

## Protein concentration in a flow chamber

The objective of this exercise is to predict the stationary concentration of paracrine proteins within a flow chamber. The model includes a layer of cells, which release, bind and unbind proteins at the cell surface. The proteins are transported within the fluid by diffusion and advection. In addition, the proteins degrade with a decay rate of  $1/\tau$ . The flow chamber is modeled in 2D. Its dimensions are  $1200\ \mu\text{m}$  and  $250\ \mu\text{m}$ . The fluid flows along the longer dimension. The layer of cell is  $400\ \mu\text{m}$ , in the middle of the longer edge.

Build the geometry of the system. Use the three following “physics” to model the system. Set the initial and boundary conditions of each “physics”, and the coupling between them. You may define constants in *Global Definitions* → *Parameters*. You should define the protein binding process at the surface (*react\_surf*) in *Model* → *Definitions* → *Variable*.

### Fluid Flow → Single-Phase Flow → Laminar Flow (spf)

Domain is flow chamber

Fluid is water

Initial velocity and pressure is 0.

Inlet flow rate is 3 ml/min (entrance thickness 2[cm])

Outlet pressure is 0 Pa

### Chemical Species Transport → Surface Reactions (chsr)

Domain is cell layer

Dependent variable: surface concentration of bound proteins  $c_s$  [mol/m<sup>2</sup>]

Initial concentration:  $c_s = 0$  [mol/m<sup>2</sup>]

Surface properties:

Density of sites:  $R_t = 1\text{e-}8$  [mol/m<sup>2</sup>] (total number of receptors on the surface)

Diffusion coefficient:  $D = 1\text{e-}8$  [m<sup>2</sup>/s]

Reaction:

Reaction rate for surface species:  $\text{react\_surf} = k_{on} \cdot (R_t - c_s) \cdot c - k_{off} \cdot c_s$ , with

$k_{on} = 30$  [m<sup>3</sup>/s/mol] (association rate),

$k_{off} = 6\text{e-}4$  [1/s] (dissociation rate)

$c$  defined below.

### Chemical Species Transport → Transport of Diluted Species (chds)

Domain is flow chamber

Dependent variable: protein concentration  $c$

Velocity field: velocity of laminar flow model

Coefficient of diffusion:  $D = 1\text{e-}8$  [m<sup>2</sup>/s]

Initial protein concentration:  $c = 0$  [mol/m<sup>3</sup>]

Inward flux at cell layer:  $\text{paracrine} - \text{react\_surf}$ , with

$\text{paracrine} = 8\text{e-}7$  [mol/m<sup>2</sup>/s] (protein production by cells)

Reaction within fluid:  $-c/\tau$ , with  $\tau = 0.05$  [s] (half-life of proteins)

Add Outflow condition to let morphogens leave the chamber.

Run a stationary study with the above flow rate, and one without flow (velocity = 0). Plot the morphogen concentration at the cell layer for these two situations.