C_b$ ), respectively, and the temperatures on the top and bottom boundaries were  $311 \text{ K}$  ( $T_t$ ) and  $285.1 \text{ K}$  ( $T_b$ ), respectively. For experiment 2, the values of  $C_t$ ,  $C_b$ ,  $T_t$  and  $T_b$  are  $1.21 \text{ mol/m}^3$ ,  $8.83 \text{ mol/m}^3$ ,  $284.8 \text{ K}$  and  $311.1 \text{ K}$ , respectively. According to Rosanne et al. [23], the effective diffusion coefficient of the compact clay for experiments 1 and 2 was  $1.7 \times 10^{-11} \text{ m}^2/\text{s}$  and  $6 \times 10^{-11} \text{ m}^2/\text{s}$ , respectively; these values were measured in pure diffusion tests without any thermal gradient. The Soret coefficients for experiments 1 and 2 were determined by inverse analysis using the measured concentration profile at  $t = 0.55 \text{ h}$  from the thermodiffusion experiments of Rosanne et al. [23], yielding values of  $-0.26$  and  $0.21 \text{ K}^{-1}$ , respectively. These values were not taken directly from Rosanne et al. [23], because their reported Soret coefficients were obtained under a numerical model with temperature-dependent diffusion coefficients, whereas the present analytical solution assumes constant coefficients evaluated at the average temperature. The same  $S_T$  values were then used to predict the concentration profiles at subsequent times ( $t = 0.83, 1.39$ , and  $2.22 \text{ h}$ ) without further adjustment.

The proposed analytical model does not consider a non-zero concentration at the bottom boundary; therefore, the boundary conditions are modified accordingly.

$$C_c(0, t) = C_t \quad (56)$$

$$C_c(H, t) = C_b \quad (57)$$

Based on the proposed analytical model, the analytical solution for the CCL is given as follows:

$$C_c(z, t) = E \exp(r_1 z) + F \exp(r_2 z) - \sum_{k=0}^{\infty} S_k \sin\left(\frac{k\pi z}{H}\right) \exp(a_c z - \delta_k t) \quad (58)$$

where

$$S_k = \frac{\int_0^H [h_c(z) - E \exp(r_1 z) - F \exp(r_2 z)] \sin\left(\frac{k\pi z}{H}\right) \exp(-a_c z) dz}{\int_0^H \sin^2\left(\frac{k\pi z}{H}\right) dz} \quad (59)$$

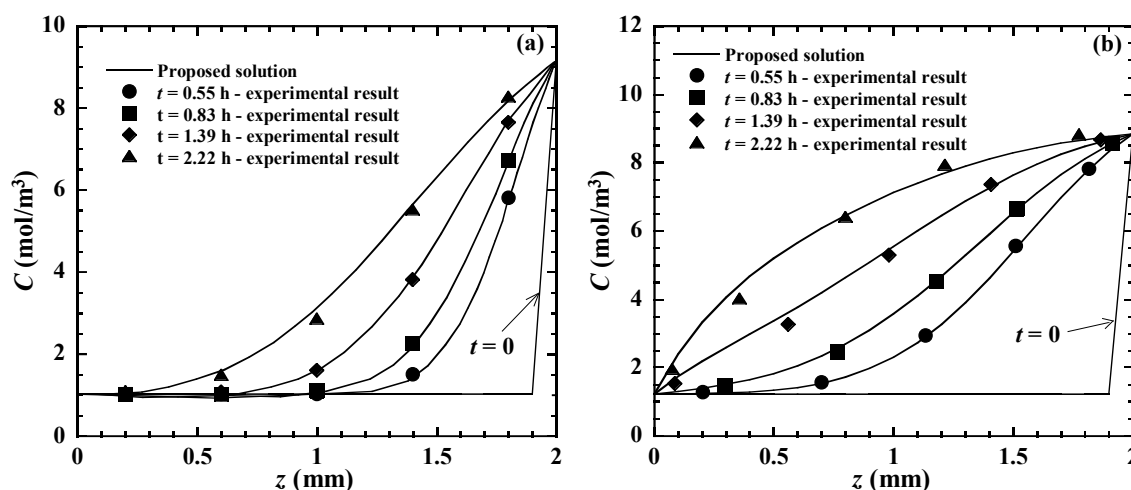
$$E + F = C_t \quad (60)$$

$$E \exp(r_1 H) + F \exp(r_2 H) = C_b \quad (61)$$

$$\delta_k = \frac{D_c}{R_{dc}} \frac{k^2 \pi^2}{H^2} + \frac{D_c a_c^2}{R_{dc}} + \lambda_c \quad (62)$$

Figure 2 compares the sodium chloride concentration profiles within the compact clay obtained from the proposed analytical solution with the experimental results of Rosanne et al. [23] at  $t = 0.55, 0.83, 1.39$  and  $2.22 \text{ h}$ . To quantitatively evaluate the agreement,

the root mean square error (RMSE) and coefficient of determination ( $R^2$ ) were calculated for each time instant as well as for the overall dataset. The results are summarized in Table 1, which confirms the excellent agreement between the proposed analytical solution and the experimental data.



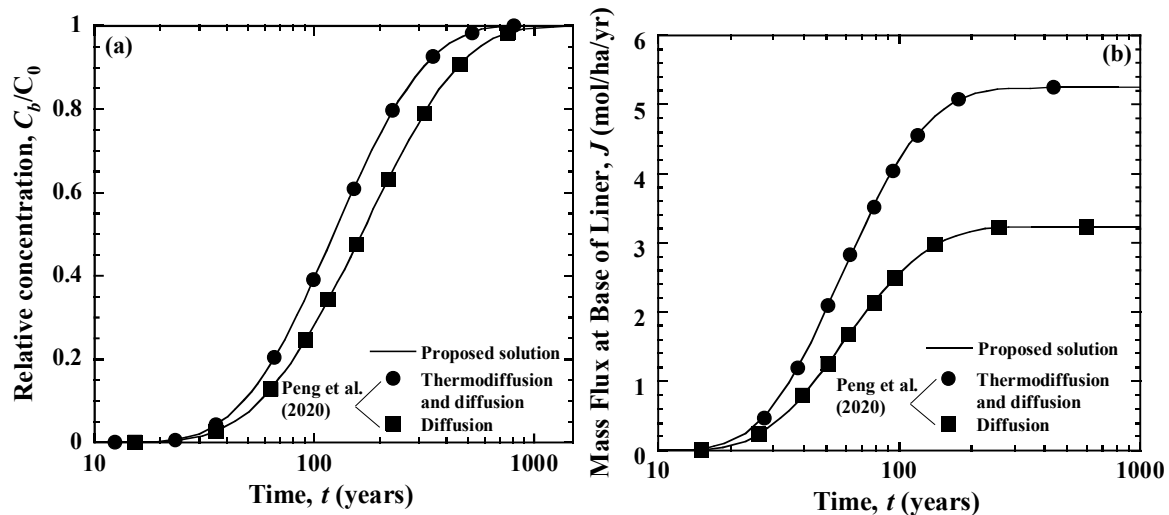
**Figure 2.** Comparison of sodium chloride concentration profile within the compact clay between the proposed analytical solution and the experimental results reported by Rosanne et al. [23]: (a) experiment 1, and (b) experiment 2.

**Table 1.** Quantitative comparison between the proposed analytical solution and experimental data of Rosanne et al. [23].

| Time $t$ (h) | Experiment 1               |         | Experiment 2               |         |
|--------------|----------------------------|---------|----------------------------|---------|
|              | RMSE (mol/m <sup>3</sup> ) | $R^2$   | RMSE (mol/m <sup>3</sup> ) | $R^2$   |
| 0.55         | 0.01507                    | 0.99995 | 0.02247                    | 0.99988 |
| 0.83         | 0.01478                    | 0.99995 | 0.01023                    | 0.99988 |
| 1.39         | 0.00777                    | 0.99999 | 0.00845                    | 0.99999 |
| 2.22         | 0.00344                    | 0.99999 | 0.26210                    | 0.98782 |
| Overall      | 0.01138                    | 0.99997 | 0.13172                    | 0.99633 |

#### 4.2. Comparisons with an Analytical Solution

In this section, a closed-form analytical solution for degradable organic contaminant transport through GMB/CCL composite liners presented by Peng et al. [26] is used to validate the proposed analytical solution. A hypothetical GMB/CCL composite liner system suggested by Peng et al. [26] is adopted here. The related parameters were given in Table 1 in Peng et al. [26]. The solution of Peng et al. [26] does not consider the defects and wrinkles occurred in GMB, so the seepage velocity is assumed to be zero in this section. The comparisons between the proposed analytical solution and the solution of Peng et al. [26] are presented in Figure 3, including (a) contaminant concentration at the base of the liner for the ZCG boundary condition, and (b) contaminant mass flux at the base of the liner for the ZC boundary condition. Two kinds of simulation were conducted with and without the effect of thermodiffusion. Figure 3 indicates that, for both boundary conditions, the proposed analytical solution is in excellent agreement with the analytical solution of Peng et al. [26].



**Figure 3.** Comparison between the proposed analytical solution and analytical solution of Peng et al. [26]: (a) contaminant concentration at the base of liner for ZCG boundary condition, and (b) contaminant mass flux at the base of liner for ZC boundary condition.

#### 4.3. Comparisons with a Numerical Model

To more comprehensively verify the proposed analytical solution, the contaminant mass flux profiles for the GMB/CCL and GMB/GCL composite liner systems calculated by the analytical solution are compared with those obtained from the finite-element software COMSOL Multiphysics 5.4. Benzene, a common organic contaminant in landfill leachates [41], is chosen as the representative contaminant. The leachate is assumed to contain a constant benzene concentration of  $100 \mu\text{g/L}$  [42]. The transport properties of Benzene for the GMB/CCL and GMB/GCL composite liner systems are presented in Table 2. The constant temperature coefficients  $\theta_{dg}$  and  $\theta_{kg}$  are 1.083 and 1.026, respectively [34].

In the COMSOL model, the GMB and CCL layers in the GMB/CCL system were discretized with 3 and 200 elements, respectively, while the GMB and GCL layers in the GMB/GCL system were discretized with 5 and 30 elements, respectively. A mesh refinement study confirmed that further refinement altered the results by less than 0.5%. The automatic Newton solver was used to solve the nonlinear system. The top boundary was set to a constant concentration  $C_g(0, t) = K_g C_0$ , and the bottom boundary was assigned as either ZC or ZCG, with flux continuity enforced at the GMB–clay interface.

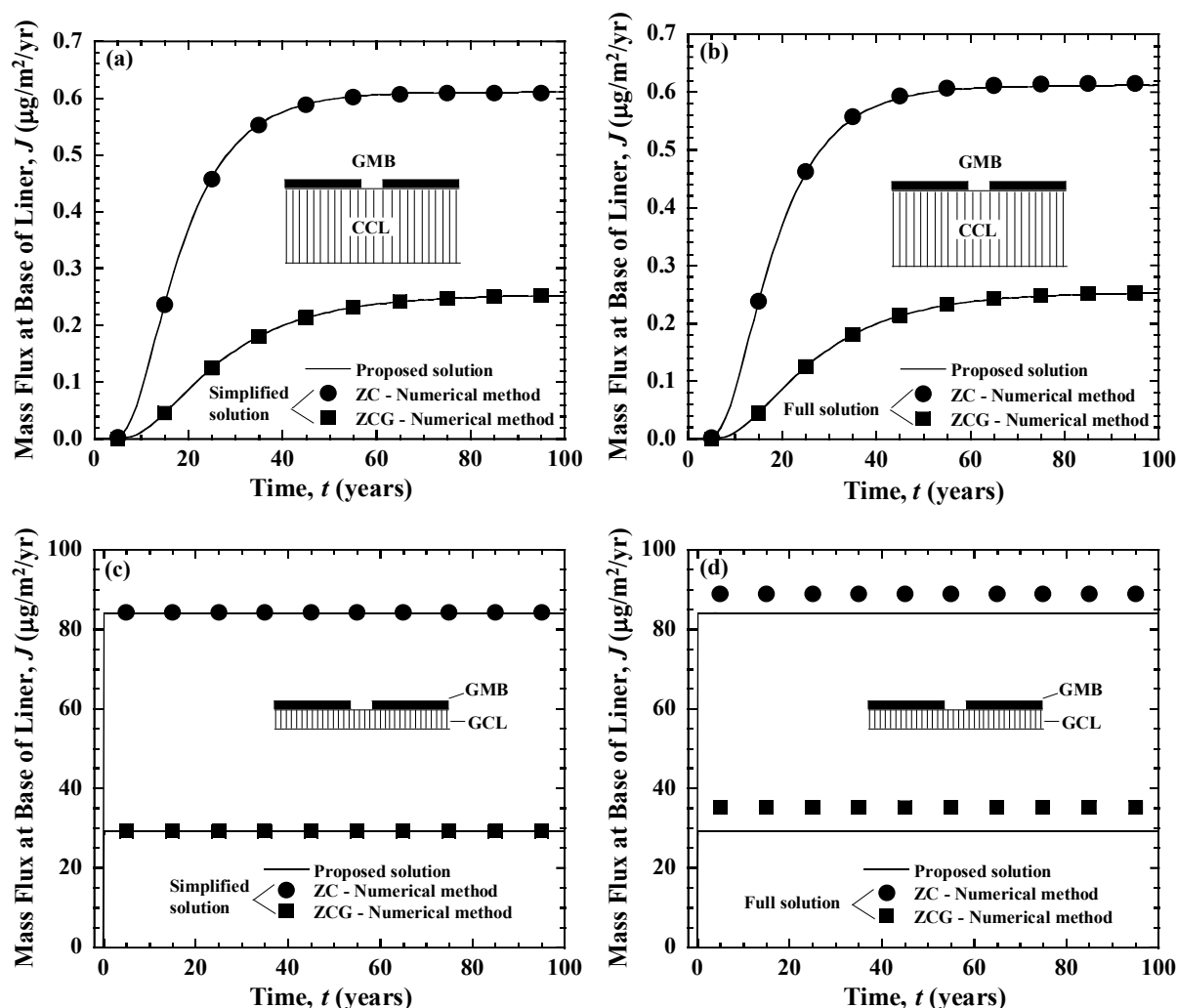
Two kinds of numerical results obtained by the COMSOL Multiphysics 5.4 are compared with the proposed analytical solution, which are presented in Figure 4. Figure 4a,c present the simplified numerical solution with the assumption of constant  $D_g$  and  $K_g$ , and Figure 4b,d present the full numerical solution with temperature-dependent  $D_g$  and  $K_g$ . Figure 4a,c show that, for both ZC and ZCG boundary conditions, the benzene mass flux curves from the proposed analytical solution agree closely with those from the simplified numerical model, confirming the accuracy of the analytical solution. For the GMB/CCL system (Figure 4a), the relative errors  $E_r$  between the analytical and numerical solutions are 0.19% and 0.28% for the ZC and ZCG boundary conditions, respectively. For the GMB/GCL system (Figure 4c), the corresponding errors are 0.19% and 0.05%, respectively.

Figure 4b shows that the proposed analytical solution can accurately predict contaminant transport in the GMB/CCL composite liner system even with constant  $D_g$  and  $K_g$ , yielding relative errors of 0.61% and 0.62% for the ZC and ZCG boundary conditions,

respectively. However, Figure 4d shows that the analytical solution predicts slightly lower mass fluxes than the full numerical solution for the GMB/GCL system, with relative errors  $E_r = 5.4\%$  and  $17.3\%$  for ZC and ZCG boundary conditions, respectively. The relative errors in the GMB/GCL system under both the ZC and ZCG conditions (Figure 4d) arise from the analytical simplification that  $D_g$  and  $K_g$  are assumed constant in the GMB, whereas the numerical solution accounts for their temperature dependence. This simplification introduces negligible error in the GMB/CCL system because the GMB thickness is only 0.15% of the CCL thickness. However, for the GMB/GCL system, the GMB thickness is 15% of the GCL thickness, making the error non-negligible. Overall, the analytical solution is sufficiently accurate for GMB/CCL systems under all conditions. For GMB/GCL systems, it captures the key trends and provides conservative estimates for preliminary design. For a final detailed design requiring high accuracy, the full numerical model with temperature-dependent properties is recommended.

**Table 2.** Benzene transport parameters for the GMB/CCL and GMB/GCL composite liner systems.

| Property                                                                              | GMB            | CCL            | GCL          |
|---------------------------------------------------------------------------------------|----------------|----------------|--------------|
| Thickness (m)                                                                         | 0.0015 [13,14] | 1 [13,14]      | 0.01 [13,14] |
| Effective diffusion coefficient at $T_r$ , $D$ ( $\times 10^{-13}$ m <sup>2</sup> /s) | 2.7 [34]       | 6000 [13,14]   | 3850 [43]    |
| Partition coefficient at $T_r$                                                        | 36 [34]        | 36 [34]        | 36 [34]      |
| Distribution coefficient at $T_r$ , $K_d$ (mL/g)                                      | -              | 0.5 [13,14]    | 4.4 [43]     |
| Porosity                                                                              | -              | 0.4 [44,45]    | 0.8 [46,47]  |
| Dry density, $\rho_d$ (kg/m <sup>3</sup> )                                            | -              | 1650 [13,14]   | 440 [13,14]  |
| Thermal conductivity, $K$ (W/mK)                                                      | 0.3 [48,49]    | 1.2 [26]       | 0.7 [36]     |
| Hydraulic conductivity, $k$ ( $\times 10^{-9}$ m/s)                                   | -              | 1 [10,11]      | 0.01 [13,14] |
| Length of the wrinkle, $L_w$ (m)                                                      | 200 [50,51]    | -              | -            |
| Width of the wrinkle, $2b$ (m)                                                        | 0.2 [50]       | -              | -            |
| Number of defects in GMB per unit area, $m_h$ (holes/ha)                              | 2.5 [52]       | -              | -            |
| Hydraulic leachate head, $h_w$ (m)                                                    |                | 0.3 [10,11]    |              |
| Interface transmissivity, $\theta$ ( $\times 10^{-8}$ m <sup>2</sup> /s)              |                | 5 [10,11]      |              |
| Half-life of benzene, $t_{1/2}$ (years)                                               |                | 20 [53]        |              |
| The temperature on the top of the liner, $T_t$ (K)                                    |                | 324.15 [7,54]  |              |
| The temperature on the top of the liner, $T_t$ (K)                                    |                | 284.15 [55,56] |              |
| The reference temperature, $T_r$ (K)                                                  |                | 295.15         |              |
| Soret coefficient, $S_T$ (K <sup>-1</sup> )                                           |                | 0.01 [23,57]   |              |



**Figure 4.** Comparison of benzene mass flux at the base of the liner between the proposed analytical solution and the COMSOL Multiphysics 5.4: (a) compared with simplified numerical solution for GMB/CCL composite liner system, (b) compared with full numerical solution for GMB/CCL liner system, (c) compared with simplified numerical solution for GMB/GCL composite liner system, and (d) compared with full numerical solution for GMB/GCL composite liner system.

## 5. Parametric Study

Based on the example in Section 4.3, the verified analytical solutions are used to investigate the effects of thermodiffusion, Soret coefficient, and thermal conductivity on benzene transport through the GMB/CL composite liner systems.

### 5.1. Effect of Thermodiffusion

Rowe [7,54] and Rowe and Hoor [19] reported that temperatures on the upper surface of landfill liners can range from 30 to 90 °C, while aquifer temperatures below the liner range from 5 to 25 °C [55,56]. Thus, the temperature difference  $\Delta T$  between the top and bottom boundaries can vary from 5 to 85 K. To illustrate the importance of considering thermodiffusion in the analysis of benzene transport through the GMB/CL liner system, Figure 5 presents the benzene mass flux  $J$  at the base of the liner for three different  $\Delta T$  ( $=0, 40$  and  $80$  K) under both ZC and ZCG conditions. The bottom temperature is kept constant at 284.15 K in all cases. Figure 5a,b present the  $J$  curves for GMB/CCL and GMB/GCL composite liner systems, respectively, and indicate that  $J$  increases with increasing  $\Delta T$  for both boundary conditions. For example, in the GMB/CCL system under the ZC

condition, the steady-state mass flux  $J_{ss}$  increases from 0.42 to 0.72  $\mu\text{g}/\text{m}^2/\text{year}$  (i.e., 71% increment) when  $\Delta T$  increases from 0 to 80 K. The GMB/GCL system exhibits much higher mass fluxes and a stronger temperature response than the GMB/CCL system because of its smaller total thickness. For all three  $\Delta T$  values, the ZC boundary condition yields higher  $J$  values and shorter breakthrough times than the ZCG condition, because advection is the only mechanism driving contaminant outflow under the ZCG condition.

To illustrate the effect of thermodiffusion in the presence of advection, Figure 6 shows the benzene mass flux under the ZC condition for three liner configurations: (i) GMB/CL with a damaged GMB (including defects and wrinkles), (ii) GMB/CL with an intact GMB, and (iii) CL alone (representing a heavily damaged or missing GMB). As expected, the mass fluxes increase significantly when the GMB is damaged or absent because advection becomes more dominant. For  $\Delta T = 40$  K,  $J_{ss}$  increases from 6.01  $\mu\text{g}/\text{m}^2/\text{year}$  for the GMB/GCL system to 117.16  $\mu\text{g}/\text{m}^2/\text{year}$  for the GCL alone. Figure 6a shows that when  $\Delta T$  increases from 0 to 40 K,  $J_{ss}$  increases by 57.7% for the intact GMB/CCL system, by 45.2% for the damaged GMB/CCL system, and by only 18.3% for the CCL alone. Thus, the relative effect of thermodiffusion decreases as advection becomes more important. Similar trends are observed in Figure 6b for GCL-based systems.

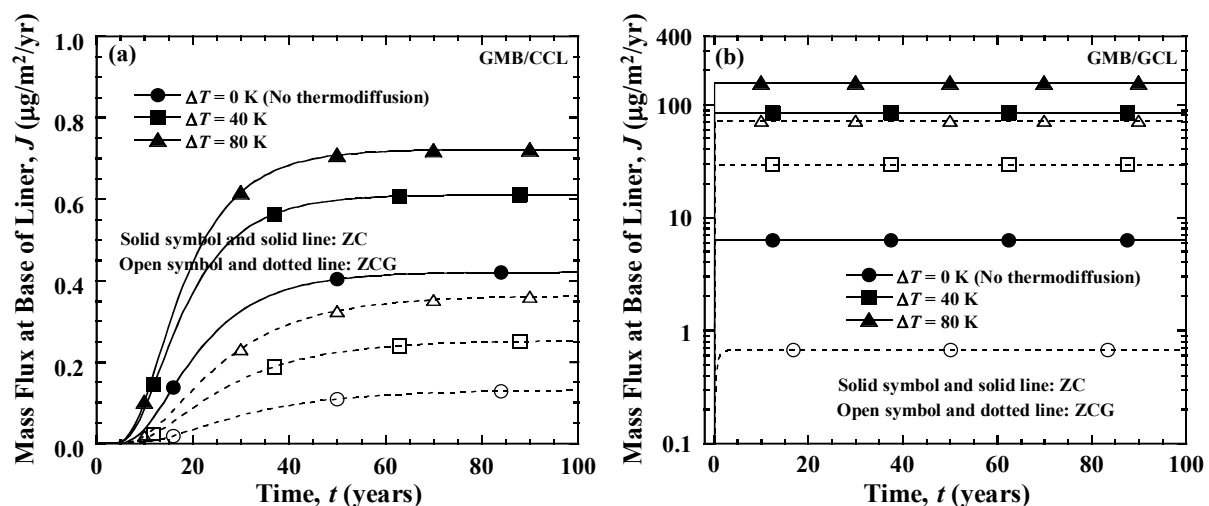
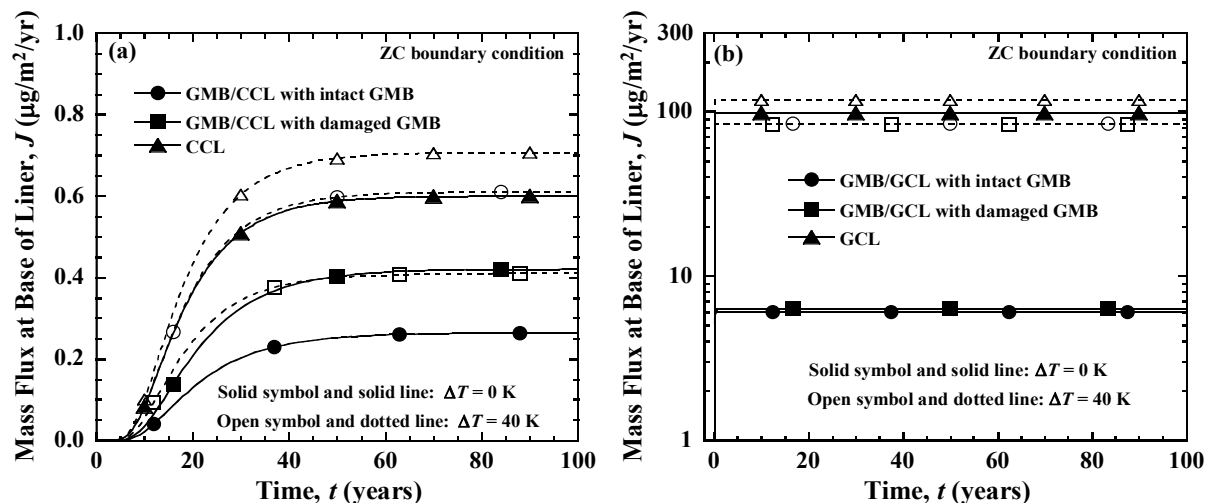


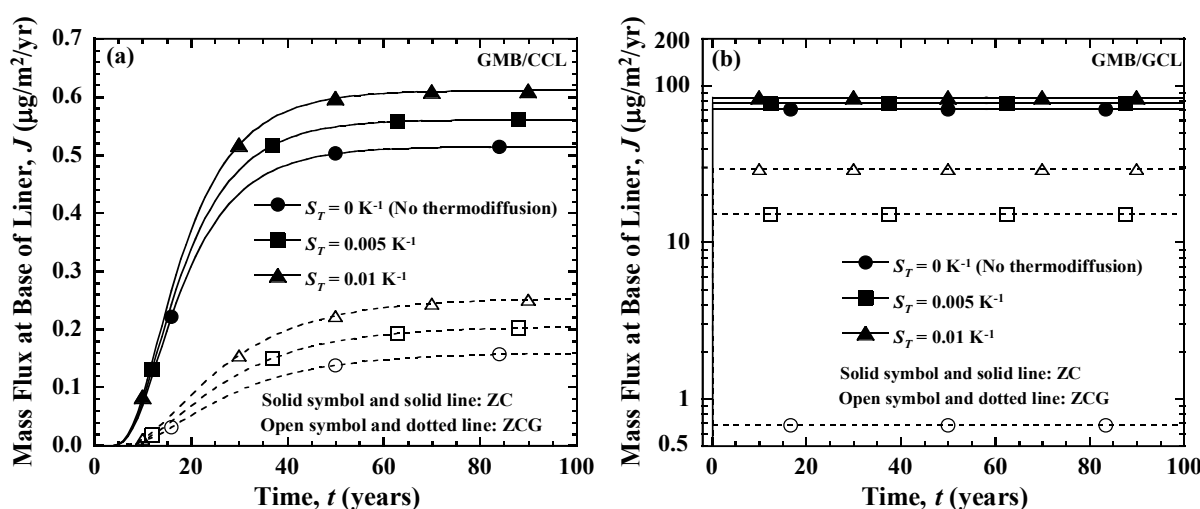
Figure 5. Benzene mass flux at the base of liner for different  $\Delta T$ : (a) GMB/CCL composite liner system, and (b) GMB/GCL composite liner system.



**Figure 6.** Benzene mass flux at the base of liner for different liner systems: (a) CCL-based liner systems, and (b) GCL-based liner systems.

### 5.2. Effect of Soret Coefficient

The Soret coefficient  $S_T$  has been reported to range from 0.005 to 0.05  $\text{K}^{-1}$  [23,57]. To illustrate the effect of the Soret coefficient on benzene transport through the GMB/CL liner system, Figure 7 presents the benzene mass flux  $J$  at the base of the liner for three different Soret coefficients  $S_T$  ( $= 0, 0.005$ , and  $0.01 \text{ K}^{-1}$ ). Figure 7a,b present the  $J$  curves for GMB/CCL and GMB/GCL composite liner systems, respectively, and indicate that  $J$  increases almost linearly with increasing  $S_T$  for both ZC and ZCG boundary conditions. Table 3 presents the values of  $J_{ss}$  for GMB/CCL and GMB/GCL composite liner system for the three different  $S_T$ . The ZCG boundary condition shows a higher relative increase in  $J_{ss}$  than the ZC condition as  $S_T$  increases, because thermodiffusion significantly raises the benzene concentration in the liner, which in turn enhances advective mass flux. For  $S_T = 0$  and ZCG condition, the GMB/GCL system gives  $J_{ss}$  of the same order as the GMB/CCL system, indicating that even a thin GCL can effectively contain contaminants when advection is the dominant transport mechanism. Under the ZC condition, however, the GMB/GCL system exhibits a steady-state mass flux two orders of magnitude higher than that of the GMB/CCL system, because diffusion becomes much more important.



**Figure 7.** Benzene mass flux at the base of liner for different  $S_T$ : (a) GMB/CCL liner system, and (b) GMB/GCL composite liner system.

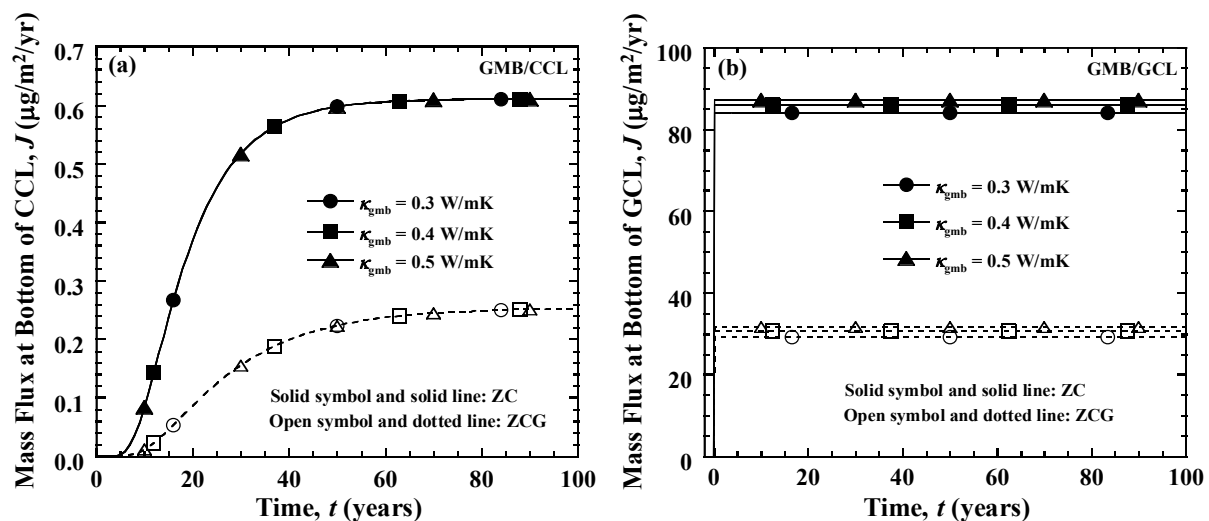
**Table 3.** Steady-state mass flux  $J_{ss}$  for GMB/CCL and GMB/GCL composite liner system for different  $S_T$ .

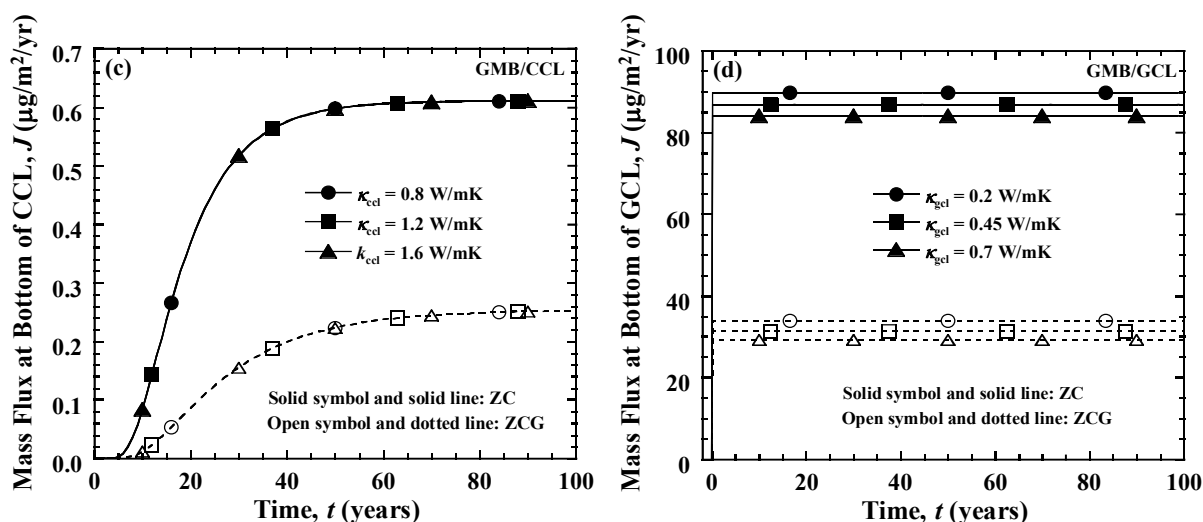
| $S_T$ ( $\text{K}^{-1}$ ) | Steady-State Mass Flux $J_{ss}$ ( $\mu\text{g}/\text{m}^2/\text{year}$ ) |                           |                                |                            |
|---------------------------|--------------------------------------------------------------------------|---------------------------|--------------------------------|----------------------------|
|                           | GMB/CCL Composite Liner System                                           |                           | GMB/GCL Composite Liner System |                            |
|                           | ZC Condition                                                             | ZCG Condition             | ZC Condition                   | ZCG Condition              |
| 0                         | 0.514                                                                    | 0.159                     | 70.370                         | 0.680                      |
| 0.005                     | 0.560 (8.9% $\uparrow$ )                                                 | 0.204 (28.3% $\uparrow$ ) | 77.010 (9.4% $\uparrow$ )      | 14.978 (2102% $\uparrow$ ) |
| 0.01                      | 0.610 (8.9% $\uparrow$ )                                                 | 0.252 (23.5% $\uparrow$ ) | 84.025 (9.1% $\uparrow$ )      | 29.137 (94.5% $\uparrow$ ) |

### 5.3. Effect of Thermal Conductivity

Hu et al. [58] reported the thermal conductivity of HDPE polymer ranging from 0.4 to 0.45 W/mK. According to the laboratory measurement data, the thermal conductivity of the GMB is around 0.3 W/mK [48,49]. Data for CCL thermal conductivity are scarce; this study adopts values for clay ranging from 0.9 to 3 W/mK [59–61]. For GCLs, laboratory measurements show thermal conductivities between 0.2 and 0.7 W/mK [36]. To illustrate the effect of thermal conductivity on benzene transport through the GMB/CL composite liner system, benzene mass flux  $J$  at the bottom of the liner system was calculated with  $\kappa_{\text{gmb}}$  (=0.3, 0.4 and 0.5 W/mK),  $\kappa_{\text{ccl}}$  (=0.8, 1.2 and 1.6 W/mK) and  $\kappa_{\text{gcl}}$  (=0.2, 0.45 and 0.7 W/mK), respectively. The chosen  $\kappa_{\text{gmb}}$  and  $\kappa_{\text{ccl}}$  are the same as those used by Peng et al. [26] for their investigation on contaminant transport through a GMB/CCL liner system.

Figure 8a,c presents the  $J$  curves for the GMB/CCL composite liner system. For either ZC or ZCG boundary condition, all the  $\kappa_{\text{gmb}}$  and  $\kappa_{\text{ccl}}$  produce the same  $J$  curves throughout the 100 yr. simulation period, because GMB is very thin relative to CCL, and, thus, the  $\kappa_{\text{gmb}}$  and  $\kappa_{\text{ccl}}$  can hardly change the temperature distribution in the GMB/CCL composite liner system. In contrast, Figure 8b,d for the GMB/GCL system show that the thermal conductivities of the GMB and GCL have significant effects. Because the GMB thickness is not negligible relative to the GCL, higher  $\kappa_{\text{gmb}}$  increases the temperature gradient in the GCL, while higher  $\kappa_{\text{gcl}}$  reduces that gradient. Consequently,  $J$  increases with increasing  $\kappa_{\text{gmb}}$  and decreasing  $\kappa_{\text{gcl}}$ .





**Figure 8.** Benzene mass flux at the base of liner for different thermal conductivities: (a) GMB/CCL composite liner system with varying GMB thermal conductivity, (b) GMB/GCL composite liner system with varying GMB thermal conductivity, (c) GMB/CCL composite liner system with varying CCL thermal conductivity, and (d) GMB/GCL composite liner system with varying GCL thermal conductivity.

## 6. Summary and Conclusions

This paper developed fully transient analytical solutions for organic contaminant transport through GMB/CCL and GMB/GCL composite liner systems, incorporating the coupled effects of advection through GMB defects, first-order degradation, and thermodiffusion. The proposed analytical solution was validated against experimental data, an existing analytical solution, and a finite-element numerical model. It is sufficiently accurate for GMB/CCL systems under all conditions. For GMB/GCL systems, it captures the general trends and provides conservative estimates for preliminary design, though the constant  $D_g$  and  $K_g$  assumption in the GMB introduces non-negligible errors. For a final detailed design requiring high accuracy, a full numerical simulation incorporating temperature-dependent properties is recommended. Using the validated solutions, a parametric study was performed to evaluate the impacts of thermodiffusion, Soret coefficient, and thermal conductivity on benzene transport. The main findings are summarized as follows:

(1) Thermodiffusion significantly accelerates benzene transport in both GMB/CCL and GMB/GCL. For the GMB/CCL system under a zero-concentration bottom boundary, increasing the temperature difference from 0 to 80 K increased the steady-state mass flux by 71%. Neglecting thermodiffusion can substantially underestimate contaminant outflow, leading to unsafe liner design.

(2) The effect of thermodiffusion is more pronounced in intact GMB liners than in damaged ones, because advection dominates when defects are present and weakens the relative contribution of thermodiffusion. The GMB/GCL system exhibits much higher benzene mass flux and stronger temperature response than the GMB/CCL system due to its smaller thickness.

(3) The benzene transport rate increases almost linearly with the Soret coefficient for both liner systems and both bottom boundary conditions. The zero-concentration-gradient condition shows a larger relative increase (up to 2102% when  $S_T$  increases from 0 to 0.005  $\text{K}^{-1}$  in the GMB/GCL system) because thermodiffusion becomes the primary driving mechanism.

(4) Thermal conductivity effects depend on the liner type. In the GMB/GCL system, higher GMB thermal conductivity and lower GCL thermal conductivity increase benzene transport by altering the temperature gradient within the GCL. In contrast, thermal conductivities of the GMB and CCL have negligible effects on the GMB/CCL system because the CCL dominates the total thickness.

(5) The proposed analytical solutions provide a computationally efficient tool for preliminary liner design, parametric sensitivity analysis, and early-stage risk assessment. They enable (i) rapid comparison of GMB/CCL and GMB/GCL systems to select environmentally preferable materials, (ii) optimization of clay liner thickness to balance containment performance against material consumption, and (iii) quantification of temperature effects to inform thermal mitigation strategies. The closed-form expressions offer explicit physical insights into the relationships between key transport parameters and liner performance, which are often obscured in numerical models. The analytical solution also serves as a reliable benchmarking tool for verifying numerical implementations.

**Author Contributions:** Y.H.: Conceptualization, data curation, writing—original draft preparation. W.-D.L.: Software, methodology, investigation, resources, supervision. J.-W.Q.: Validation, writing—review and editing, formal analysis. J.W.: Formal analysis, investigation, writing—original draft, writing—review and editing. H.-F.P.: Data curation, writing—review and editing, supervision. All authors have read and agreed to the published version of the manuscript.

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**Data Availability Statement:** Dataset available on request from the authors. The data are not publicly available due to large volume of raw simulation data and the complexity of the source code involved.

**Conflicts of Interest:** The authors declare no conflicts of interest.

## Appendix A

The general solution to the governing Equations (33) and (34) can be written as follows:

$$w_g(z, t) = \sum_{k=1}^{\infty} S_k f_{k,g}(z) \exp(a_g z - \delta_k t) \quad (A1)$$

$$w_c(z, t) = \sum_{k=1}^{\infty} S_k f_{k,c}(z) \exp(a_c z - \delta_k t) \quad (A2)$$

where  $f_{k,g}(z)$  and  $f_{k,c}(z)$  are determined by the following equations:

$$D_g \frac{\partial^2 f_{k,g}(z)}{\partial z^2} - \frac{(v_a - A_g S_T D_g K_g)^2}{4 D_g K_g^2} f_{k,g}(z) + \delta_k f_{k,g}(z) = 0 \quad (A3)$$

$$\frac{D_c}{R_{dc}} \frac{\partial^2 f_{k,c}(z)}{\partial z^2} - \frac{(v_c - A_c S_T D_c)^2}{4 D_c R_{dc}} f_{k,c}(z) + \delta_k f_{k,c}(z) - \lambda f_{k,c}(z) = 0 \quad (A4)$$

$$f_{k,g}(z) \Big|_{z=0} = 0 \quad (A5)$$

$$\exp(a_g z) f_{k,g}(z) \Big|_{z=L_g} = K_c \exp(a_c z) f_{k,c}(z) \Big|_{z=L_g} \quad (\text{A6})$$

$$\left\{ \left( A_g S_T D_g + a_g D_g - v_a / K_g \right) \exp(a_g z) f_{k,g}(z) + D_g \exp(a_g z) \frac{\partial f_{k,g}(z)}{\partial z} \right\} \Big|_{z=L_g} =$$

$$\left\{ \left( A_c S_T n_c D_c + a_c n_c D_c - v_c n_c \right) \exp(a_c z) f_{k,c}(z) + n_c D_c \exp(a_c z) \frac{\partial f_{k,c}(z)}{\partial z} \right\} \Big|_{z=L_g} \quad (\text{A7})$$

$$f_{k,c}(z) \Big|_{z=H} = 0 \quad (\text{A8})$$

and

$$\left( a_c f_{k,c}(z) + \frac{\partial f_{k,c}(z)}{\partial z} \right) \Big|_{z=H} = 0 \quad (\text{A9})$$

The solution to Equations (A3) and (A4) can be expressed as follows:

$$f_{k,g}(z) = \begin{cases} H_k \sin(\xi_{k,g} z) & \text{when } \delta_k \geq \frac{(v_a - A_g S_T D_g K_g)^2}{4 D_g K_g^2} \\ H_k \sinh(\xi_{k,g} z) & \text{when } \delta_k < \frac{(v_a - A_g S_T D_g K_g)^2}{4 D_g K_g^2} \end{cases} \quad (\text{A10})$$

$$f_{k,c}(z) = \begin{cases} G_k \sin(\xi_{k,c} z) + Q_k \cos(\xi_{k,c} z) & \text{when } \delta_k \geq \frac{(v_c - A_c S_T D_c)^2}{4 D_c R_{dc}} + \lambda \\ G_k \sinh(\xi_{k,c} z) + Q_k \cosh(\xi_{k,c} z) & \text{when } \delta_k < \frac{(v_c - A_c S_T D_c)^2}{4 D_c R_{dc}} + \lambda \end{cases} \quad (\text{A11})$$

where  $H_k$ ,  $G_k$  and  $Q_k$  are the parameters to be determined by substituting Equations (A10) and (A11) into Equations (A6) to (A7) and Equation (A8) or Equation (A9) as follows:

$$[\mathbf{M}][H_k \ G_k \ Q_k]^T = 0 \quad (\text{A12})$$

in which matrix  $\mathbf{M}$  is a matrix that depends on  $\delta_k$ . A non-zero solution of Equation (A12) only exists if the determinant of the matrix  $\mathbf{M}$  is zero. The values of  $\delta_k$  can be obtained by the following equation:

$$N_{7k} (N_{1k} N_{6k} - N_{3k} N_{4k}) + N_{8k} (N_{2k} N_{4k} - N_{1k} N_{5k}) = 0 \quad (\text{A13})$$

Depending on the relative magnitude of  $\delta_k$ ,  $\frac{(v_a - A_g S_T D_g K_g)^2}{4 D_g K_g^2}$  and  $\frac{(v_c - A_c S_T D_c)^2}{4 D_c R_{dc}} + \lambda$ ,  $N_{1k}$  to  $N_{8k}$  can be determined by one of the following three cases:

**Case 1.** When  $\delta_k \geq \frac{(v_a - A_g S_T D_g K_g)^2}{4 D_g K_g^2}$  and  $\delta_k \geq \frac{(v_c - A_c S_T D_c)^2}{4 D_c R_{dc}} + \lambda$ ,

$$N_{1k} = \sin(\xi_{k,g} L_g) \exp(a_g L_g) \quad (\text{A14})$$

$$N_{2k} = K_c \sin(\xi_{k,c} L_g) \exp(a_c L_g) \quad (\text{A15})$$

$$N_{3k} = K_c \cos(\xi_{k,c} L_g) \exp(a_c L_g) \quad (A16)$$

$$N_{4k} = (A_g S_T D_g + a_g D_g - v_a / K_g) \sin(\xi_{k,g} L_g) \exp(a_g L_g) + D_g \xi_{k,g} \cos(\xi_{k,g} L_g) \exp(a_g L_g) \quad (A17)$$

$$N_{5k} = (A_c S_T n_c D_c + a_c n_c D_c - v_c n_c) \sin(\xi_{k,c} L_g) \exp(a_c L_g) + n_c D_c \xi_{k,c} \cos(\xi_{k,c} L_g) \exp(a_c L_g) \quad (A18)$$

$$N_{6k} = (A_c S_T n_c D_c + a_c n_c D_c - v_c n_c) \cos(\xi_{k,c} L_g) \exp(a_c L_g) - n_c D_c \xi_{k,c} \sin(\xi_{k,c} L_g) \exp(a_c L_g) \quad (A19)$$

$$N_{7k} = \begin{cases} \sin(\xi_{k,c} H) & \text{for ZC bottom boundary} \\ \xi_{k,c} \cos(\xi_{k,c} H) + a_c \sin(\xi_{k,c} H) & \text{for ZCG bottom boundary} \end{cases} \quad (A20)$$

$$N_{8k} = \begin{cases} \cos(\xi_{k,c} H) & \text{for ZC bottom boundary} \\ -\xi_{k,c} \sin(\xi_{k,c} H) + a_c \cos(\xi_{k,c} H) & \text{for ZCG bottom boundary} \end{cases} \quad (A21)$$

**Case 2.** When  $\frac{(v_a - A_g S_T D_g K_g)^2}{4D_g K_g^2} \leq \delta_k < \frac{(v_c - A_c S_T D_c)^2}{4D_c R_{dc}} + \lambda$   $N_{1k}$  and  $N_{4k}$  are the same as Equations (A14) and (A17), respectively, and others can be expressed as follows:

$$N_{2k} = K_c \sinh(\xi_{k,c} L_g) \exp(a_c L_g) \quad (A22)$$

$$N_{3k} = K_c \cosh(\xi_{k,c} L_g) \exp(a_c L_g) \quad (A23)$$

$$N_{5k} = (A_c S_T n_c D_c + a_c n_c D_c - v_c n_c) \sinh(\xi_{k,c} L_g) \exp(a_c L_g) + n_c D_c \xi_{k,c} \cosh(\xi_{k,c} L_g) \exp(a_c L_g) \quad (A24)$$

$$N_{6k} = (A_c S_T n_c D_c + a_c n_c D_c - v_c n_c) \cosh(\xi_{k,c} L_g) \exp(a_c L_g) + n_c D_c \xi_{k,c} \sinh(\xi_{k,c} L_g) \exp(a_c L_g) \quad (A25)$$

$$N_{7k} = \begin{cases} \sinh(\xi_{k,c} H) & \text{for ZC} \\ \xi_{k,c} \cosh(\xi_{k,c} H) + a_c \sinh(\xi_{k,c} H) & \text{for ZCG} \end{cases} \quad (A26)$$

$$N_{8k} = \begin{cases} \cosh(\xi_{k,c} H) & \text{for ZC bottom boundary} \\ \xi_{k,c} \sinh(\xi_{k,c} H) + a_c \cosh(\xi_{k,c} H) & \text{for ZCG bottom boundary} \end{cases} \quad (A27)$$

**Case 3.** When  $\frac{(v_c - A_c S_T D_c)^2}{4D_c R_{dc}} + \lambda \leq \delta_k < \frac{(v_a - A_g S_T D_g K_g)^2}{4D_g K_g^2}$   $N_{2k}$ ,  $N_{3k}$  and  $N_{5k}$  to  $N_{8k}$  are the same as Equations (A15), (A16) and (A18) to (A21), respectively, and  $N_{1k}$  and  $N_{4k}$  can be expressed as follows:

$$N_{1k} = \sinh(\xi_{k,g} L_g) \exp(a_g L_g) \quad (A28)$$

$$N_{4k} = (A_g S_T D_g + a_g D_g - v_a / K_g) \sinh(\xi_{k,g} L_g) \exp(a_g L_g) + D_g \xi_{k,g} \cosh(\xi_{k,g} L_g) \exp(a_g L_g) \quad (A29)$$

Using the orthogonal relation, the following equation can be obtained (see Appendix B):

$$(\delta_k - \delta_m) \left[ \int_0^{L_g} f_{m,g}(z) f_{k,g}(z) dz + n_g R_{dc} \eta K_c \int_{L_g}^H f_{m,c}(z) f_{k,c}(z) dz \right] = \begin{cases} = 0 & (k \neq m) \\ \neq 0 & (k = m) \end{cases} \quad (A30)$$

$$\text{where } \eta = \exp \left[ 2(a_c - a_g) L_g \right]$$

Based on the initial conditions, we can obtain that

$$\sum_{k=1}^{\infty} S_k \int_0^{L_g} f_{k,g}(z) f_{m,g}(z) dz = \int_0^{L_g} [h_g(z) - u_g(z)] f_{k,g}(z) \exp(-a_g z) dz \quad (A31)$$

$$n_c R_{dc} \eta K_c \sum_{k=1}^{\infty} S_k \int_{L_g}^H f_{k,c}(z) f_{m,c}(z) dz = n_g R_{dc} \eta K_c \int_{L_g}^H [h_c(z) - u_c(z)] f_{k,c}(z) \exp(-a_c z) dz \quad (A32)$$

The following equation can be obtained by accumulating Equations (A31) and (A32)

$$\sum_{k=1}^{\infty} S_k \left[ \int_0^{L_g} f_{k,g}(z) f_{m,g}(z) dz + n_c R_{dc} \eta K_c \int_{L_g}^H f_{k,c}(z) f_{m,c}(z) dz \right] = \int_0^{L_g} [h_g(z) - u_g(z)] f_{k,g}(z) \exp(-a_g z) dz + n_c R_{dc} \eta K_c \int_{L_g}^H [h_c(z) - u_c(z)] f_{k,c}(z) \exp(-a_c z) dz \quad (A33)$$

Uniting Equation (A30), the value of  $S_k$  can be expressed as follows:

$$S_k = \frac{\int_0^{L_g} [h_g(z) - u_g(z)] f_{k,g}(z) \exp(-a_g z) dz + n_c R_{dc} \eta K_c \int_{L_g}^H [h_c(z) - u_c(z)] f_{k,c}(z) \exp(-a_c z) dz}{\int_0^{L_g} f_{k,g}^2(z) dz + n_c R_{dc} \eta K_c \int_{L_g}^H f_{k,c}^2(z) dz} \quad (A34)$$

## Appendix B

Based on Equations (A3) and (A4), it can be obtained that

$$\begin{aligned} & (\delta_k - \delta_m) \left[ \int_0^{L_g} f_{m,g}(z) f_{k,g}(z) dz + n_g R_{dc} \eta K_c \int_{L_g}^H f_{m,c}(z) f_{k,c}(z) dz \right] \\ &= \int_0^{L_g} \left[ D_g \frac{\partial^2 f_{k,g}(z)}{\partial z^2} - \frac{(v_a - A_g S_T D_g K_g)^2}{4 D_g K_g^2} f_{k,g}(z) \right] f_{m,g}(z) dz \\ &+ \int_0^{L_g} f_{k,g}(z) \left[ D_g \frac{\partial^2 f_{m,g}(z)}{\partial z^2} - \frac{(v_a - A_g S_T D_g K_g)^2}{4 D_g K_g^2} f_{m,g}(z) \right] dz \\ &+ n_c R_{dc} \eta K_c \int_{L_g}^H \left[ \frac{D_c}{R_{dc}} \frac{\partial^2 f_{k,c}(z)}{\partial z^2} - \frac{(v_c - A_c S_T D_c)^2}{4 D_c R_{dc}} f_{k,c}(z) - \lambda f_{k,c}(z) \right] f_{m,c}(z) dz \\ &+ n_c R_{dc} \eta K_c \int_{L_g}^H f_{k,c}(z) \left[ \frac{D_c}{R_{dc}} \frac{\partial^2 f_{m,c}(z)}{\partial z^2} - \frac{(v_c - A_c S_T D_c)^2}{4 D_c R_{dc}} f_{m,c}(z) - \lambda f_{m,c}(z) \right] dz \\ &= -D_g \int_0^{L_g} \frac{\partial^2 f_{k,g}(z)}{\partial z^2} f_{m,g}(z) dz + D_g \int_0^{L_g} f_{k,g}(z) \frac{\partial^2 f_{m,g}(z)}{\partial z^2} dz \\ &- n_c D_c \eta K_c \int_{L_g}^H \frac{\partial^2 f_{k,c}(z)}{\partial z^2} f_{m,c}(z) dz + n_c D_c \eta K_c \int_{L_g}^H f_{k,c}(z) \frac{\partial^2 f_{m,c}(z)}{\partial z^2} dz \end{aligned} \quad (A35)$$

where

$$\begin{aligned} & -D_g \int_0^{L_g} \frac{\partial^2 f_{k,g}(z)}{\partial z^2} f_{m,g}(z) dz + D_g \int_0^{L_g} f_{k,g}(z) \frac{\partial^2 f_{m,g}(z)}{\partial z^2} dz \\ &= D_g \left[ \left( f_{k,g}(z) \frac{\partial f_{m,g}(z)}{\partial z} - \frac{\partial f_{k,g}(z)}{\partial z} f_{m,g}(z) \right) \right]_{z=L_g} - \left( f_{k,g}(z) \frac{\partial f_{m,g}(z)}{\partial z} - \frac{\partial f_{k,g}(z)}{\partial z} f_{m,g}(z) \right) \Big|_{z=0} \\ &= D_g \left( f_{k,g}(L_g) \frac{\partial f_{m,g}(L_g)}{\partial z} - f_{k,g}(0) \frac{\partial f_{m,g}(0)}{\partial z} \right) - D_g \left( \frac{\partial f_{k,g}(L_g)}{\partial z} f_{m,g}(L_g) - \frac{\partial f_{k,g}(0)}{\partial z} f_{m,g}(0) \right) \end{aligned} \quad (A36)$$

Similarly,

$$\begin{aligned}
& -n_c D_c \eta K_c \int_{L_g}^H \frac{\partial^2 f_{k,c}(z)}{\partial z^2} f_{m,c}(z) dz + n_c D_c \eta K_c \int_{L_g}^H f_{k,c}(z) \frac{\partial^2 f_{m,c}(z)}{\partial z^2} dz \\
& = n_c D_c \eta K_c \left[ \left( f_{k,c}(z) \frac{\partial f_{m,c}(z)}{\partial z} - \frac{\partial f_{k,c}(z)}{\partial z} f_{m,c}(z) \right) \right]_{z=H} - \left( f_{k,c}(z) \frac{\partial f_{m,c}(z)}{\partial z} - \frac{\partial f_{k,c}(z)}{\partial z} f_{m,c}(z) \right) \bigg|_{z=L_g} \\
& = n_c D_c \eta K_c \left( f_{k,c}(H) \frac{\partial f_{m,c}(H)}{\partial z} - f_{k,c}(L_g) \frac{\partial f_{m,c}(L_g)}{\partial z} \right) - n_c D_c \eta K_c \left( \frac{\partial f_{k,c}(H)}{\partial z} f_{m,c}(H) - \frac{\partial f_{k,c}(L_g)}{\partial z} f_{m,c}(L_g) \right)
\end{aligned} \quad (A37)$$

According to Equations (A5) to (A9), we can obtain that

$$\begin{aligned}
& D_g f_{k,g}(L_g) \frac{\partial f_{m,g}(L_g)}{\partial z} - n_c D_c \eta K_c f_{k,c}(L_g) \frac{\partial f_{m,c}(L_g)}{\partial z} = \\
& \eta K_c (A_g S_T n_c D_c + n_c D_c a_c - v_c n_c) f_{k,c}(L_g) f_{m,c}(L_g) - (A_g S_T D_g + a_g D_g - v_a / K_g) f_{k,g}(L_g) f_{m,g}(L_g)
\end{aligned} \quad (A38)$$

$$\begin{aligned}
& D_g \frac{\partial f_{k,g}(L_g)}{\partial z} f_{m,g}(L_g) - n_c D_c \eta K_c \frac{\partial f_{k,c}(L_g)}{\partial z} f_{m,c}(L_g) = \\
& \eta K_c (A_g S_T n_c D_c + n_c D_c a_c - v_c n_c) f_{k,c}(L_g) f_{m,c}(L_g) - (A_g S_T D_g + a_g D_g - v_a / K_g) f_{k,g}(L_g) f_{m,g}(L_g)
\end{aligned} \quad (A39)$$

Uniting Equations (A38) and (A39) can obtain that

$$\begin{aligned}
& \left[ D_g f_{k,g}(L_g) \frac{\partial f_{m,g}(L_g)}{\partial z} - n_c D_c \eta K_c f_{k,c}(L_g) \frac{\partial f_{m,c}(L_g)}{\partial z} \right] - \\
& \left[ D_g \frac{\partial f_{k,g}(L_g)}{\partial z} f_{m,g}(L_g) - n_c D_c \eta K_c \frac{\partial f_{k,c}(L_g)}{\partial z} f_{m,c}(L_g) \right] = 0
\end{aligned} \quad (A40)$$

Substituting Equations (A36) and (A37) into (A35) and uniting Equation (A40) can determine that the right-hand side of Equation (A35) equals zero. Furthermore, we can then obtain the following equation:

$$\int_0^{L_g} f_{m,g}(z) f_{k,g}(z) e dz + n_g R_{dc} \eta K_c \int_{L_g}^H f_{m,c}(z) f_{k,c}(z) dz = 0 \quad (k \neq m) \quad (A41)$$

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