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Existence and uniqueness of solution for molecular diffusion of CO_2 in CH_4 under unknown boundary conditions in enhanced gas recovery (EGR) process

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Abstract

This study is intended to provide a one-dimensional inverse nonlinear problem to investigate molecular diffusion of CO_2 in CH_4 in a hydrocarbon reservoir. Generally, boundary fluxes at the top and the bottom of the reservoir are non-zero. Furthermore, it is not practically possible to identify the exact boundary conditions, therefore we are faced with an inverse problem which is discussed with two non-zero and unknown boundary conditions via the auxiliary problems. We will consider the case where the governing boundary conditions are defined as $f(u(0,t))$ and $f(u(1,t))$ so that u and f are unknown . We will provide the conditions for f where the desired problem has a unique solution. Assuming an over-specified data $u(0,t)=\psi(t)$ with several admissible conditions for ψ , we will prove the existence and uniqueness of solution (u^*, f^*) for the problem. In order to achieve this goal, we will demonstrate that a defined transfer T_ψ has a unique fixed point. Accordingly, we need to prove that T_ψ is a contraction. During this process, we will apply the other governing equations and functions such as Abel integral equation, Jacobi function, Volterra operators, Lipschitz function and Holder function on the discussed inverse problems.

***Keywords**: Molecular Diffusion; Fick's first law; Fixed point; Contraction; Jacobi function; Volterra operator; Abel equation; Lipschitz function.*

1. Introduction

One of the most practical methods for EGR (Enhanced Gas Recovery) from a hydrocarbon reservoir, is CO_2 injection in the reservoir. In this method, high pressure CO_2 is injected in the reservoir, and the remaining hydrocarbon flows into the wellbore. About 80% (or more) of natural gas is methane (CH_4). Therefore a molecular diffusion between CO_2 and CH_4 can be introduced. At $t=0$ under the known temperature and pressure, the density of CO_2 is more than CH_4 , thus a vertical diffusion will occur between the gases. When the gas equilibrium is reached, the process will stop.

In this study, we assume that the reservoir is horizontal and uniform. Also, its upper half and lower half are respectively filled by pure methane and pure carbon dioxide. Uniformity of the reservoir means that the pressure and temperature are constant, so the gases have the same and fixed temperature.

Fick's first law will govern the behavior of each of the gases. On the other hand, we are faced with a vertical diffusion in the reservoir so the resulted diffusion equation will be one-dimensional nonlinear equation (ODE) which along with the governing boundary conditions will show a type of nonlinear inverse problems (NIP). In addition, it is not practically possible to identify the exact boundary conditions, thus this problem will be discussed with unknown boundary conditions. In recent years, an important mathematically challenging and well-studied class of these problems is, to prove the existence and uniqueness of solution and investigate the unknown functions that appear in the partial differential equations. In this regard, one may find some studies in the literature which have been often carried out on heat conduction problems. For example, Rosch has investigated the identification of unknown boundary functions as optimal control problems [1-2]. Some researchers have employed the boundary element method to approximate the unknown boundary functions [3-4].

2. Mathematical formulation [5-6]

We consider that:

a) Attribute 1 is for CO_2 and attribute 2 is for CH_4.
b) l : Thickness of the reservoir
c) D_{12} : Effective diffusion coefficient of the composition of two gases.
d) ρ : Mass density of the composition of two gases.
e) ρ_i : Mass density of i^{th} the gas $\quad i=1,2$
f) C_i : Concentration of i^{th} gas $\quad i=1,2$
g) C : Concentration of the gas composition
h) J_i^* : Molar concentration of i^{th} gas $\quad i=1,2$
i) z : Height
j) Δx_i : Mole fraction of i^{th} gas $\quad i=1,2$
k) v_i : Speed of i^{th} gas $\quad i=1,2$
l) N_i : Molar flux of i^{th} gas $\quad i=1,2$
m) $\bar{v}_i$: Partial molar volume of i^{th} gas $\quad i=1,2$
n) v^* : Molecular velocity

Generally, D_{12} is a function of temperature and pressure of the gas composition. When we ignore the changes in pressure and temperature and assume that the reservoir is uniform, we actually consider D_{12} is constant. We follow the problem assuming that D_{12} is constant.

As we know N_i and J_i^* are respectively defined as follows:

$$N_i = C_i v_i \qquad i=1,2 \tag{1}$$

$$J_i^* = C_i(v_i - v^*) \qquad i=1,2 \tag{2}$$

We put in the recent equation the following relation:

$$v^* = \frac{\sum_{j=1}^{2} C_j v_j}{C} \tag{3}$$

And then, we have:

$$J_i^* = C_i v_i - \frac{C_i}{C}\sum_{j=1}^{2} C_j v_j \qquad i=1,2 \tag{4}$$

Regarding $x_i = \frac{C_i}{C}$, $i = 1,2$ and (1):

$$J_i^* = N_i - x_i \sum_{k=1}^{2} N_k \qquad i = 1,2 \tag{5}$$

Now, if ρ is constant (uniform mass density), Fick's first law will be defined according to the following equation:

$$J_i^* = -D_{12} \frac{\partial \rho_i}{\partial z} \qquad i = 1,2 \tag{6}$$

In the case that ρ is not constant, the law will be stated as follow:

$$J_i^* = -CD_{12} \frac{\partial x_i}{\partial z} \qquad i = 1,2 \tag{7}$$

In the more general case, we assume that ρ is not constant. According to equations (5) and (7):

$$N_i = x_i \left(N_1 + N_2\right) - CD_{12} \frac{\partial x_i}{\partial z} \qquad i = 1,2 \tag{8}$$

In addition, the following equation is for N_i and $\bar{V}_i$:

$$\bar{V}_1 N_1 + \bar{V}_2 N_2 = 0 \tag{9}$$

Using equations (8) and (9), we have:

$$N_1 = \frac{-CD_{12} \frac{\partial x_1}{\partial z}}{1 - x_1 \left(1 - \frac{\bar{V}_1}{\bar{V}_2}\right)} \tag{10}$$

Similarly:

$$N_2 = \frac{-CD_{12} \frac{\partial x_2}{\partial z}}{1 - x_2 \left(1 - \frac{\bar{V}_2}{\bar{V}_1}\right)} \tag{11}$$

If the concentration of each of the gases is shown as $C_i = C_i(z,t)$, $i = 1,2$, as the concentration of the gas composition is fixed, we can write

$$C_1(z,t) + C_2(z,t) = C \,. \tag{12}$$

On the other hand $C_i = Cx_i$ so $x_1 + x_2 = 1$. Therefore, equations (10) and (11) can be written:

$$N_1 = \frac{-D_{12} \frac{\partial C_1}{\partial z}}{1 - x_1 \left(1 - \frac{\bar{V}_1}{\bar{V}_2}\right)} \quad \text{and} \quad N_2 = \frac{-D_{12} \frac{\partial C_2}{\partial z}}{x_1 + (1 - x_1) \frac{\bar{V}_2}{\bar{V}_1}} \tag{13}$$

Regardless of chemical reactions, Molar balance equation would be:

$$\frac{\partial C_i}{\partial t} + \frac{\partial N_i}{\partial z} = 0 \tag{14}$$

Substituting equation (13) in equation (14), we have:

$$\frac{\partial C_1}{\partial t}+\frac{\partial\left(\frac{-D_{12}\frac{\partial C_1}{\partial z}}{1-x_1\left(1-\frac{\bar{V}_1}{\bar{V}_2}\right)}\right)}{\partial z}=0 \quad \text{and} \quad \frac{\partial C_2}{\partial t}+\frac{\partial\left(\frac{-D_{12}\frac{\partial C_2}{\partial z}}{x_1+(1-x_1)\left(\frac{\bar{V}_2}{\bar{V}_1}\right)}\right)}{\partial z}=0 \qquad (15)$$

As for the ideal gases, $\bar{v}_i$ is constant:

$$\bar{V}_i=\frac{RT}{P} \qquad i=1,2 \qquad (16)$$

So (15) can be written as:

$$\frac{\partial C_i}{\partial t}+\frac{\partial\left(-D_{12}\frac{\partial C_i}{\partial z}\right)}{\partial z}=0 \qquad i=1,2 \qquad (17)$$

Finally, we have the diffusion equation as follow:

$$\frac{\partial C_i}{\partial t}=D_{12}\frac{\partial^2 C_i}{\partial z^2} \qquad i=1,2 \qquad (18)$$

Now, we consider boundary flows at the top and the bottom of the reservoir. In other words, we have the following boundary conditions (fluxes at the top and bottom of the reservoir is not zero):

$$\left.\frac{\partial C_i}{\partial z}\right|_{z=0}=g_{i0}(t) \quad \text{and} \quad \left.\frac{\partial C_i}{\partial z}\right|_{z=l}=g_{i1}(t) \qquad i=1,2 \qquad (19)$$

In real terms, $g_{i0}(t)$ and $g_{i1}(t)$ cannot be accurately identified. So, in this case, we are faced with an inverse problem with the boundary conditions. Assuming $\tilde{t}=\frac{D_{12}}{l}t$ and $\tilde{z}=\frac{1}{l}z$, we define $\tilde{C}_i$ so that $\tilde{C}_i(\tilde{z},\tilde{t})=\frac{l}{C}C_i(z,t)$. Now we can write:

$$\frac{\partial C_i}{\partial t}=\frac{CD_{12}}{l^2}\frac{\partial \tilde{C}_i}{\partial \tilde{t}} \quad \text{and} \quad \frac{\partial C_i}{\partial z}=\frac{C}{l}\frac{\partial \tilde{C}_i}{\partial \tilde{z}} \qquad i=1,2 \qquad (20)$$

On the other hand:

$$\frac{\partial C_i}{\partial t}=\frac{CD_{12}}{l^2}\frac{\partial \tilde{C}_i}{\partial \tilde{t}}=\frac{1}{l}\frac{\partial}{\partial \tilde{z}}\left(D_{12}\frac{C}{l}\frac{\partial \tilde{C}_i}{\partial \tilde{z}}\right)=\frac{CD_{12}}{l^2}\frac{\partial^2 \tilde{C}_i}{\partial \tilde{z}^2} \qquad i=1,2 \qquad (21)$$

Regarding equation(20) we can result:

$$\frac{\partial \tilde{C}_i}{\partial \tilde{t}}=\frac{\partial^2 \tilde{C}_i}{\partial \tilde{z}^2} \qquad i=1,2 \qquad (22)$$

Also, the boundary conditions (19) will change as follows:

$$\left.\frac{\partial \tilde{C}_i}{\partial \tilde{z}}\right|_{\tilde{z}=0}=\tilde{g}_{i0}(\tilde{t}) \quad \text{and} \quad \left.\frac{\partial \tilde{C}_i}{\partial \tilde{z}}\right|_{\tilde{z}=1}=\tilde{g}_{i1}(\tilde{t}) \qquad i=1,2 \qquad (23)$$

In an optimistic mode, we assume that:

$$\tilde{g}_{i0}(\tilde{t})=f(\tilde{C}_i(0,\tilde{t})) \quad \text{and} \quad \tilde{g}_{i1}(\tilde{t})=f(\tilde{C}_i(1,\tilde{t})) \qquad i=1,2 \qquad (24)$$

where f is an unknown function. We provide the conditions in which, the problem has a unique solution.

3. Existence and uniqueness of the solution

Consider the following inverse problem:

$$\frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial x^2} \qquad 0<x<1 \qquad 0<t<T \tag{25}$$

$$u(x,0)=\varphi(x) \qquad 0\le x\le 1 \tag{26}$$

$$\frac{\partial u}{\partial x}(0,t)=g(t) \qquad 0\le t\le T \tag{27}$$

$$\frac{\partial u}{\partial x}(1,t)=h(t) \qquad 0\le t\le T \tag{28}$$

We consider the solution of this problem as $u=v+w$, where v and w are respectively the solutions of the following inverse problems as auxiliary problems.

$$\frac{\partial v}{\partial t}=\frac{\partial^2 v}{\partial x^2} \qquad 0<x<1 \qquad 0<t<T \tag{29}$$

$$v(x,0)=0 \qquad 0\le x\le 1 \tag{30}$$

$$\frac{\partial v}{\partial x}(0,t)=g(t) \qquad 0\le t\le T \tag{31}$$

$$\frac{\partial v}{\partial x}(1,t)=h(t) \qquad 0\le t\le T \tag{32}$$

And:

$$\frac{\partial w}{\partial t}=\frac{\partial^2 w}{\partial x^2} \qquad 0<x<1 \qquad 0<t<T \tag{33}$$

$$w(x,0)=\varphi(x) \qquad 0\le x\le 1 \tag{34}$$

$$\frac{\partial w}{\partial x}(0,t)=0 \qquad 0\le t\le T \tag{35}$$

$$\frac{\partial w}{\partial x}(1,t)=0 \qquad 0\le t\le T \tag{36}$$

Now, we discuss one of the basic properties of Jacobi function which will be used in this topic [7-9]. Jacobi function is defined as follows:

$$\theta(x,t)=\sum_{n=-\infty}^{+\infty}K(x+2n,t) \qquad x\in\Re \qquad t>0 \tag{37}$$

Or:

$$\theta(x,t)=K(x,t)+\sum_{n=1}^{+\infty}\big(K(x+2n,t)+K(x-2n,t)\big) \qquad x\in\Re \qquad t>0 \tag{38}$$

$$\theta(0,t)=K(0,t)+\sum_{n=1}^{+\infty}\big(K(2n,t)+K(-2n,t)\big)=K(0,t)+2\sum_{n=1}^{+\infty}K(2n,t) \quad t>0 \tag{39}$$

If we define the function H so that $H(t)=\frac{1}{\sqrt{\pi t}}\sum_{n=1}^{+\infty}e^{-\frac{n^2}{t}}$ then:

$$\theta(0,t)=\frac{1}{\sqrt{4\pi t}}+H(t) \qquad t>0 \tag{40}$$

In this case, the function H is located in the set $C^{\infty}(0,\infty)$ such that:

$$H^n(0)=0 \qquad \forall n \in N \tag{41}$$

The following theorem is an important application of Jacobi function:

Theorem 1: Problem (29) to (32) has a solution as follow [8]:

$$v(x,t)=-2\int_0^t \theta(x,t-\eta)g(\eta)d\eta+2\int_0^t \theta(x-1,t-\eta)h(\eta)d\eta \tag{42}$$

Therefore, the solution of problem (25) to (28) will be:

$$u(x,t)=w(x,t)-2\int_0^t \theta(x,t-\eta)g(\eta)d\eta+2\int_0^t \theta(x-1,t-\eta)h(\eta)d\eta \tag{43}$$

And then for $x=0$:

$$u(0,t)=w(0,t)-2\int_0^t \theta(0,t-\eta)g(\eta)d\eta+2\int_0^t \theta(0-1,t-\eta)h(\eta)d\eta \tag{44}$$

Now we define:

$$S(t)=\frac{1}{2}\left(w(0,t)-u(0,t)\right)+\int_0^t \theta(-1,t-\eta)h(\eta)d\eta=\int_0^t \theta(0,t-\eta)g(\eta)d\eta \tag{45}$$

Equation (45) is an Abel integral equation. According to equation (40) we can write the recent equation as:

$$S(t)=\int_0^t\left(\frac{1}{\sqrt{4\pi(t-\eta)}}+H(t-\eta)\right)g(\eta)d\eta=\frac{1}{\sqrt{4\pi}}\int_0^t g(\eta)\frac{d\eta}{\sqrt{t-\eta}}+\int_0^t H(t-\eta)g(\eta)d\eta \tag{46}$$

If $S(t)$ is absolutely continuous and $S'(t)$ is bounded then, as equation (46) is an Abel integral equation it can be written as follow:

$$g(t)=\frac{2}{\sqrt{\pi}}\left(\frac{S(0)}{\sqrt{t}}+\int_0^t \frac{S'(\eta)}{\sqrt{t-\eta}}d\eta+\int_0^t E(t,\eta)g(\eta)d\eta\right) \tag{47}$$

where:

$$E(t,\eta)=\frac{1}{\sqrt{t-\eta}}+\int_\eta^t \frac{H'(t-\lambda)}{\sqrt{t-\lambda}}d\lambda \tag{48}$$

Now, Let us consider the case where functions g and h are defined as:

$$g(t)=f(u(0,t)) \qquad \text{and} \qquad h(t)=f(u(1,t)) \tag{49}$$

where the function f is unknown. For problem (25) to (28), over-specified data $u(0,t)=\psi(t)$ is considered so that function ψ is true in conditions (I) and (II):

(I) Function ψ in $[0,T]$ is absolutely differentiable and $\psi(0)=\varphi(0)$ also ψ is monotonic on $[0,T]$. Now, we write equation (45) as follow:

$$S(t)=\frac{1}{2}\left(w(0,t)-\psi(t)\right)+\int_0^t \theta(-1,t-\eta)f(u(1,\eta))d\eta \tag{50}$$

Based on equation(34), it is clear that:

$$S(0)=\frac{1}{2}\left(w(0,0)-\psi(0)\right)+\int_0^0 \theta(-1,-\eta)f(u(1,\eta))d\eta=0 \tag{51}$$

On the other hand:

$$S'(\eta)=\frac{1}{2}\left(w'(0,\eta)-\psi'(t)\right)+\int_0^\eta \theta'(-1,\lambda-\eta)f(u(1,\lambda))d\lambda \tag{52}$$

By substituting equations (52) and (51) in equation (47), we will have:

$$f(u(0,t)) = f(\psi(t)) = \frac{2}{\sqrt{\pi}}\int_0^t E(t,\eta) f(\psi(\eta))d\eta + \frac{1}{\sqrt{\pi}}\int_0^t \left\{ w'(0,\eta) - \psi'(t) + 2\int_0^\eta \theta'(-1,\lambda-\eta) f(u(1,\lambda))d\lambda \right\} \frac{d\eta}{\sqrt{t-\eta}} \quad (53)$$

The right side of the above equation is a nonlinear function of $f(t)$. Since the final term includes $f(u(1,t))$ and also $u(1,t)$ depends on f, therefore the value of u is depends on x, t and f. In other words $u(x,t) \equiv u(x,t;f)$. In addition, $u(x,t;f)$ should be located in the domain of f, in other words we consider the following condition:

(II) Regarding ψ is monotonic on $[0,T]$ then $\forall t \in [0,T]$, $u(1,t;f) \in [\psi(0),\psi(T)]$.

We write the left side of equation (53) as below:

$$fo\,\psi(t) = T_\psi[fo\,\psi](t) \quad (54)$$

Assuming $fo\,\psi = y$, we will have:

$$y(t) = T_\psi[y](t) \quad (55)$$

We mean to demonstrate T_ψ has a unique fixed point. In order to achieve this goal, we need to prove that T_ψ is a contraction. The following operators are defined:

$$d_1[f](t) = \frac{2}{\pi}\int_0^t E(t,\eta) f(\eta)d\eta \quad (56)$$

$$d_2[f](t) = \frac{2}{\pi}\int_0^t \theta'(-1,t-\eta) f(\eta)d\eta \quad (57)$$

$$a[f](t) = \int_0^t \frac{f(\eta)}{\sqrt{t-\eta}}d\eta \quad (58)$$

where d_1 and d_2 are Volterra linear operators and a is Abel linear operator. Also, function d_3 is defined as:

$$d_3(t) = \frac{1}{\pi}a[w'(0,t) - \psi'(t)] \quad (59)$$

With regards to the above definitions, equation (53) can be written as below:

$$y(t) = T_\psi[y](t) = d_1[y](t) + d_2(t) + a\big(d_2[T_\psi[y]]\big)(t) \quad (60)$$

To continue the discussion, we need some of the following lemmas. Before referring to the lemmas, we refer to the following definition.

Function f $x = x_0$ is a continuous Holder function of order α if there is a constant number such as r and a small sized neighborhood of x_0, so that for each x of this neighborhood we have:

$$\left| f(x) - f(x_0) \right| \le r\left| x - x_0 \right|^\alpha \quad (61)$$

The space of single-variable functions whose m^{th} derivative is a continuous Holder function of order $0 < \alpha \le 1$ on $[a,b]$ is shown by $C^{m+\alpha}[a,b]$. When $\alpha = 1$ we are faced with the continuity of Lipschitz . The space of single-variable continuous functions of Lipschitz on $[a,b]$ is shown by $lip[a,b]$. Also, the below relations respectively define a half-norm and a norm in this space:

$$\underset{a\le x_1\le x_2\le b}{|f|_1} = Sup\frac{|f(x_1)-f(x_2)|}{|x_1-x_2|} \tag{62}$$

$$\|f\|_1 = |f|_1 + \|f\|_\infty \tag{63}$$

The space of functions with a half-power fractional derivative on $[a,b]$ is shown by $H[a,b]$, and we define a half-norm in this space as follow:

$$\underset{a\le x_1\le x_2\le b}{|f|_H} = Sup\frac{|f(x_1)-f(x_2)|}{|x_1-x_2|^{\frac{1}{2}}} \tag{64}$$

Also, the below relation defines a norm in this space:

$$\|f\|_H = |f|_H + \|f\|_\infty \tag{65}$$

Lemma 1: If functions σ, h_1 and h_2 belong to space $lip[0,T]$, then there will be a constant number such as c so that $\|a[\sigma(h_1)]-a[\sigma(h_2)]\|_H \le c\|h_1-h_2\|_\infty$.

Proof: First, we define:

$$P(t) = a[\sigma(h_1)](t) - a[\sigma(h_2)](t) = a[\sigma(h_1)-\sigma(h_2)] \tag{66}$$

According to equation (58), we can write:

$$|P(t_1)-P(t_2)| = \left|\int_0^{t_1}\frac{1}{\sqrt{t_1-\tau}}[\sigma(h_1)(\tau)-\sigma(h_2)(\tau)]d\tau - \int_0^{t_2}\frac{1}{\sqrt{t_2-\tau}}[\sigma(h_1)(\tau)-\sigma(h_2)(\tau)]d\tau\right| \tag{67}$$

And then:

$$|P(t_1)-P(t_2)| \le \left|\int_0^{t_1}\frac{1}{\sqrt{t_1-\tau}}d\tau - \int_0^{t_2}\frac{1}{\sqrt{t_2-\tau}}d\tau\right|.\|\sigma(h_1)-\sigma(h_2)\|_\infty$$

$$= \left|2\sqrt{t_1}-2\sqrt{t_2}\right|.\|\sigma(h_1)-\sigma(h_2)\|_\infty$$

Or:

$$\frac{|P(t_1)-P(t_2)|}{|t_1-t_2|^{1/2}} \le 2\|\sigma(h_1)-\sigma(h_2)\|_\infty \tag{68}$$

On the other hand:

$$\|p\|_\infty \le \left|\int_0^{t}\frac{1}{\sqrt{t-\tau}}d\tau\right|.\|\sigma(h_1)-\sigma(h_2)\|_\infty = \left|2\sqrt{t}\right|.\|\sigma(h_1)-\sigma(h_2)\|_\infty$$

$$\le A\|\sigma(h_1)-\sigma(h_2)\|_\infty \tag{69}$$

According to equations (65), (68) and (69) we can write:

$$\|p\|_H = Sup\frac{|P(t_1)-P(t_2)|}{|t_1-t_2|^{1/2}} + \|p\|_\infty \le 2\|\sigma(h_1)-\sigma(h_2)\|_\infty + A\|\sigma(h_1)-\sigma(h_2)\|_\infty$$

$$= (2+A)\|\sigma(h_1)-\sigma(h_2)\|_\infty \tag{70}$$

σ is a continuous Lipschitz function, so:

$$\|\sigma(h_1)-\sigma(h_2)\|_\infty \le B\|h_1-h_2\|_\infty \tag{71}$$

Finally, from (70) and (71) we will have:

$$\|p\|_H \le c\|h_1-h_2\|_\infty \tag{72}$$

Lemma 2: We assume that f_1 and f_2 are Lipschitz functions .The following problem is considered:

$$\frac{\partial u^i}{\partial t}=\frac{\partial^2 u^i}{\partial x^2} \qquad 0<x<1 \qquad 0<t<T \qquad i=1,2 \tag{73}$$

$$u^i(x,0)=\varphi(x) \qquad 0\le x\le 1 \qquad i=1,2 \tag{74}$$

$$\frac{\partial u^i}{\partial x}(0,t)=f_i(u^i(0,t)) \qquad 0\le t\le T \tag{75}$$

$$\frac{\partial u^i}{\partial x}(1,t)=f_i(u^i(1,t)) \qquad 0\le t\le T \tag{76}$$

$$u^i(0,t)=\psi(x) \qquad 0\le x\le 1 \qquad i=1,2 \tag{77}$$

The solution of above problem is true in the following inequality:

$$\left\|u^{(1)}(1,t)-u^{(2)}(1,t)\right\|_H \le c\left\|f_1-f_2\right\|_\infty \tag{78}$$

where T is sufficiently small and constant c depends on T and Lipschitz norms of f_1 & f_2.

Proof: Function q is defined as below:

$$q(t)=u^{(1)}(1,t)-u^{(2)}(1,t)=\int_0^t L(t-\tau)\Big(f_1(u^{(1)}(1,\tau))-f_2(u^{(2)}(1,\tau))\Big)d\tau \tag{79}$$

where $L(T)$ is single kernel at coordinates origin. Assuming $0\le t_2<t_1\le T$, we write:

$$\begin{aligned}
q(t_1)-q(t_2)&=\int_0^{t_1} L(t_1-\tau)\Big(f_1(u^{(1)}(1,\tau))-f_2(u^{(2)}(1,\tau))\Big)d\tau\\
&-\int_0^{t_2} L(t_2-\tau)\Big(f_1(u^{(1)}(1,\tau))-f_2(u^{(2)}(1,\tau))\Big)d\tau\\
&=\int_0^{t_2}\Big(L(t_1-\tau)-L(t_2-\tau)\Big)\Big(f_1(u^{(1)}(1,\tau))-f_1(u^{(2)}(1,\tau))\Big)d\tau\\
&+\int_0^{t_2}\Big(L(t_1-\tau)-L(t_2-\tau)\Big)\Big(f_1(u^{(2)}(1,\tau))-f_2(u^{(2)}(1,\tau))\Big)d\tau\\
&+\int_{t_2}^{t1} L(t_1\text{-}\tau)\Big(f_1\big(u^{(1)}(1,\tau)\big)-f_1\big(u^{(2)}(1,\tau)\big)\Big)d\tau\\
&+\int_{t_2}^{t_1} L(t_1-\tau)\Big(f_1(u^{(2)}(1,\tau))-f_2(u^{(2)}(1,\tau))\Big)d\tau=I_1+I_2+I_3+I_4
\end{aligned}$$

Now, we consider the recent integrals as follows:

$$\begin{aligned}
\left|I_1\right|&=\left|\int_0^{t_2}\Big(L(t_1-\tau)-L(t_2-\tau)\Big)\Big(f_1(u^{(1)}(1,\tau))-f_1(u^{(2)}(1,\tau))\Big)d\tau\right|\\
&\le\int_0^{t_2}\left|L(t_1-\tau)-L(t_2-\tau)\right|.\left\|f_1\right\|_1.\left|u^{(1)}(1,\tau)-u^{(2)}(1,\tau)\right|d\tau
\end{aligned}$$

$$\leq \int_0^{t_2}\int_{t_2}^{t_1}\frac{\partial L}{\partial s}(s-\tau).d\tau.\left\|f_1\right\|_1.\underset{0\leq t\leq T}{Sup}\left|u^{(1)}(1,t)-u^{(2)}(1,t)\right| \leq c_1\sqrt{t_1-t_2}.\left\|f_1\right\|_1.\underset{0\leq t\leq T}{Sup}\left|u^{(1)}(1,t)-u^{(2)}(1,t)\right|$$

$$\left|I_2\right| = \left|\int_0^{t_2}\left(L(t_1-\tau)-L(t_2-\tau)\right)\left(f_1(u^{(2)}(1,\tau))-f_2(u^{(2)}(1,\tau))\right)d\tau\right|$$

$$\leq \int_0^{t_2}\left|L(t_1-\tau)-L(t_2-\tau)\right|.\left|f_1(u^{(2)}(1,\tau))-f_2(u^{(2)}(1,\tau))\right|d\tau$$

$$\leq \int_0^{t_2}\int_{t_2}^{t_1}\frac{\partial L}{\partial s}(s-\tau)d\tau.\left\|f_1-f_2\right\|_\infty \leq c_2\sqrt{t_1-t_2}.\left\|f_1-f_2\right\|_\infty$$

$$\left|I_3\right| = \left|\int_{t_2}^{t_1}L(t_1-\tau)\left(f_1(u^{(1)}(1,\tau))-f_1(u^{(2)}(1,\tau))\right)d\tau\right|$$

$$\leq \int_{t_2}^{t_1}\left|L(t_1-\tau)\right|.\left\|f_1\right\|_1.\left|u^{(1)}(1,\tau)-u^{(2)}(1,\tau)\right|d\tau \leq c_3\sqrt{t_1-t_2}.\left\|f_1\right\|_1.\underset{0\leq t\leq T}{Sup}\left|u^{(1)}(1,t)-u^{(2)}(1,t)\right|$$

$$\left|I_4\right| = \left|\int_{t_2}^{t_1}L(t_1-\tau)\left(f_1(u^{(2)}(1,\tau))-f_2(u^{(2)}(1,\tau))\right)d\tau\right|$$

$$\leq \int_{t_2}^{t_1}\left|L(t_1-\tau)\right|.\left|f_1(u^{(2)}(1,\tau))-f_2(u^{(2)}(1,\tau))\right|d\tau \leq c_4\sqrt{t_1-t_2}.\left\|f_1-f_2\right\|_\infty$$

With respect to the recent relations:

$$\left|q(t_1)-q(t_2)\right| = \left|I_1+I_2+I_3+I_4\right| \leq \left|I_1\right|+\left|I_2\right|+\left|I_3\right|+\left|I_4\right|$$

$$\leq \sqrt{t_1-t_2}\left((c_1+c_3).\left\|f_1\right\|_1.\underset{0\leq t\leq T}{Sup}\left|u^{(1)}(1,t)-u^{(2)}(1,t)\right|+(c_2+c_4).\left\|f_1-f_2\right\|_\infty\right)$$

We can conclude:

$$\frac{\left|q(t_1)-q(t_2)\right|}{\left|t_1-t_2\right|^{\frac{1}{2}}} \leq \left((c_1+c_3).\left\|f_1\right\|_1.\left\|q\right\|_\infty+(c_2+c_4).\left\|f_1-f_2\right\|_\infty\right) \tag{80}$$

If we define $c_5 = \max\left\{(c_1+c_3).\left\|f_1\right\|_1,(c_2+c_4)\right\}$ then, according to equation (64):

$$\underset{a\leq t_1\leq t_2\leq b}{\left|q\right|_H} = Sup\frac{\left|q(t_1)-q(t_2)\right|}{\left|t_1-t_2\right|^{\frac{1}{2}}} \leq c_5\left(\left\|q\right\|_\infty+\left\|f_1-f_2\right\|_\infty\right) \tag{81}$$

On the other hand, regarding equation (64) we can conclude:

$$\left\|q\right\|_\infty \leq \sqrt{t}\left|q\right|_H \tag{82}$$

Therefore:

$$\left\|q\right\|_H = \left|q\right|_H+\left\|q\right\|_\infty \leq \sqrt{t}\left|q\right|_H+\left|q\right|_H = (1+\sqrt{t})\left|q\right|_H$$

$$\leq (1+\sqrt{t})c_5\left(\sqrt{t}|q|_H + \| f_1 - f_2\|_\infty\right) \leq c_6\left(\sqrt{t}|q|_H + \| f_1 - f_2\|_\infty\right) \tag{83}$$

Eventually,we have: $\|q\|_H \leq \dfrac{c_6}{1-c_6\sqrt{T}}\| f_1 - f_2\|_\infty$ (84)

As mentioned earlier, we mean to demonstrate that T_ψ is a contraction. We consider equation (60) and define y_1 and y_2 so that $y_1(r) = T_\psi[y_1](t) = f_1 o\psi(t)$, $y_2(r) = T_\psi[y_2](t) = f_2 o\psi(t)$. where f_1 and f_2 are true in lemma 2. Regarding equation (60) we can write:

$$\|T_\psi[y_1] - T_\psi[y_2]\|_H \leq \|d_1[y_1] - d_1[y_2]\|_H + \|a(d_2[T_\psi[y_1]]) - a(d_2[T_\psi[y_2]])\|_H \tag{85}$$

In according to Lemma 1, the right side of the above relation can be written:

$$\|a(d_2[T_\psi[y_1]]) - a(d_2[T_\psi[y_2]])\|_H \leq c\|T_\psi[y_1] - T_\psi[y_2]\|_H = c\| f_1(u^1(1,t)) - f_2(u^2(1,t))\|_\infty$$

$$\leq c\| f_1(u^1(1,t)) - f_1(u^2(1,t))\|_\infty + c\| f_1(u^2(1,t)) - f_2(u^2(1,t))\|_\infty$$

$$\leq c\| f_1\|_1 \|u^1(1,t) - u^2(1,t)\|_\infty + c\| f_1 - f_2\|_\infty$$

$$\leq c_0\left(\|u^1(1,t) - u^2(1,t)\|_\infty + \| f_1 - f_2\|_\infty\right) \tag{86}$$

where $c_0 = \max\{c, \| f_1\|_1\}$

Therefore, with regards to equation (86) we can write equation(85) as:

$$\|T_\psi[y_1] - T_\psi[y_2]\|_H \leq c_0\left(\|u^1(1,t) - u^2(1,t)\|_\infty + \| f_1 - f_2\|_\infty\right) \tag{87}$$

On the other hand, according to equation (64) we can generally conclude that:

$$\| f\|_\infty \leq \sqrt{t}| f|_H \leq \sqrt{T}| f|_H \tag{88}$$

So:

$$\|T_\psi[y_1] - T_\psi[y_2]\|_H \leq c_0\sqrt{T}\left(\|u^1(1,t) - u^2(1,t)\|_H + \| f_1 - f_2\|_H\right) \tag{89}$$

Now, regarding the recent relation and equation (84) we can write:

$$\|T_\psi[y_1] - T_\psi[y_2]\|_H \leq c_0\sqrt{T}\left(\frac{c_6}{1-c_6\sqrt{T}}\| f_1 - f_2\|_\infty + \| f_1 - f_2\|_H\right)$$

$$\leq c_0\sqrt{T}\left(\frac{c_6}{1-c_6\sqrt{T}}\sqrt{T}\| f_1 - f_2\|_H + \| f_1 - f_2\|_H\right)$$

$$\leq c_0\sqrt{T}\left(\frac{c_6}{1-c_6\sqrt{T}}\sqrt{T} + 1\right)\| f_1 - f_2\|_H \tag{90}$$

Or:

$$\|T_\psi[y_1] - T_\psi[y_2]\|_H \leq \frac{c'}{1-c'\sqrt{T}}\sqrt{T}\| f_1 - f_2\|_H \tag{91}$$

Therefore, for T which is small enough ($2c'\sqrt{T} < 1$), T_ψ is a contraction in space H. According to the principle of contraction Mapping, T_ψ has only and only a unique fixed point such as y^* and there is only and only one f^* corresponding to y^* s.t $y^* = f^* O\psi$. In other words, if conditions (I) and (II) are established then problem (25) to (28) assuming equation(49) will has a pair of unique solution (u^*, f^*) in $[0,t^*]$ s.t $0 \le t^* \le T$.

4. Conclusion

The present study has shown that a molecular diffusion problem is arisen in a hydrocarbon reservoir, under the unknown boundary conditions as $f(u(0,t))$ and $f(u(1,t))$ (u and f are unknown) with considering an over-specified data as $u(0,t) = \psi(t)$ has a unique solution as (u^*, f^*) in $[0,T]$. In according to the below conditions, the problem can be extended on all the time:

1- we limit f to uniform Lipschitz functions.

2- f is limited to non-negative functions so that $f(0) = 0$, by applying the Maximum principle [10], u remains uniformly bounded.

It is very interesting to extend the discussion on the above problem when the temperature and pressure are not constant, e.g. when the reservoir is not uniform

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