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VARIATIONAL METHODS IN ANALYSIS AND MATHEMATICAL PHYSICS

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OPTIMAL CONTROL OF AN IMMOBILIZED ENZYME SYSTEM

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OPTIMAL CONTROL

OF AN IMMOBILIZED ENZYME SYSTEM

This lecture presents an application of the optimal control techniques for an immobilized enzyme system. This work has been done by J. HENRY (INRIA) and G. GELLF (University of Compiègne).

INTRODUCTION.

Enzymes are proteins which are a catalytic activity for many biochemical reactions. A continuous use of this catalytic activity is of a great interest in numerous industrial applications. Here the modelization and the control of a packed bed enzyme reactor are considered. We present successively the following points :

- Physical problem and its mathematical formulation,

- Theorical results for the state equation and the optimal control problem,

- Discretization and numerical results.

For details, we refer to G. GELLF - J. HENRY [1], J. HENRY [2].

I - PHYSICAL PROBLEM and MATHEMATICAL FORMULATION.

In a packed bed enzyme reactor, the enzymes are immobilized by a cocrossliking procedure into purely proteic particles. The particles are packed into a thermostated column which is continuously

flowed through by the substrate. The outlet product concentration is mesured as a function of : flow rate, inlet substrate concentration, enzyme activity and kinetics.

The optimal control problem is to determine the flow rate to obtain a given output substrate concentration.

I-1) The state equation.

We consider the two-dimensional case. We denote by S (x,t) the substrate concentration. We have two phases : the bulk solution and the enzyme insoluble phase (membraneous phase). In this modelization, the membraneous phase is assumed to be plane.

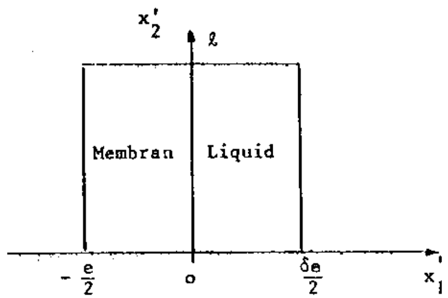

Figure 1.1.

Leet e be the thickness of the membran. The thickness the bulk solution is equal to $\frac{\delta e}{2}$, $\delta = \frac{\gamma}{1-\gamma}$ (γ voidage coefficient of the column). So the domain Ω, where we consider, the phenomena is given figure 1.1.

We consider the case without diffusion in the direction of the flow (ox'_2). So we have for $S(x'_1, x'_2, t)$ the following equations :

in the liquid phase :

$$\frac{\partial S}{\partial t'} + c'(x'_1)\frac{\partial S}{\partial x'_2} - D_L \frac{\partial^2 S}{\partial x_1'^2} = 0 \quad (1.1)$$

in the membraneous phase :

(1.2) $$\frac{\partial S}{\partial t'} - D_M \frac{\partial^2 S}{\partial x_1'^2} + V_M \frac{S}{K_M + S} = 0$$

with the boundary conditions :

(1.3) $$S(x_1', 0, t') = S_e(t')$$

(1.4) $$\frac{\partial S}{\partial x_1'}\left(\frac{\delta e}{2}, x_2', t'\right) = 0$$

the transmission conditions :

(1.5) $$S(0_-, x_2', t') = S(0_+, x_2', t')$$

(1.6) $$D_M \frac{\partial S}{\partial x_1'}(0_-, x_2', t') = D_L \frac{\partial S}{\partial x_1'}(0_+, x_2', t')$$

and the initial condition :

(1.7) $$S(x_1', x_2', 0) = S_0(x_1', x_2')$$

By using the following dimensionless parameters :

$$s = \frac{S}{K_M} \;;\; x_1 = \frac{2x_1'}{e} \;;\; x_2 = \frac{x_2'}{\ell} \;;\; t = t'\frac{c_m}{\ell}$$

$$\sigma = \frac{V_M \ell}{K_M c_m} \;;\; \mu_M = \frac{4 D_M \ell}{e^2 c_m} \;;\; \mu_L = 4\frac{D_L \ell}{e^2 c_m} \;;\; c(x_1) = \frac{c'(x_1')}{c_m}$$

with

$$\frac{\delta_e}{2} c_m = \int_0^{\frac{\delta_e}{2}} c'(x_1')\, dx_1'$$

we obtain for the state equation :

(1.8) $$\frac{\partial s}{\partial t} + c(x_1)\frac{\partial s}{\partial x_2} - \mu_L \frac{\partial^2 s}{\partial x_1^2} = 0 \qquad 0 \le x_1 \le \delta ,\; 0 \le x_2 \le 1$$

(1.9) $$\frac{\partial s}{\partial t} - \mu_M \frac{\partial^2 s}{\partial x_1^2} + \sigma \frac{s}{1+|s|} = 0 \qquad -1 \le x_1 \le 0 ,\; 0 \le x_2 \le 1$$

with the corresponding boundary conditions:

(1.10) $$s(x_1, 0, t) = \alpha(t)$$

(1.11) $$\frac{\partial s}{\partial x_1}(\delta, x_2, t) = 0$$

and the initial condition

(1.12) $$s(x_1, x_2, 0) = s_0(x_1, x_2)$$

We obtain the following variational equation (we suppose c (x,t) = d (t) c (x_1)).

(1.13) $$\begin{cases} \left(\frac{\partial s}{\partial t}, \varphi\right) + d(t)\left(c(x_1)\frac{\partial s}{\partial x_2}, \varphi\right)_L + a(s,\varphi) + (f(s),\varphi)_M = 0 \qquad \forall \varphi \in V = H^1(-1,\delta) \\ s(x_1, 0, t) = d(t) \in L^2(0,T) \;;\; s(x_1, x_2, 0) = s_0 \ge 0 \end{cases}$$

with

$$a(y,\varphi) = \mu_M \int_{\Omega_M} \frac{\partial y}{\partial x_1}\frac{\partial \varphi}{\partial x_1} dx_1 dx_2 + \mu_L \int_{\Omega_L} \frac{\partial y}{\partial x_1}\frac{\partial \varphi}{\partial x_1} dx_1 dx_2$$

$$f(s) = \sigma \frac{s}{1+|s|}$$

$$(\varphi,\psi)_L = \int_{\mathcal{O}_L} \varphi \psi \, d\mathcal{O} \;;\; (\varphi,\psi)_M = \int_{\mathcal{O}_M} \varphi\psi \, d\mathcal{O}$$

$$\mathcal{O}_L =]0,\delta[\;;\; \mathcal{O}_M =]-1,0[\;;\; \mathcal{O} =]-1,\delta[$$

$$\Omega_L = \mathcal{O}_L \times]0,1[\;;\; \Omega_M = \mathcal{O}_M \times]0,1[\;;\; \Omega = \mathcal{O} \times]0,1[$$

I-2) The optimal control problem.

- The control variable is d(t).
- The admissible space of control $\mathcal{U}_{ad}$

(1.20) $$\mathcal{U}_{ad} = \{ d \in L^\infty(0,T) \mid 0 < d_0 \le d \le d_1 \}$$

- The observation

$$(1.21) \quad z(t) = \int_0^S c(x_1)\, s(x_1,1,t)\, dx_1$$

- The functional :

$$(1.22) \quad J(d) = \frac{1}{2}\int_0^T |z(t) - z_d(t)|^2\, dt \qquad \text{(where } z_d \text{ is a given function)}$$

Then, we have the optimal control problem :

$$(1.23) \begin{cases} \text{To find } d^*(t) \in \mathcal{U}ad \text{ s.t.} \\ J(d^*) \le J(d) \quad \forall d \in \mathcal{U}ad \end{cases}$$

II - THEORICAL RESULTS.

In this chapter, the main theoritical results are presented. For details of the demonstration, we refer to J. HENRY [2].

II-1) State equation.

We suppose that :

$$\left| \begin{array}{l} d \in \mathcal{U}_{ad} \cap W^{1,\infty}(0,T) \;;\; d \in H^1(0,T) \\ s^0 \in H^1(0,1; L^2(\mathcal{O})) \cap L^1(0,1; \mathcal{D}(A)) \;;\; s = \alpha(0) \end{array} \right.$$

Then we have the proposition :

Proposition 2.1. The problem (1.13) has a unique solution in $L^2(\mathbb{R}, \mathcal{V})$ of the form $s = s^0 + y$.

where s^0 is solution of (1.8)-(1.12) with $\sigma = o$.

The solution is obtain as the limit of the problem with diffusion on the direction ox_2, by using, in particular, techniques of singular perturbation.

II-2) Optimal control problem.

Proposition 2.2: The optimal control problem (1.23) has a solution $d^* \in ad$.

Idea of the demonstration :

If we consider d_n a minimizing sequence of J. We obtain the a priori estimates

$s_n = s(d_n)$ is bounded in $L^2(\mathcal{Q}, \mathcal{V})$ $\qquad \mathcal{Q}_0 =]0,T[\times]0,1[\;\; ((t,x_2))$

$\dfrac{\partial s_n}{\partial t} + d_n \tilde{c} \dfrac{\partial s_n}{\partial x_2}$ is bounded in $L^2(\mathcal{Q}, \mathcal{V}')$.

(Where $\tilde{c}$ is the extension by zero of c in Ω.)

$f(s_n)$ is bounded in $L^\infty(Q_M)$

By using lemmas of compacity for Sobolev spaces and monotonicity method, we prove that there exist a subsequence $\{d_\mu, s_\mu\}$ such that

$d_\mu \longrightarrow d^*$ in $L^\infty(0,T)$ weak-star

$s_\mu \longrightarrow s$ in $L^r(\mathcal{Q}, \mathcal{V})$ strongly.

$\dfrac{\partial s_\mu}{\partial t} + d_\mu \tilde{c} \dfrac{\partial s_\mu}{\partial x_2} \longrightarrow \dfrac{\partial s}{\partial t} + d^* \tilde{c} \dfrac{\partial s}{\partial x_2}$ in $L^2(\mathcal{Q}, \mathcal{V}')$ strongly

Then we deduce that :

$$J(d_\mu) \longrightarrow J(d^*)$$

which proves the existence of an optimal control d^*. $\square$

We have the following necessary optimality conditions:

Proposition 2.3. If (d^*, s^*) is a solution of the optimal control (1.23) there exists p^* such that (d^*,s^*,p^*) verifies the necessary optimality conditions :

$$
(2.1)\quad \begin{cases} \left(\dfrac{\partial s^*}{\partial t}, \varphi\right) + d^*\left(c(x_1)\dfrac{\partial s^*}{\partial x_2}, \varphi\right)_L + a(s^*,\varphi) + (\beta(s^*),\varphi)_\Pi = 0 \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \forall \varphi \in \mho \\ s^*(x_1, 0, t) = \alpha(t)\ ; \quad s^*(x_1, x_2, 0) = s_0 \end{cases}
$$

$$
(2.2)\quad \begin{cases} \left(-\dfrac{\partial p^*}{\partial t}, \psi\right) - d^*\left(c(x_1)\dfrac{\partial p^*}{\partial x_2}, \psi\right)_L + a(p^*,\psi) + (\beta'(s^*)p^*, \psi)_\Pi = 0 \\ p^*(x_1, 1, t) = \dfrac{1}{d^*}\left(z^* - z_d(t)\right)\ ; \quad p^*(x_1,x_2,T) = 0 \qquad \forall \psi \in \mho \end{cases}
$$

$$
(2.3)\quad \int_{\mathcal{R}} \left(c(x_1)\frac{\partial s^*}{\partial x_2}, p^*\right)_L (d - d^*)\, dx_2\, dt \leq 0 \qquad \forall d \in \mathcal{U}_{ad} \cap W^{1,\infty}(0,T)
$$

The principal points of the demonstration are :

Point 1 : We prove the existence and the uniqueness of a solution for the adjoint system (2.2).

Point 2 : To obtain the optimality conditions, classicaly we define:

$$
(2.4)\qquad \eta_\lambda = \frac{1}{\lambda}\left(s(d+\lambda w) - s(d)\right)
$$

then η_λ is solution of :

$$
(2.5)\quad \begin{cases} \left(\dfrac{\partial \eta_\lambda}{\partial t}, \psi\right) + (d+\lambda w)\left(c\dfrac{\partial \eta_\lambda}{\partial x_2}, \psi\right)_L + a(\eta_\lambda, \psi) \\ \qquad + \left(\beta'(s(d) + \theta_\lambda \eta_\lambda)\eta_\lambda, \psi\right)_\Pi = -w\left(\dfrac{\partial s(d)}{\partial x_2}, \psi\right)_L \quad \forall \psi \in \mho \\ \eta_\lambda(x_1', 0, t) = 0 \quad ; \quad \eta_\lambda(x_1, x_2, 0) = 0 \end{cases}
$$

With a-priori estimates, by passing at the limit, we obtain that ;

$$
\eta_\lambda \longrightarrow \hat{s}_d(w) \quad \text{in} \quad L^2(\mathcal{R}, \mho) \quad \text{weakly}
$$

solution of :

$$
(2.6)\quad \begin{cases} \left(\dfrac{\partial}{\partial t}\hat{s}_d(w), \psi\right) + d\left(c\dfrac{\partial}{\partial x_2}\hat{s}_d(w), \psi\right)_L + a(\hat{s}_d(w), \psi) \\ \qquad + \left(\beta'(s(d))\hat{s}_d(w), \psi\right)_\Pi = -w\left(c\dfrac{\partial s(d)}{\partial x_2}, \psi\right)_L \\ \qquad\qquad\qquad\qquad\qquad\qquad \forall \psi \in \mho \\ \hat{s}_d(w)(x_1, 0, t) = 0 \ ; \quad \hat{s}_d(w)(x_1, x_2, 0) = 0 \end{cases}
$$

Because the application $w \to \hat{s}_d(w)$ is linear, continuous from $L^\infty(0,T)$ into $W = \left\{ s \mid s \in L^2(\mathcal{R}, \mho)\ ,\ \dfrac{\partial s}{\partial t} + d\tilde{c}\dfrac{\partial s}{\partial x_2} \in L^2(\mathcal{R}, \mho') \right\}$

we deduce that $d \to s(d)$ is G-differentiable.

Then J is G-differentiable and we have :

$$
\langle J'(d), w \rangle = \int_0^T (z(t) - z_d(t)) \int_0^\delta c(x_1)\, \hat{s}_d(w)(x_1, 1, t)\, dx_1\, dt
$$

If we introduce the adjoint state p solution of (2.2), we obtain :

$$
(2.7)\quad \langle J'(d), w \rangle = \int_0^T \int_0^\delta d\, c(x_1)\, p(x_1, 1, t)\, \hat{s}_d(w)(x_1, 1, t)\, dx_1\, dt.
$$

If we take $\phi = \hat{s}_d(w)$ in (2.2) and if we integrate on $[0,1] \times [0,T]$ we obtain :

$$\int_0^T\int_0^1 \left(-\frac{\partial p}{\partial t}, \hat{s}\right) dx_1 dx_2 dt + \int_0^T\int_0^1 (c(x_1) d \frac{\partial \hat{s}_d(w)}{\partial x_2}, p)_L \, dx_2 dt$$

$$+ \int_0^T\int_0^1 a(p, s_d(w))\, dx_2 dt + \int_0^T\int_0^1 (g'(s(d))p, \hat{s}_d(w))_M \, dx_2 dt$$

$$= \int_0^T\int_0^\delta d\, c(x_1)\, p(x_1,1,t)\, \hat{s}_d(w)(x_1,1,t)\, dx_1 dt = \langle J_d', w\rangle$$

Then, with (2.6), we obtain :

$$\langle J'(d), w\rangle = -\int_{R_0} \left(c \frac{\partial}{\partial x_2} s(d), p(d)\right)_L w \, dx_2 \, dt$$

From which, we deduce (2.3).

$\square$

III - DISCRETIZATION AND NUMERICAL RESULTS.

We have use the following finite-difference scheme

Step 1 :

in Q_M $$s_{i,j}^{n+1/2} = s_{i,j}^{n} - k\sigma \frac{s_{i,j}^n}{1+s_{i,j}^n}$$

in Q_L $$s_{i,j}^{n+1/2} = s_{i,j}^{n}\left(1 - k^2\frac{c_i^2}{h_2^2}\right) - s_{i,j+1}^{n}\left(\frac{kc_i}{2h_2} - \frac{k^2c_i^2}{2h_2^2}\right) + s_{i,j-1}^{n}\left(\frac{kc_i}{2h_2} + k^2\frac{c_i^2}{2h_2^2}\right)$$

Step 2 :

in Q_M $$s_{i,j}^{n+1} - k\frac{\mu_M}{h_1^2}\left(s_{i-1,j}^{n+1} - 2s_{i,j}^{n+1} + s_{i+1,j}^{n+1}\right) = s_{i,j}^{n+1/2}$$

in Q_L $$s_{i,j}^{n+1} - \frac{k\mu_L}{h_1^2}\left(s_{i-1,j}^{n+1} - 2s_{i,j}^{n+1} + s_{i+1,j}^{n+1}\right) = s_{i,j}^{n+1/2}$$

- Optimization.

A conjugate gradient algorithm (Polak-Ribière) with projection is used to compute an optimal control.

- Numerical results.

Some numerical results are given Figures 3.1 - 3.2.

- $z_d(t)$ is obtained as the solution of the system for $d(t) = 0{,}5$ and $\alpha(t) = 1$.

- The constraints for $d(t)$ are $0{,}1 \le d \le 1$.

- We presented the computed optimal control for perturbations on $\alpha(t)$

i) Figure 3-1 for

$$\alpha(t) = \begin{cases} 1+0{,}5 \sin 2\pi t & t<0{,}5 \\ 1 & t\ge 0{,}5 \end{cases}$$

ii) Figure 3-2 for

$$\alpha(t) = \begin{cases} 1+0{,}2 \sin \pi t & t< 1 \\ 1 & t\ge 1 \end{cases}$$

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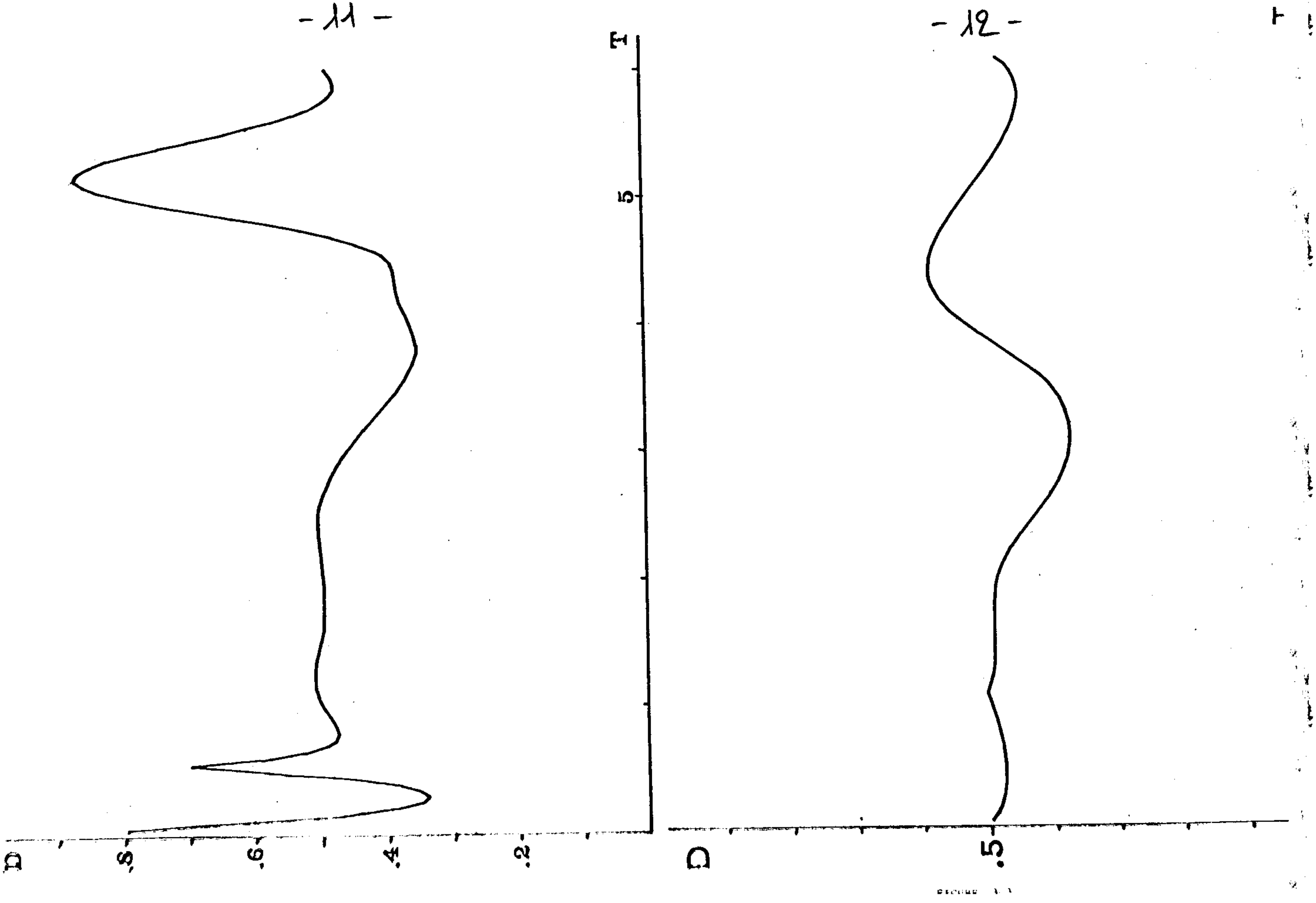
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