

Optimal dosage in a micro-pipe

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1 Introduction

Optimization of scalar dispersion in pipe is a long standing problem related to several field of science and engineering, including classical chemical, biological and environmental problems. One of the most interesting challenge is the feeding of a biological system with an optimal concentration of substances. In this context, this project propose an optimal model for scalar intake in a micro-pipe, using an adjoint-based optimization technique. The system is considered in an input/output framework where we measure the concentration profile in a target section in order to control the inlet. The problem is modelled in 2-dimension by the advection-diffusion equation (also known as scalar transport equation) considering a fully developed laminar flow.

2 Problem formulation

In order to model the dispersion of a substance in a micro-pipe, we consider the dimensionless 2-D, isotropic, homogeneous advection-diffusion-reaction equation. The fluid is considered incompressible while the flow is laminar and fully developed, resulting in parabolic velocity profile (Poiseuille profile):

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} - \frac{1}{Pe} \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right) + rC - S = 0 \quad (1)$$

$$0 \leq x \leq L \quad -D/2 \leq y \leq D/2 \quad 0 \leq t \leq T$$

$$u = U(1 - y^2) \quad (2)$$

with homogeneous conditions on the streamline boundary

$$C(0, y, t) = 0 \quad C(L, y, t) = 0 \quad (3)$$

and no-flux conditions on the pipe walls.

$$\left. \frac{\partial C}{\partial y} \right|_{y=-D/2} = 0 \quad \left. \frac{\partial C}{\partial y} \right|_{y=D/2} = 0 \quad (4)$$

The initial condition is given by

$$C(x, y, 0) = 0 \quad (5)$$

$C(x, y, t)$ is the concentration of a scalar quantity of interest, $u(y)$ is the non-dimensional velocity field, Pe is the Peclet non-dimensional number, r is the non-dimensional reaction rate, $S(x, y, t)$ is the non-dimensional emission rate and U is the center-line velocity. $Pe = \frac{UD}{d}$ measures the relative importance of advection compared to diffusion (with an homogeneous and isotropic diffusivity d and a pipe dimension D). We can also define the Schmidt number $Sc = \frac{\nu}{d}$, where ν is the kinematic viscosity, and consider that $Pe = ReSc$.

A sketch of the computational domain is shown in Figure 1. The source term $S(x, y, t)$ represent a 2-

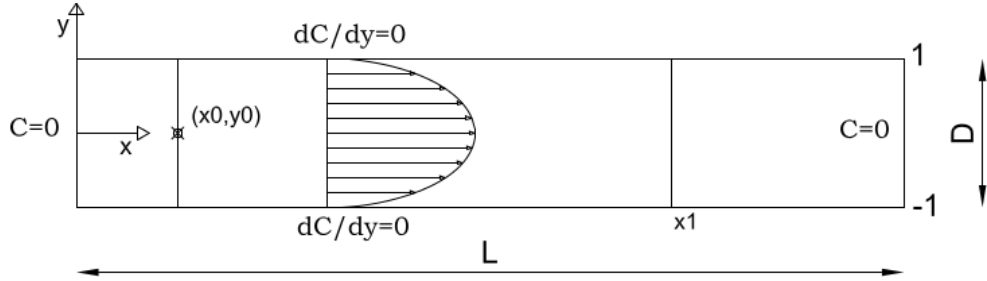


Figure 1: Domain for the control problem and boundary conditions

dimensional fixed point source located in (x_0, y_0) :

$$S(x, y, t) = s(t)\delta(x - x_0)\delta(y - y_0) \quad (6)$$

where $s(t)$ represent the inlet quantity at time dt (control term) and δ is the Dirac delta. Considering its properties, the following relation is obtained:

$$\iiint S(x, y, t) dx dy dt = \iiint [s(t)\delta(x - x_0)\delta(y - y_0)] dx dy dt = \int s(t) dt \quad (7)$$

In order to reach a certain concentration at the target section X_1 or, in other terms, to minimize the discrepancy with a target concentration, the following objective function J is chosen:

$$J = \iint f[C(x, y, T) - C_0]^2 dx dy + \frac{1}{2}\gamma \int [s(t)]^2 dt \quad (8)$$

where $f = e^{-(x-x_1)^6}$ is a bell shaped function centred in X_1 , C_0 is the target concentration to be reached in x_1 and γ is a regularization term. The second term of the objective function represents the cost of the

scalar inlet quantity and it also has the purpose to put a limit on the control. Linearizing the equation, setting $C \rightarrow C + \delta C$ and $s \rightarrow s + \delta s$:

$$\delta J = \iint f \delta C [C(x, y, T) - C_0] dx dy + \gamma \int [s(t) \delta s] dt \quad (9)$$

3 Optimization

Optimization is done using Lagrange multipliers , in order reach the optimal solution in a very quick way.

If we consider (1),(3),(8), the Lagrangian function is defined as:

$$\begin{aligned} \delta \mathcal{L} = & \iint f \delta C [C(x, y, T) - C_0] dx dy + \gamma \int [s \delta s] dt - \\ & \iiint a \left[\frac{\partial \delta C}{\partial t} + U \frac{\partial \delta C}{\partial x} - \frac{1}{Pe} \nabla^2 \delta C - \delta S + r \delta C \right] dx dy dt - \iint b [\delta C(0, y, T) - 0] dy dt \\ & - \iint c [\delta C(L, y, t) - 0] dy dt - \iint d \left[\frac{\partial \delta C(x, 1, t)}{\partial y} - 0 \right] dx dt - \\ & \iint e \left[\frac{\partial \delta C(x, -1, t)}{\partial y} - 0 \right] dx dt - \iint g [\delta C(x, y, 0) - 0] dx dy \end{aligned} \quad (10)$$

were $\delta \mathcal{L}(C, s, a, b, c, d, e, g)$ is the linearized Lagrangian, $a(x, y, t), b(y, t), c(y, t), d(x, t), e(x, t), g(x, y)$ are the Lagrangian multipliers. Thus, setting the gradient of \mathcal{L} equal to zero, we are looking for the stationary point, obtaining the necessary conditions for the problem resolution:

- $\frac{\partial \mathcal{L}}{\partial a} = 0 \rightarrow \frac{\partial \delta C}{\partial t} + U \frac{\partial \Delta C}{\partial x} - \frac{1}{Pe} \nabla^2 \delta C - S + r \Delta C = 0$
- $\frac{\partial \mathcal{L}}{\partial b, c} = 0 \rightarrow C(0, y, T) = 0 ; C(L, y, t) = 0$
- $\frac{\partial \mathcal{L}}{\partial d, e, g} = 0 \rightarrow \frac{\partial C}{\partial y} \Big|_{y=-D/2} = 0 ; \frac{\partial C}{\partial y} \Big|_{y=D/2} = 0 ; C(x, y, 0) = 0$
- $\frac{\partial \mathcal{L}}{\partial C} = 0 \rightarrow$

$$-\frac{\partial a}{\partial t} - U \frac{\partial a}{\partial x} - \frac{1}{Pe} \nabla^2 a + rC = 0 \quad (11)$$

$$a(x, y, T) = 2f(C(x, y, T) - C_0) \quad (12)$$

$$a(X, y, t) = a(0, y, t) = 0 \quad (13)$$

$$\frac{\partial a}{\partial y} \Big|_{y=D/2} = \frac{\partial a}{\partial y} \Big|_{y=-D/2} = 0 \quad (14)$$

- $\frac{\partial \mathcal{L}}{\partial s} = 0$

$$s(t) = -\frac{a(x_0, y_0, t)}{\gamma} \quad (15)$$

The equation (11) is the *adjoint equation* while the (12),(13) and (14) are the boundary and initial conditions that define the adjoint problem. Eq.(15) is called *optimality condition* and define the optimal control of $s(t)$.

4 Numerical approach

The optimization problem is solved numerically, in 2-dimensions and the partial derivatives are discretized using a finite difference methods implemented in Matlab environment. The following iterative scheme is used:

- forward integration of the state equation;
- evaluation of the cost function;
- backward integration of the adjoint and accuracy check;
- update the control function via the optimality equation.

These steps have been embedded inside a loop stopping when convergence on \mathbf{J} is reached. Both the direct and the adjoint system are discretized using the simple FTCS scheme (Forward Time, Central Space) that is explicit, first order accurate in time and second order accurate in space. The diffusion part use a 5-point stencil. The discrete form of the direct equation (1) is:

$$\frac{C_{i,j}^{n+1} - C_{i,j}^n}{\Delta t} + u \frac{C_{i+1,j}^n - C_{i-1,j}^n}{2 \Delta s} = \frac{1}{Pe} \frac{C_{i+1,j}^n + C_{i-1,j}^n + C_{i,j+1}^n + C_{i,j-1}^n - 4 C_{i,j}^n}{\Delta s^2} - r C_{i,j}^n + S^n \quad (16)$$

that leads to the the following system:

$$C_{i,j}^{n+1} = \left(1 - \frac{4 \Delta t}{Pe \Delta s^2} - r \Delta t\right) C_{i,j}^n + \left(\frac{\Delta t}{Pe \Delta s^2} - \frac{u \Delta t}{2 \Delta s}\right) C_{i+1,j}^n + \left(\frac{\Delta t}{Pe \Delta s^2} + \frac{u \Delta t}{2 \Delta s}\right) C_{i-1,j}^n + \left(\frac{\Delta t}{Pe \Delta s^2}\right) C_{i,j+1}^n + \left(\frac{\Delta t}{Pe \Delta s^2}\right) C_{i,j-1}^n + S_{i,j} \Delta t \quad (17)$$

where i and j indicate respectively the streamwise and spanwise index, n represent the time index. Introducing the linear operator \mathbf{A} , the vectorial form of the system is:

$$\hat{C}^{m+1} = \mathbf{A} \hat{C}^n + \Delta t \hat{S}^n \quad (18)$$

The matrix \mathbf{A} is structured using a natural rowwise ordering, composed by a tridiagonal matrix T and two diagonal matrix $I_f I_b$. The resulting scheme is:

$$A = \begin{bmatrix} T & I_f & & & \\ I_b & T & I_f & & \\ & & \ddots & \ddots & \ddots \\ & & & I_b & T \end{bmatrix} \quad T = \begin{bmatrix} k1 & k2 & & & \\ k2 & k1 & k2 & & \\ & \ddots & \ddots & \ddots & \\ & & & k2 & k1 \end{bmatrix} \quad I_f = \begin{bmatrix} k3 & & & & \\ & \ddots & & & \\ & & & & \\ & & & & k3 \end{bmatrix} \quad I_b = \begin{bmatrix} k4 & & & & \\ & \ddots & & & \\ & & & & \\ & & & & k4 \end{bmatrix}$$

where $k1 = (1 - \frac{4 \Delta t}{Pe \Delta s^2} - r \Delta t)$, $k2 = (\frac{\Delta t}{Pe \Delta s^2})$, $k3(y) = (\frac{\Delta t}{Pe \Delta s^2} - \frac{u \Delta t}{2 \Delta s})$, $k4(y) = (\frac{\Delta t}{Pe \Delta s^2} + \frac{u \Delta t}{2 \Delta s})$.

Stability is performing using Von Neumann analysis leading to Courant-Friedrichs-Lewy (CFL) condition:

$$\Delta t \leq \frac{\Delta s}{u} \quad (19)$$

It requires that the time step must be smaller than the time it takes fluid to travel between grid points.

The same approach is used for the adjoint equation and the resulting scheme is:

$$\frac{a_{i,j}^{n-1} - a_{i,j}^n}{\Delta t} - u \frac{a_{i+1,j}^n - a_{i-1,j}^n}{2\Delta s} = \frac{1}{Pe} \frac{a_{i+1,j}^n + a_{i-1,j}^n + a_{i,j+1}^n + a_{i,j-1}^n - 4a_{i,j}^n}{\Delta s^2} \quad (20)$$

$$a^{n-1} = \mathbf{A}^* a^n \quad (21)$$

where the matrix \mathbf{A}^* is:

$$\mathbf{A}^* = \begin{bmatrix} T & I_b & & & \\ I_f & T & I_b & & \\ & \ddots & \ddots & \ddots & \\ & & & I_f & T \end{bmatrix}$$

We can note that the diffusion part of the equation is self-adjoint ($L = L^*$), so $T = T'$, while time derivative and advection part produces a change in the sign of the adjoint.

The accuracy of the adjoint has been checked using the equality $\langle C, \mathbf{A}a \rangle = \langle a, \mathbf{A}^T C \rangle + B.T.$ that leads to:

$$\iint [a(x, y, T)C(x, y, T)] dx dy = \iint [a(x, y, t)S(x, y, t)] dx dy \quad (22)$$

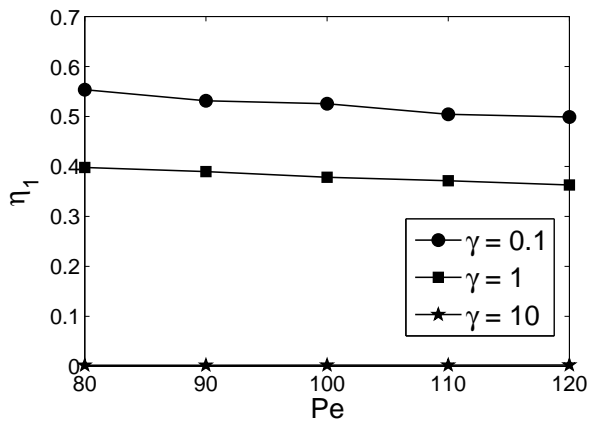
which in all simulation has been less than 10^{-10} , next to machine precision.

5 Results

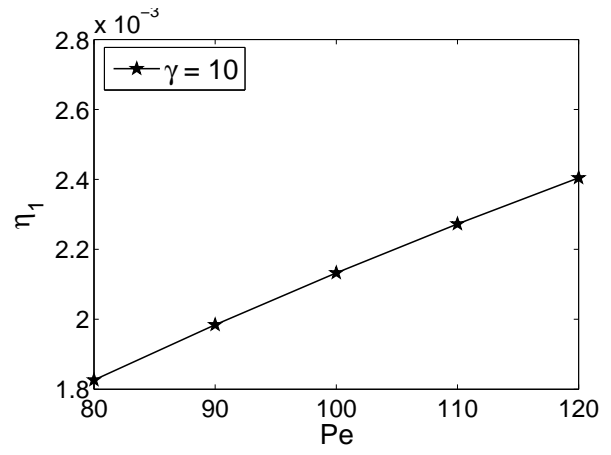
The optimization model is implemented in Matlab environment for a generic case of micro-pipe with a fixed point source in the centerline. The target section is located in the final part of the pipe. The computational test have the following characteristics: $L=6$, $D=1$, $Sc=100$, $Pe=[80,90,100,110,120]$, $\gamma=[0.1,1,10]$, $C_0=10$, $ds=0.02$, $dt=0.002$, $T=7$, $r=0.01$, $x_0=0.012$ L, $y_0=0$, $x_1=0.6$ L. Considering that $Re = \frac{Pe}{Sc}$ the simulated flow have $Re=[0.8,0.9,1,1.1,2]$.

In order to evaluate the result of the optimization system in respect to the target value, an *efficiency variable* is defined as:

$$\eta_1 = \frac{\frac{1}{D} \int_0^D C(x_1, y, T) dy}{C_0} \quad (23)$$



(a) global view



(b) $\gamma = 10$

Figure 2: Efficiency of the optimization system as a function of Peclet number and γ parameter. A detailed view for the case $\gamma=10$ is shown in the right figure.

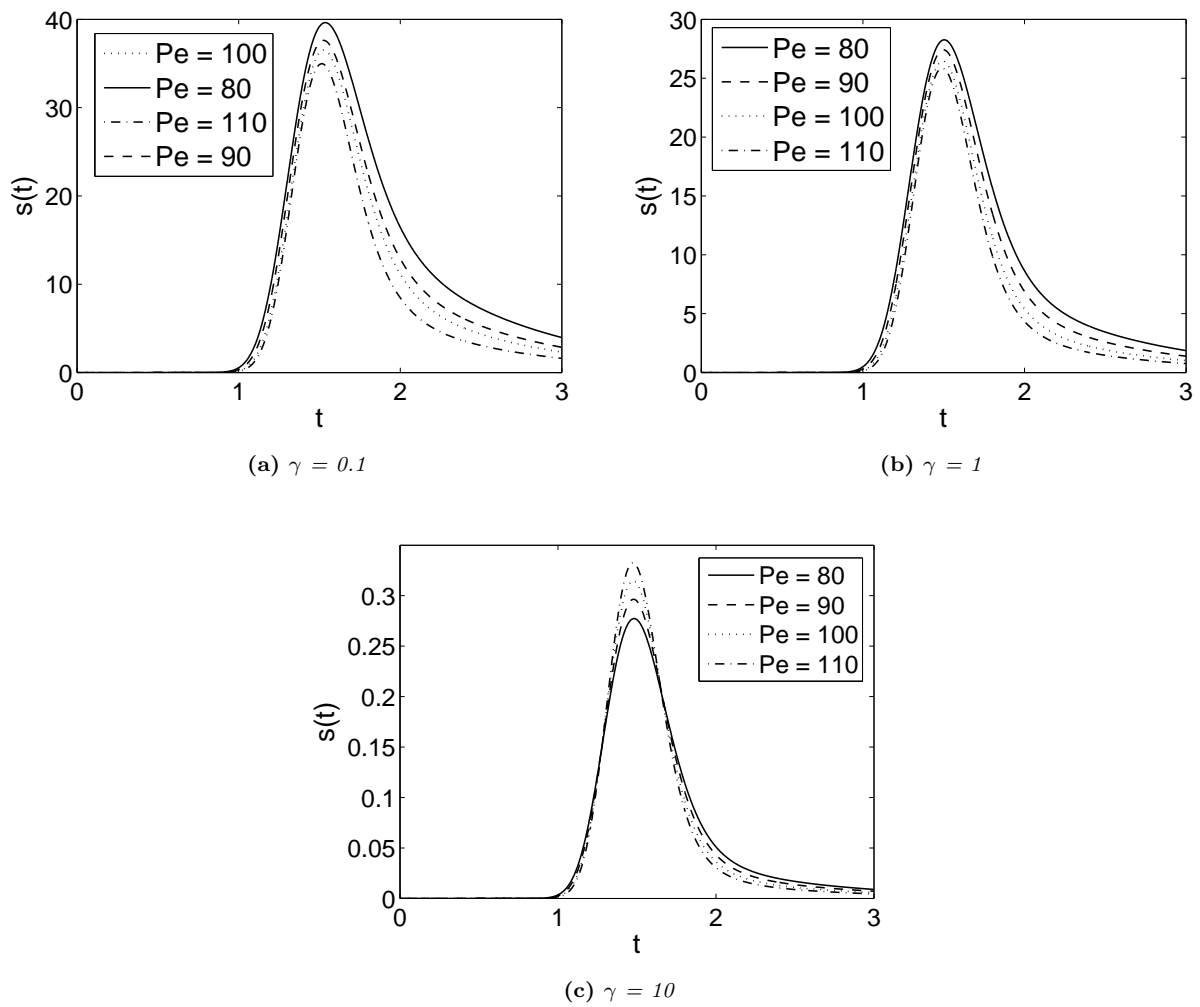


Figure 3: Optimal intake curve $s(t)$ as a function of the Peclet number and γ parameter.

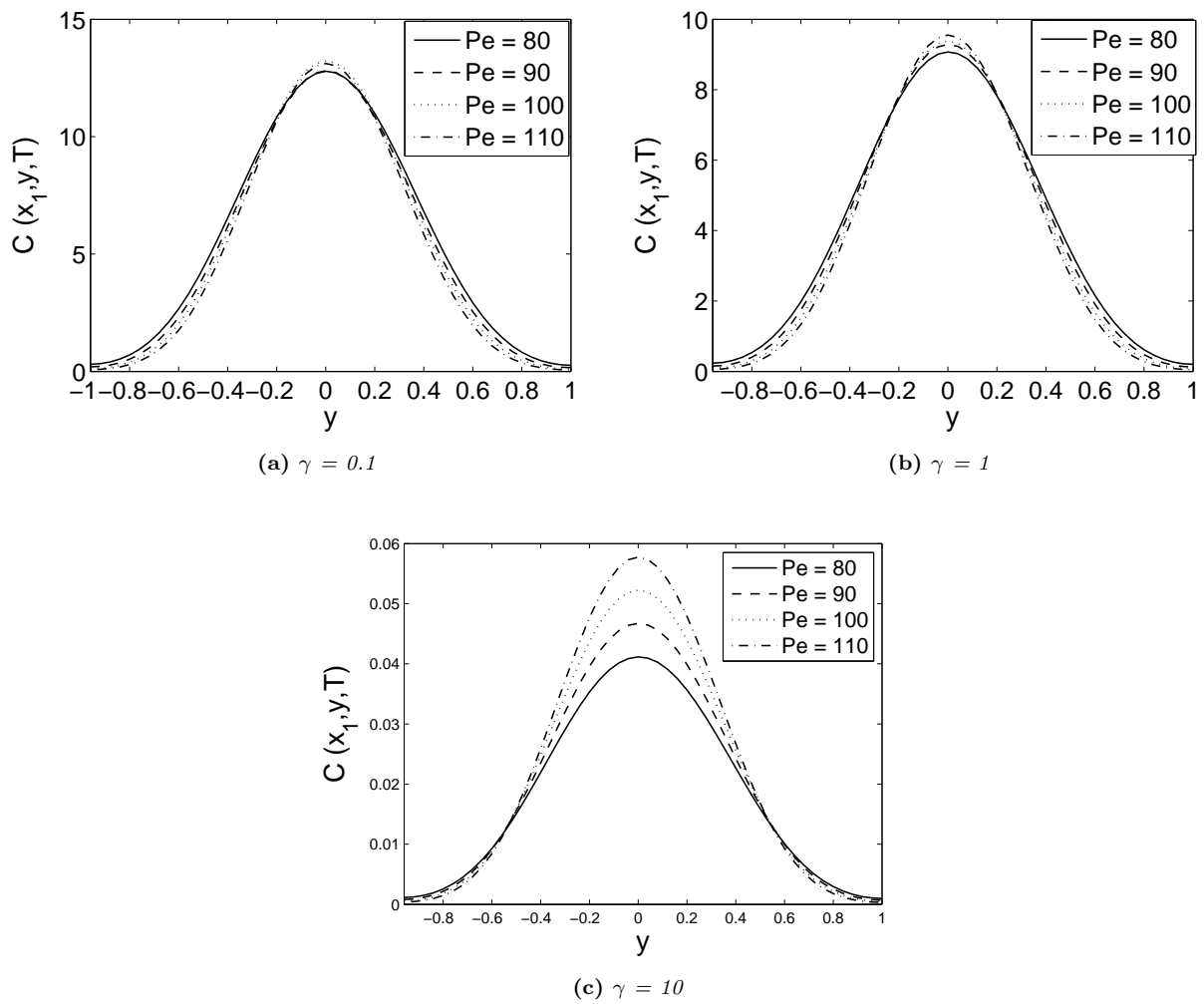
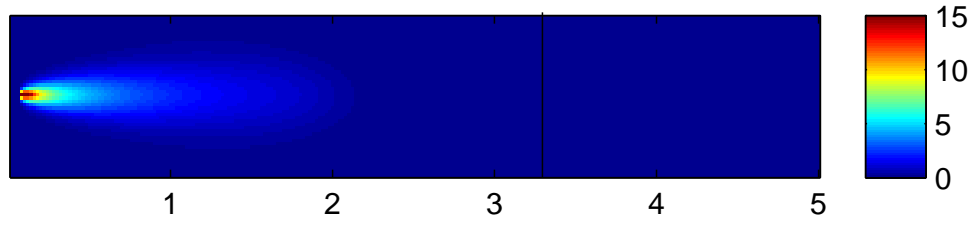
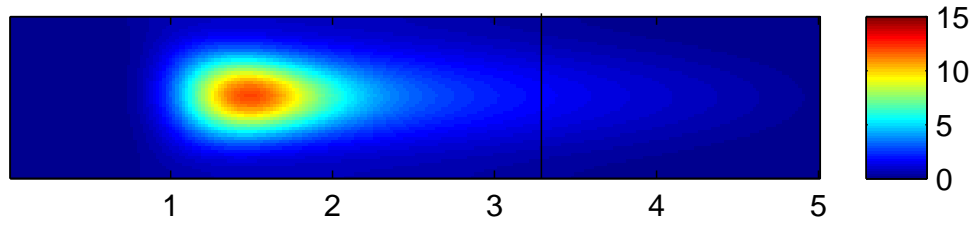


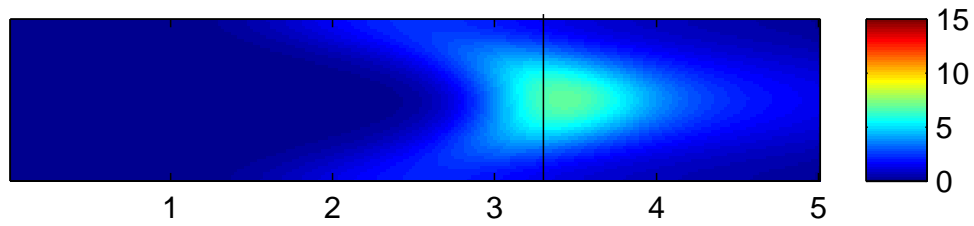
Figure 4: Concentration profile in the target section as a function of the Peclet number and γ parameter.



(a) $t = 2$

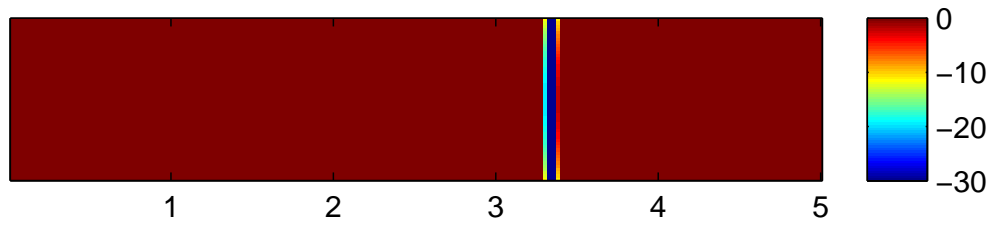


(b) $t = 5$

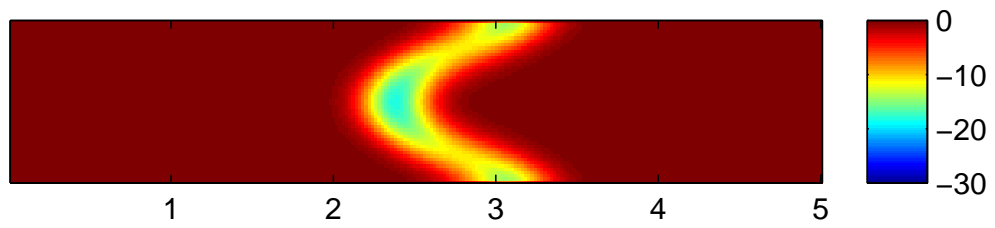


(c) $t = 7$

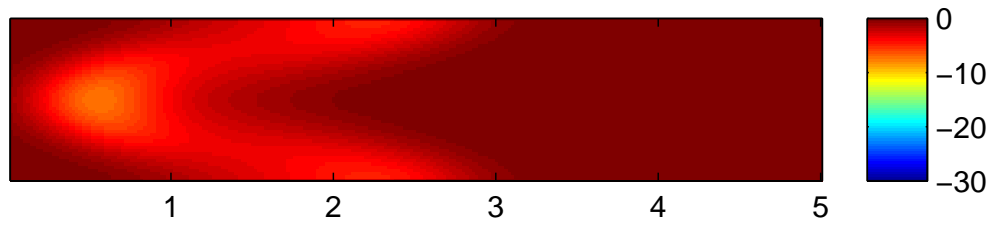
Figure 5: Concentration maps in the case $Pe=100, \gamma=1$ and $T=7$ for some significant frames.



(a) $t = 7$



(b) $t = 5$



(c) $t = 2$

Figure 6: Adjoint variable values in the case $Pe=100, \gamma=1$ and $T=7$ for some significant frames.

6 Conclusions

A model for compute the optimal nutrient intake has been build using an adjoint-based approach. The mathematical problem is based on the advection-diffusion-reaction equation solved iteratively using the finite difference technique. The model, developed in Matlab environment, is applied to a generical domain able to simulate the behaviour in micro-pipe-like condition, very common in biological, chemical and environmental systems. The efficiency of the optimization system is tested considering different flow condition and objective function paramenters, respectively varying the Peclet number and γ . The results indicates that:

- the parameter γ is critical for the behavior of the system. While for $\gamma < 1$ the efficiency is inversely proportional to Pe number, for $\gamma > 1$ the behaviour is reverse. This is because lower Peclet flow "lose" less costly material travelling toward the target. ;
- the performance in term of homogeneous target concentration decrease very quickly increasing γ ;
- the target region show a concentration deficit near the surface due to low spanwise disperision. This problem could be solved using a moving or multipoint source.

7 References

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