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A Parabolic Inverse Problem in Chromatography

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1 Introduction

In this talk we shall prove a uniqueness result for a parabolic inverse problem arisen in GPC (Gel Permeation Chromatography), the fundamental technology to measure the size of moleculars. The mathematical model of GPC is proposed by Deisler-Wilhelm [1] in 1953. They derived a system of parabolic equations about the concentration of the "mobil phase" and of the "gel phase" with the interaction term between both phases at the interface of the solute and the gel.

In the present paper we neglect the interaction and pick up the mobile phase only. We also suppose that the flow and the diffusion is one-dimensional, and that the column I may be regarded as an interval $[0,l]$.

Then the equation of continuity is expressed as

$$\frac{\partial u}{\partial t}+\frac{\partial j}{\partial x}=0 \qquad (0<x<\infty),$$

where j denotes the flux so that

$$j=-D(x)\frac{\partial u}{\partial x}+V(x)u,$$

where D is the diffusion coefficient. The Peclet number, assumed to be a constant in the case of low Reinold's number, is given as

$$p=a\frac{V(x)}{D(x)},$$

where a denotes the size of moleculars. Thus, our equation is given as

$$\frac{\partial u}{\partial t}=\frac{\partial}{\partial x}\left\{V(x)\left(K\frac{\partial u}{\partial x}-u\right)\right\} \qquad (0<x<\infty,\ 0<t<T) \tag{1.1}$$

with $K=a/p$, where the input and the output of chromatography are described as

$$VK\frac{\partial u}{\partial x}\bigg|_{x=0}=f(t) \qquad (0<t<T) \tag{1.2}$$

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and

(1.3) $$u|_{x=l} = g(t) \qquad (0 < t < T)$$

respectively. We suppose that

(1.4) $$u|_{t=0} = 0 \qquad (0 < x < \infty)$$

and also

(1.5) $$u \in O(1) \qquad (\text{as } x \to \infty)$$

Furthermore, we admit the discontinuity of the velocity $V = V(x)$ at $x = l$, in which case we impose

(1.6) $$u|_{x=l-0} = u|_{x=l+0} \qquad (0 < t < T)$$

and

(1.7) $$V\frac{\partial u}{\partial x}\bigg|_{x=l-0} = V\frac{\partial u}{\partial x}\bigg|_{x=l+0} \qquad (0 < t < T)$$

as the interior boundary conditions. In the actual problem the output is desired to obey a sharp (pulse-like) shape. Otherwise we cannot measure the response time precisely. To this end it is believed that the gel should be located uniformly. For its examination it will be useful to know the inside velocity $V = V(x)$, which is desired to be constant. Thus, we want to determine $V = V(x)$ $(0 \le x \le l)$ by $f = f(t)$ $(0 < t < T)$ and $g = g(t)$ $(0 < t < T)$. This is a parabolic inverse problem and our uniqueness theorem is stated as follows.

Theorem 1 *Under the assumption that*

(1.8)

$$V \in C^2[0,l], \quad V(x) = \textit{constant } (= V(l+0)) \quad \textit{on} \quad [l, +\infty) \quad \textit{and} \quad V(x) > 0, \quad (x \in [0, \infty))$$

the input

(1.9) $$f \in L^1(0,T) \quad \textit{with} \quad f \not\equiv 0$$

and the output

$$(1.10) \qquad g : \textit{absolutely continuous on } [0,T] \quad \textit{with} \quad g(0) = 0$$

determine the velocity $V = V(x)$ $(0 \le x < \infty)$ *and the constant* $K > 0$ *in (1.1)-(1.7).*

We think that the assumptions (1.8) is reasonable at least as a first approximation. Our result is related to the work of Pierce [4] in 1979, which has established the uniqueness of $(p, h, H) \in C^1[0,1] \times R \times R$ in

$$(1.11) \qquad \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - p(x)u \qquad (0 < x < 1, 0 < t < T)$$

with

$$(1.12) \qquad u|_{t=0} = 0 \qquad (0 < x < 1)$$

and

$$(1.13) \qquad -\frac{\partial u}{\partial x} + hu\Big|_{x=0} = 0 \quad (0 < t < T),$$

from the input

$$(1.14) \qquad \frac{\partial u}{\partial x} + Hu\Big|_{x=1} = f(t) \not\equiv 0 \quad (0 < t < T)$$

and the output

$$(1.15) \qquad u|_{x=1} = g(t) \quad (0 < t < T).$$

Main differences are (i) location of inputs and outputs, (ii) order of unknown coefficients, and (iii) discontinuity of unknown coeficients.

As for the point (iii), it should be noted that $V(x)$ is supposed to be constant outside the column (i.e., $x \in [l, \infty]$), and that the location of discontinuity $x = l$ is prescribed implicitly. This would make the situation easier to assure the uniqueness in our inverse problem with the discontinuity.

As for the point (ii), we recall the work Murayama [3]. It has established the generic uniqueness of $\alpha = \alpha(x)$ and $a = a(x)$ in

$$(1.16) \qquad \frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(\alpha(x)\frac{\partial u}{\partial x}\right) \qquad (0 < x < 1, 0 < t < T)$$

with

$$u|_{t=0} = a(x) \tag{1.17}$$

and

$$\left.\frac{\partial u}{\partial x}\right|_{x=0,1} = 0 \tag{1.18}$$

from the outputs

$$u|_{x=0} = f_0(t) \quad \text{and} \quad u|_{x=1} = f_1(t) \qquad (\,0 < t < T\,) \tag{1.19}$$

by prescribing the parameter

$$L = \int_0^1 \frac{dx}{\sqrt{a(x)}} \tag{1.20}$$

We note that such a parameter as L is not prescribed in our theorem. Finally, our problem is rather more close to that of Suzuki [6] regarding the point (i). In fact, the infinite degree of nonuniqueness of $(\,p, h, H\,)$ is proven in

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - p(x)u \qquad (\,0 < x < 1,\ 0 < t < T\,) \tag{1.21}$$

with

$$u|_{t=0} = a(x) \qquad (\,0 < x < 1\,) \tag{1.22}$$

and

$$-\frac{\partial u}{\partial x} + h\,u\Big|_{x=0} = \frac{\partial u}{\partial x} + H\,u\Big|_{x=1} = 0 \qquad (\,0 < t < T\,) \tag{1.23}$$

for the outputs

$$u|_{x=0} = f_0(t) \quad \text{and} \quad u|_{x=x_1} = f_1(t) \qquad (\,0 < t < T\,) \tag{1.24}$$

with $x_1 \neq 1$, in spite that the generic uniqueness of $(\,p, h, H, a\,)$ has been established in the same problem of $x_1 = 1$ by [3] or [5]. This suggests that uniqueness is rather crucial in our theorem. The generic uniqueness actually holds for $x_1 \geq \frac{1}{2}$ by adding the output

$$g_1 = \left.\frac{\partial u}{\partial x}\right|_{x=x_1} \qquad (\,0 < t < T\,) \tag{1.25}$$

to f_0 and f_1 in (1.24). However, it looks hard to pick up such an output g_1 in the actual situation of ours.

2 Spectral data

For $P = (p,\, h,\, H) \in C^0[0,1] \times \boldsymbol{R} \times \boldsymbol{R}$, let A_P be the Sturm-Liouville operator $-\frac{d^2}{dx^2} + p(x)$ under the boundary condition $(-\frac{d}{dx} + h)\cdot|_{x=0} = (\frac{d}{dx} + H)\cdot|_{x=1} = 0$. Its eigenvalues and eigenfunctions are denoted by $\{\lambda_n\}_{n=0}^{\infty}$ and $\{\varphi_n(\,\cdot\,; P)\}_{n=0}^{\infty}$, respectively, the latter being normalized as $\|\varphi_n\|_{L^2(0,1)} = 1$, and $\varphi_n(0) > 0$.

We call the quantities $S(P) := \{\lambda_n,\, \dfrac{\varphi_n(1)}{\varphi_n(0)}\}_{n=0}^{\infty}$ the spectral data. The following assertion follows from Gel'fand-Levitan's theory [2] :

Theorem 2 *The coefficients $P = (p,\, h,\, H)$ is recoverd by the spectral data S(P).*

The proof is given in [5] for instance, under the assumption of $p \in C^1[0,1]$. We can extend the results to the general case $p \in C^0[0,1]$ by the method of [7].

3 Outline of the Proof

The unique solvability of

(3.1) $$\frac{\partial u}{\partial t} = KV_+\{\frac{\partial^2 u}{\partial x^2} - \frac{1}{K}\frac{\partial u}{\partial x}\} \qquad (l < x < +\infty,\ 0 < t < +\infty)$$

with

(3.2) $$u|_{t=0} = 0$$

and

(3.3) $$u|_{x=l} = g(t), \qquad u \in O(1) \quad \text{as } x \to +\infty \qquad (0 < t < +\infty)$$

is well known. Here, $V_+ = V(x)$ $(l < x < +\infty)$ is a positive constant. We first calculate the value

(3.4) $$m(t) = KV_+\frac{\partial u}{\partial x}\bigg|_{x=l+0} \qquad (0 < t < T)$$

Next we consider

(3.5) $$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\{KV(x)(\frac{\partial u}{\partial x} - \frac{1}{K}u)\} \qquad (0 < x < l,\ 0 < t < T)$$

with

$$u|_{t=0} = 0 \qquad (0 < x < l)\,, \tag{3.6}$$

$$KV\frac{\partial u}{\partial x}\bigg|_{x=0} = f(t)\,, \quad u|_{x=l} = g(t) \qquad (0 < t < T)\,, \tag{3.7}$$

and

$$KV\frac{\partial u}{\partial x}\bigg|_{x=l-0} = m(t) \qquad (0 < t < T)\,. \tag{3.8}$$

Introducing the Liouville transformation

$$z = \int_0^x \frac{dy}{\sqrt{KV(y)}}\,, \tag{3.9}$$

we can deduce the equation

$$\frac{\partial U}{\partial t} = \frac{\partial^2 U}{\partial z^2} - p(z)U \qquad (0 < z < L\,, 0 < t < T)\,, \tag{3.10}$$

with

$$U|_{t=0} = 0 \qquad (0 < z < L)\,, \tag{3.11}$$

$$-\frac{\partial U}{\partial z} + hU\bigg|_{z=0} = F(t)\,, \quad \frac{\partial U}{\partial z} + HU\bigg|_{z=L} = M(t) \qquad (0 < t < T)\,, \tag{3.12}$$

and

$$U|_{z=L} = J(t) \qquad (0 < t < T) \tag{3.13}$$

in the previous section. Here, the non-homogeneous term $F = F(t), M = M(t)$, and $J = J(t)$ is determined by the functions $f = f(t)$ and $g = g(t)$. We want to derive a closed relation for f and g through (3.10)-(3.13). Namely,

$$\int_0^t K_3(t-s)g'(s)ds = \int_0^t K_4(t-s)f(s)ds \qquad (0 < t < T)\,. \tag{3.14}$$

Therefore, the input $f \not\equiv 0$ and the output g determine the meromorphic function

$$\frac{\hat{K}_4(\lambda)}{\hat{K}_3(\lambda)} \quad \text{in} \quad \lambda \in C\,, \tag{3.15}$$

which determines the values

$$K,\ V(l \pm 0),\ V'(l-0)$$

as well as the spectrtal data

$$\left\{\lambda_n,\ \frac{\varphi_n(L)}{\varphi_n(0)}\right\}_{n=0}^{\infty} \tag{3.16}$$

of Ap.

From theorem 2 in §2, the latters determine

$$p = p(z)\ (0 \leq z \leq)\ ,\ h \text{ and } H \tag{3.17}$$

so does $V(x) = \dfrac{1}{Kz'(x)^2} \quad (0 \leq x \leq l)$.

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