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Solving Advection-Diffusion Equations via Sobolev Space Notions

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Abstract In this paper, the time-dependent advection-diffusion equation is studied. After introducing these equations in various engineering fields such as gas adsorption, solid dissolution, heat and mass transfer in falling film or pipe and other equations similar to transport phenomena, a new method has been proposed to find their solutions. Among the various works on solving these PDEs by numerical and somewhat analytical methods, a general analytical framework for solving these equations is presented. Using advanced components of Sobolev spaces, weak solutions and some important integral inequalities, an analytical method for the existence and uniqueness of the weak solution of these PDEs is presented, which is the best solution in the proposed structure. Then, with a reduced system of ODE, one can solve the problem of the general parabolic boundary value problem, which includes PDE transport phenomena. Besides, the new approach supports the infinite propagation speed of disturbances of (time-dependent) diffusion-time equations in semi-infinite media.

Keywords: *advection-diffusion equation, Sobolev spaces, weak solutions, Harnack's inequality, semi-infinite media*

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1. Introduction

Transport phenomena are a way that chemical engineers group together three areas of study that have certain ideas in common: fluid mechanics, heat transfer and mass transfer, [1,2]. The idea behind the conservation of mass and energy results in a general form of the equation of change, including several common terms such as accumulation, diffusion, and convection.

A known form of such partial differential equations is a time-dependent advection-diffusion equation and describes physical phenomena where mass and/or energy are transferred inside a physical system due to two processes: diffusion and convection.

These equations are equally important in soil physics, biophysics, petroleum engineering and chemical engineering for describing similar processes, [3,4,5,6]. Such PDEs can be solved analytically only in special cases, [6,7,8]; however, a large number of advanced numerical methods have been developed to approximate the solution to the equations, [9,10,11,12].

Among various boundary value problems in the field of phenomena transport, in Section 2, we introduce some of its known problems such as gas absorption and solid dissolution in falling film, advection-diffusion in semi-infinite media and heat and mass transfer inside a circular pipe. Then in some functional analysis ingredients have been given which result in the presentation of the general framework. A tabular comparison has been done between four known problems of transport phenomena and our general initial/boundary problem has been presented in Section 2.

Finally, after the explanation of the motivation of the proposed methodology in Section 3, the main result expressed and proved in Theorem 1 (Section 4).

Also, our new approach that is proving the existence and uniqueness of the weak solution of the general problem results in the reduction of the general initial/boundary PDE to a system of ODE which easily has been solved.

The other advantage of the proposed methodology is that the maximum of the function in some interior of the film at a positive time can be estimated by the minimum of it in the same region at a later time. This fact supports infinite propagation speed of disturbances of advection-diffusion equations which has been proved in Corollary 1.

2. Various Applications of Advection-Diffusion Equations in Engineering

The first equation applies to gas absorption in falling film, [1]. For example, consider absorption of gas component A diffusing into a laminar falling liquid film (B) leads to the following problem

$$\begin{cases} v_{\max}\left(1-\left(\frac{x}{\delta}\right)^2\right)\frac{\partial c_A}{\partial z}=D_{AB}\frac{\partial^2 c_A}{\partial x^2}, \\ u_{\max},\delta,D_{AB}:\text{constant}, \\ c_A:\text{dependent variable}, \\ x,z:\text{independent variable}, \end{cases} \quad (1)$$

where δ is the thickness of the falling liquid film, $v_{\max}$ is the maximum velocity, $c_A(x,z)$ is the concentration of A and D_{AB} is the diffusion coefficient of A in the film B.

The boundary conditions are

$$\begin{cases} z=0, c_A=c_{A_0}, \\ x=0, c_A=c_{A_i}, \\ x=\delta, \frac{\partial c_A}{\partial x}=0. \end{cases} \quad (2)$$

The first boundary condition corresponds to the fact that the film consists of a constant concentration of A (i.e., c_{A_0} at top, and the second indicated that at the liquid-gas interface the concentration of A is determined by the solubility of A in B (i.e., c_{A_i}). The third one states that A cannot diffuse through the solid wall.

The other problem deals with solid dissolution in falling film, [1,2]. In the case of dissolution of a solid matter (A) into a falling liquid film near the wall, as the notion above, we have the following problem

$$\begin{cases} ax\frac{\partial c_A}{\partial z}=D_{AB}\frac{\partial^2 c_A}{\partial x^2}, \\ D_{AB}:\text{constant}, \\ c_A:\text{dependent variable}, \\ x,z:\text{independent variable}, \end{cases} \quad (3)$$

with the boundary conditions

$$\begin{cases} z=0, c_A=c_{A_0}, \\ x=0, c_A=c_{A_i}, \\ x=\delta, c_A=c_{A_0}. \end{cases} \quad (4)$$

where c_{A_0} is the concentration of A at top, δ is the thickness of the falling film, and c_{A_i} is the solubility of A in the film. The third problem is advection-diffusion equation with variable coefficients in semi-infinite media, [5,6]. A one-dimensional linear advection-diffusion equation, derived on the principle of conservation of mass, is

$$\begin{cases} \frac{\partial c_A}{\partial t}=\frac{\partial}{\partial x}\left(D(x,t)\frac{\partial c_A}{\partial x}-u(x,t)c_A\right), \\ c_A:\text{dependent variable}, \\ x:\text{independent variable}, \end{cases} \quad (5)$$

where D and u are called dispersion coefficient and velocity of the flow field, respectively, and $c_A(x,t)$ is the dispersing solute concentration at a position x along the longitudinal direction at time, t.

The initial and boundary conditions may be written as

$$\begin{cases} x\geq 0; t=0, c_A(x,t)=0, \\ x=0; t>0, c_A(x,t)=c_{A_0}, \\ x\to\infty; t>0, \frac{\partial c_A}{x}=0. \end{cases} \quad (6)$$

The last equation is about heat and mass transfer in a fully-developed laminar flow inside a circular pipe, [2]. The energy equation inside a circular pipe in the region far away from the entrance with a fully developed and parabolic velocity distribution can be written as

$$\begin{cases} \left(1-\left(\frac{r}{R}\right)^2\right)\frac{\partial T}{\partial z}=\left(\frac{\kappa}{2\rho c_p U_m}\right)\left(\frac{\partial^2 T}{\partial r^2}+\frac{1}{r}\frac{\partial T}{\partial r}\right), \\ R,\kappa,\rho,c_p,U_m:\text{constant}, \\ T:\text{dependent variable}, \\ r,z:\text{independent variable}, \end{cases} \quad (7)$$

where T is temperature of the fluid, κ is the thermal conductivity of the fluid, c_p is the specific heat of the fluid at constant pressure, R is the radius of pipe, U_m is the average velocity of the fluid over the cross-section, and ρ is the density of the fluid.

The boundary conditions are

$$\begin{cases} z=0, T=T_0, \\ r=R, T=T_{wall}, \\ r=0, \frac{\partial T}{\partial r}=0. \end{cases} \quad (8)$$

Now, we study some analytic notions which are needed in the sequel.

3. Statement of the Problem

As the standard notions of functional analysis, [13,14,15], Assume U be an open, bounded subset of $\mathbf{R}^n$ and consider the Sobolev space $W^{k,p}(U)$ consists of all locally summable functions $u:U\to\mathbf{R}$ such that for each multiindex α with $|\alpha|\leq k$, $D^\alpha U$ exists in the weak sense which means that for all test functions $C_c^\infty(U)$, $\int_U uD^\alpha\phi dx=(-1)^{|\alpha|}\int_U v\phi dx$ and the weak derivation belongs to $L^p(U)$. We denote by $W_0^{k,p}(U)$ the closure of $C_c^\infty(U)$ in $W^{k,p}(U)$ and $W^{k,2}(U)$ with $H^k(U)$, then $H^0(U)=L^2(U)$.

Consider a variation of the initial/boundary-value problems mentioned in Section 2, such as

$$\begin{cases} u_t + Pu = f, \text{ in } U_T \\ u = 0, \text{ on } \partial U \times [0,T], \\ u = g, \text{ on } U \times \{t=0\}, \end{cases} \quad (9)$$

where $U_T := U \times (0,T]$ for some fixed time $T > 0$, ∂U is the boundary of U, $f : U_T \to \mathbf{R}$ and $g : U \to \mathbf{R}$ are given, and $u : \overline{U_T} \to \mathbf{R}$ is the unknown; $u = u(x,t)$. The letter P denotes for each time t a second-order partial differential operator, having the nondivergece form

$$Pu = -\sum_{i,j=1}^{n} a^{ij}(x,t) u_{x_i x_j} + \sum_{i=1}^{n} b^i(x,t) u_{x_i} + c(x,t)u, \quad (10)$$

for given coefficients $a^{ij}, b^i, c \ (i,j = 1,...,n)$.

Assume for now that $a^{ij}, b^i, c \in L^\infty(U_T)$, $(i,j=1,...,n)$, $f, g \in L^2(U_T)$ and $a^{ij} = a^{ji}$ $(i,j=1,...,n)$. The time-dependent bilinear form has been defined as

$$F[u,v;t] = \int_U \sum_{i,j=1}^{n} a^{ij}(x,t) u_{x_i} v_{x_j} dx + \int_U \sum_{i=1}^{n} b^i(x,t) u_{x_i} v + c(x,t) uv dx \quad (11)$$

for $u, v \in H_0^1(U)$, $0 \le t \le T$ almost everywhere.

The initial/boundary value problem (9) covers four problems mentioned in Section 2, and all of them can be expressed in the form of (10).

In fact, considering the open subset U as an open subset containing the falling film/semi-infinite media results in the following comparable results.

Then the problem of existence and uniqueness of the solution of the boundary value problems (1)-(8) reduced to the existence and uniqueness of the solution of initial/boundary value problem (9). For this purpose, the weak solutions of it will be searched.

4. Weak Solutions of Advection-Diffusion Equations

Let $u = u(x,t)$ is a smooth solution of our parabolic problem (9). Now switch the viewpoint, by associating with u a mapping $u : [0,T] \to H_0^1(U)$ defined by $[u(t)](x) := u(x,t)$, $(x \in U, 0 \le t \le T)$.

Returning to problem (9), similarly define $f : [0,T] \to L^2(U)$ defined by $[f(t)](x) := f(x,t)$, $(x \in U, 0 \le t \le T)$.

Then if we fix a function $v \in H_0^1(U)$, multiply the PDE (3) by v and integrate by parts, to find

$$(u', v) + F[u,v;t] = (f, v) \quad \left(' = \frac{d}{dt}\right) \quad (12)$$

for each $0 \le t \le T$, the pairing $(.,.)$ denoting inner product in $L^2(U)$ and F is defined as the equation (11). Then

$$u_t = g^0 - \sum_{j=1}^{n} g^j_{x_j}, \quad \text{in } U_T \quad (13)$$

for $g^0 = f - \sum_{i=1}^{n} b_i u_{x_i} - cu$ and $g^j = f - \sum_{i=1}^{n} ai^j u_{x_i}$, $(i,j=1,...,n)$. Then the right hand side of (13) lies in the Sobolev space $H^{-1}(U)$:

$$\|u_t\|_{H^{-1}(U)} \le \left(\sum_{j=0}^{n} \left\| g^j \right\|^2_{L^2(U)} \right)^{\frac{1}{2}} \le c\left(\|u\|_{H_0^1(U)} + \|f\|_{L^2(U)} \right). \quad (14)$$

Estimation (14) suggests it may be reasonable to look for a weak solution with $u' \in H^{-1}(U)$ for almost everywhere time $0 \le t \le T$; in which case the first term in (6) can be expressed as $\langle u', v \rangle$, $\langle .,. \rangle$, being the pairing of $H^{-1}(U)$ and $H_0^1(U)$. But a function $u \in L^2\left(0,T; H_0^1(U)\right)$ with $u' \in L^2\left(0,T; H_0^{-1}(U)\right)$ which satisfies in equation (12) for each $v \in H_0^1(U)$ and almost everywhere time $0 \le t \le T$, and $u(0) = g$ is a weak solution of the parabolic initial/boundary value problem (9).

Theorem 1. The weak solution of advection-diffusion PDEs (1), (3), (5) and (7) with initial/boundary conditions (2), (4), (6) and (8), respectively, exists and is unique.

Proof. As mentioned before, it suffices to prove this for initial/boundary problem (9). The proof arranged in four steps:

Step 1. Let the functions $\phi_k = \phi_k(x)$, $(k = 1,...,n)$ are smooth, $\{\phi_k\}_{k=1}^n$ is an orthogonal basis of $H_0^1(U)$ and is an orthonormal basis of $L^2(U)$.

Fix a positive integer m. a function $u_m : [0,T] \to H_0^1(U)$ of the form

$$u_m(t) := \sum_{k=1}^{m} \rho_m^k(t) \phi_k, \quad (15)$$

will be found where we want to select the coefficients $\rho_m^k(t)$, $(0 \le t \le T, k = 1,...,m)$ so that

$$\rho_k^m(0,) = (g, \phi_k) \quad (k = 1,...,m) \quad (16)$$

and

$$\begin{aligned} &(u'_m, \phi_k) + F[u_m, \phi_k; t] = (f, \phi_k) \\ &(0 \le t \le T, k = 1,...,m) \end{aligned} \quad (17)$$

where, $(.,.)$ denotes the inner product in $L^2(U)$.

Thus a function u_m of the form (15) can be found that satisfies the projection (16) of problem (9) onto the finite dimensional subspace spanned by $\{\phi_k\}_{k=1}^n$.

For this purpose, assuming u_m has the structure (15), at first note from orthonormal property of $\{\phi_k\}_{k=1}^n$ in $L^2(U)$, $\left(u_m'(t),\phi_k\right)=\left(\rho_k^m\right)'(t)$.

Also, $e^{kl}(t)=F[\phi_l,\phi_k;t]$; $F[u_m,\phi_k;t]=\sum_{l=1}^m e^{kl}(t)\rho_m^l(t)$, $(k,l=1,...,m)$. Then (17) becomes the linear system of ODE

$$\left(\rho_k^m\right)'(t)+\sum_{l=1}^m e^{kl}(t)\rho_m^l(t)=f^k(t),\ (k=1,...,m) \quad (18)$$

subject to the initial conditions (16).

According to standard existence theory for ordinary differential equations, there exists a unique absolutely continuous function $\rho_m(t):=\left(\rho_m^1(t),...,\rho_m^m(t)\right)$ satisfying (16) and (18) for almost everywhere $0\le t\le T$.

Step 2. Now propose to send m to infinity and to show a subsequence of our solutions u_m of the approximate problems (16), (17) converges to a weak solution of (9).

For this some uniform estimates such as energy estimates will be necessary which states there exists a constant c, depending only on U, T and the coefficients of L, such that

$$\begin{aligned}&\max_{0\le t\le T}\|u_m(t)\|_{L^2(U)}+\|u_m(t)\|_{L^2(0,T;H_0^1(U))}\\&+\|u_m'(t)\|_{L^2(0,T;H_0^{-1}(U))}\\&\le c\left(\|f\|_{L^2(0,T;L^2(U))}+\|g\|_{L^2(U)}\right),\quad \forall m=1,2.\end{aligned} \quad (19)$$

According to the energy estimates (19), the sequence $\{u_m\}_{m=1}^\infty$ is bounded in $L^2(0,T,H_0^1(U))$, and $\{u_m'\}_{m=1}^\infty$ is bounded in $L^2(0,T,H_0^{-1}(U))$.

Consequently there exists a subsequence $\{u_{m_l}\}_{l=1}^\infty\subset\{u_m\}_{m=1}^\infty$ and a function $L^2(0,T,H_0^1(U))$ with $u'\in L^2(0,T,H_0^{-1}(U))$ such that

$$\begin{cases}u_{m_l}\to u & \text{weakly in } L^2(0,T,H_0^1(U))\\ u_{m_l}'\to u' & \text{weakly in } L^2(0,T,H_0^{-1}(U))\end{cases} \quad (20)$$

Next fix an integer N and choose a function $v\in C^1\left([0,T];H_0^1(U)\right)$ having the form

$$v(t)=\sum_{k=1}^N\rho^k(t)\phi_k, \quad (21)$$

where $\left\{\rho^k\right\}_{k=1}^N$ are given smooth functions. We choose $m\ge N$, multiply (17) by $e^k(t)$, sum $k=1,...,N$, and then integrate with respect to t find

$$\int_0^T\langle u_m,v\rangle+F[u_m,v;t]dt=\int_0^T(f,v)\,dt, \quad (22)$$

Set $m=m_l$ and recall (20), to find upon passing to weak limits that

$$\int_0^T\langle u,v\rangle+F[u,v;t]dt=\int_0^T(f,v)\,dt. \quad (23)$$

This equality then holds for all functions $v\in L^2\left(0,T;H_0^1(U)\right)$, as functions of the form (21) are dense in this space. Hence in particular

$$\langle u,v\rangle+F[u,v;t]=(f,v),\quad \forall v\in H_0^1(U),0\le t\le T \quad (24)$$

furthermore we have $u\in C\left([0,T];L^2(U)\right)$.

Step 3. In order to prove $u(0)=g$, first note from (23) that

$$\begin{aligned}&\int_0^T-\langle u,v\rangle+F[u,v;t]dt=\int_0^T(f,v)\,dt+(u(0),v(0)),\\&\forall v\in C1\left([0,T];H_0^1(U)\right);v(T)=0.\end{aligned} \quad (25)$$

Similarly, from (22), deduce that identity (26):

$$\begin{aligned}&\int_0^T-\langle v',u_m\rangle+F[u_m,v;t]dt\\&=\int_0^T(f,v)\,dt+(u_m(0),v(0)),\end{aligned} \quad (26)$$

Set $m=m_l$ and once again employ (20) to find

$$\int_0^T-\langle v,u\rangle+F[u,v;t]dt=\int_0^T(f,v)\,dt+(g,v(0)). \quad (27)$$

Since $u_{m_l}(0)\to g$ in $L^2(U)$.

As $v(0)$ is arbitrary, comparing (25) and (27), concludes that $u(0)=g$.

Step 4. Also a weak solution of (9) is unique. Since it suffices to check that the only weak solution of (9) with $f\equiv g\equiv 0$ is $u\equiv 0$.

To prove this, observe that by setting $v=u$ in identity (24) (for $f\equiv 0$) results

$$\frac{d}{dt}\left(\frac{1}{2}\|u\|_{L^2(U)}^2\right)+F[u,u;t]=\langle u,u\rangle B[u,u;t]=0 \quad (28)$$

Since $F[u,u;t]\ge\beta\|u\|_{H_0^1(U)}^2-\gamma\|u\|_{L^2(U)}^2\ge-\gamma\|u\|_{L^2(U)}^2$, then Gronwall's inequality, and (28) imply $u\equiv 0$.

The structure of the proof can be coincided in Figure 1.

Corollary 1. The uniformly PDE (9) can well describe the (time-dependent) advection-diffusion and heat and mass-transfer phenomena in some inconvenient falling films such as semi-infinite media with more propagation.

Proof. Assume $u\in C_1^2(U_T)$ solves $u_t+Pu=0$ and $u\ge 0$ in U_T. Suppose $V\subset\subset U$ is connected. Then Harnak's inequality, states that for each $0<t_1<t_2\le T$, there exists a constant c such that $\sup_V u(.,t_1)\le c\inf_V u(.,t_2)$. The constant c depends only

on V, t_1, t_2 and the coefficient of P (of course, if the coefficients are continuous or bounded, it is manageable, too). Then, Harnack's inequality states that if u is a nonnegative solution of our parabolic PDE, then the maximum of u in some interior at a positive time can be estimated by the minimum of u in the same region at a later time.

Assume $u \in C_1^2(U_T) \bigcap C\left(\overline{U_T}\right)$ and $c \equiv 0$ in U_T. Suppose also U is connected. If $u_t + Pu \le 0$ in U_T and u attains its maximum over $\overline{U_T}$ at a point $(x_0, u_0) \in U_T$, likewise, if $u_t + Pu \ge 0$ in U_T and u attains its maximum over U_T at a point $(x_0, u_0) \in U_T$ then of Harnack inequality we have u is constant on U_{T_0}.

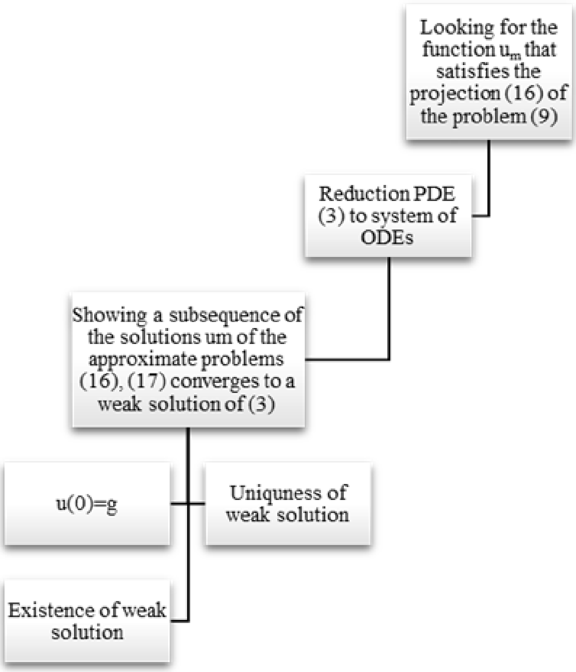

Figure 1. Structure of the proof of Theorem 1

5. Conclusion

In this paper, a novel methodology was presented to examine existence and uniqueness of the weak solution of gas absorption and solid dissolution in falling film, advection-diffusion in semi-infinite media and heat and mass transfer inside a circular pipe which are the most important problems in the field of phenomena transport. In fact, some advanced functional analysis ingredients have been caused to present a general framework for these PDEs and showed that weak solution is the best one in this structure.

The main advantage of our approach is that it provides a general methodology which outperforms the numerical methods. Also it results in the reduction of the general initial/boundary PDE to a system of ODE which easily can be solved. The other benefit is that it supports infinite propagation speed of disturbances of advection-diffusion equations in some awkward falling films such as semi-infinite media.

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