LESSON 17: REACTION OF SOLUTE WITH DISPERSION

In estuaries and along coastal plain rivers the transport of the solute/pollutant strongly depends also on dispersion. The equation of the transport is the following:

$$\frac{\partial C}{\partial t} + \frac{Q}{A}\frac{\partial C}{\partial x} = \frac{1}{A}\frac{\partial}{\partial x}\left(K_x \frac{\partial C}{\partial x}\right) \mp rC$$

The dynamics of $\tilde{O}$ and BOD is then described by the following system of equations:

$$\begin{cases} \dfrac{\partial B}{\partial t} + \dfrac{Q}{A}\dfrac{\partial B}{\partial x} = \dfrac{1}{A}\dfrac{\partial}{\partial x}\left(K_x A \dfrac{\partial B}{\partial x}\right) - r_d B \\ \dfrac{\partial \tilde{O}}{\partial t} + \dfrac{Q}{A}\dfrac{\partial \tilde{O}}{\partial x} = \dfrac{1}{A}\dfrac{\partial}{\partial x}\left(K_x A \dfrac{\partial \tilde{O}}{\partial x}\right) + r_d B - r_a \tilde{O} \end{cases}$$

The solution of the full equations is only numerical. However an analytical solution is possible under the following assumptions:

- Stationarity, i.e. $\partial/\partial t = 0$
- Homogeneous reach, i.e. K_x, Q and A are constant $\longrightarrow$ $U = \dfrac{Q}{A}$

The two equations of the system now read:

$$\begin{cases} \dfrac{d^2 B}{dx^2} - \dfrac{U}{K_x}\dfrac{dB}{dx} - \dfrac{r_d}{K_x} B = 0 & (1) \\ \dfrac{d^2 \tilde{O}}{dx^2} - \dfrac{U}{K_x}\dfrac{d\tilde{O}}{dx} - \dfrac{r_a}{K_x}\tilde{O} + \dfrac{r_d}{K_x} B = 0 & (2) \end{cases}$$

Let's solve eq. (1). It is an homogenous II order differential equation, that in the most general form reads:

$$\frac{d^2 y}{dx^2} - a_1 \frac{dy}{dx} - a_0 y = 0$$

Its solution is given by the characteristic polynomial: $P(\lambda) = \lambda^2 - a_1\lambda - a_0 = 0$
The solution is then:

$$\lambda_{1,2} = \frac{a_1 \pm \sqrt{{a_1}^2 + 4a_0}}{2} \longrightarrow \lambda_{1,2} = \frac{1}{2}\left(\frac{U}{K_x} \pm \sqrt{\frac{U^2}{{K_x}^2} + \frac{4r_d}{K_x}}\right)$$

By rearranging the roots solution:

$$\lambda_{1,2} = \frac{1}{2}\left(\frac{U}{K_x} \pm \frac{U}{K_x}\sqrt{1 + \frac{4 r_d K_x}{U^2}}\right) \longrightarrow \lambda_{1,2} = \frac{U}{2K_x}(1 \pm m_d)$$

with: $m_d = \sqrt{1 + \frac{4 r_d K_x}{U^2}} > 1$

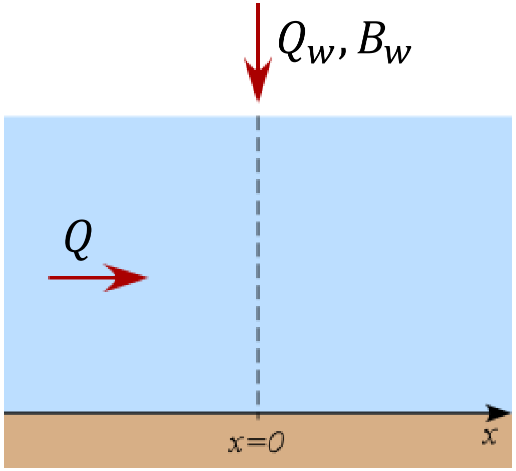
Being $m_d > 0$ both λ_1 and λ_2 are real ($\lambda_1, \lambda_2 \in \mathcal{R}$), i.e. the solution of the equation is:

$$y = c_1 e^{\lambda_1 x} + c_2 e^{\lambda_2 x} \longrightarrow B = c_1 e^{\lambda_1 x} + c_2 e^{\lambda_2 x}$$

In this case $\lambda_1 > 0$ and $\lambda_2 < 0$, moreover $|\lambda_1| > |\lambda_2|$.
The two constants of integration c_1 and c_2 can be defined as following.

Let's consider the discharge of BOD in $x = 0$. Because $K_x \neq 0$, BOD spreads also upstream ($x < 0$). The BCs are:

a. $x = 0 \longrightarrow B = B_0$
b. $x \to +\infty \longrightarrow B = 0$
c. $x \to -\infty \longrightarrow B = 0$



BOD DISTRIBUTION

By applying the conditions (b) and (c), we find respectively:

$$B = c_1 e^{\lambda_1 \infty} + c_2 \cancelto{0}{e^{\lambda_2 \infty}} = 0 \quad \longrightarrow \quad c_1 = 0 \ \text{for } x > 0$$

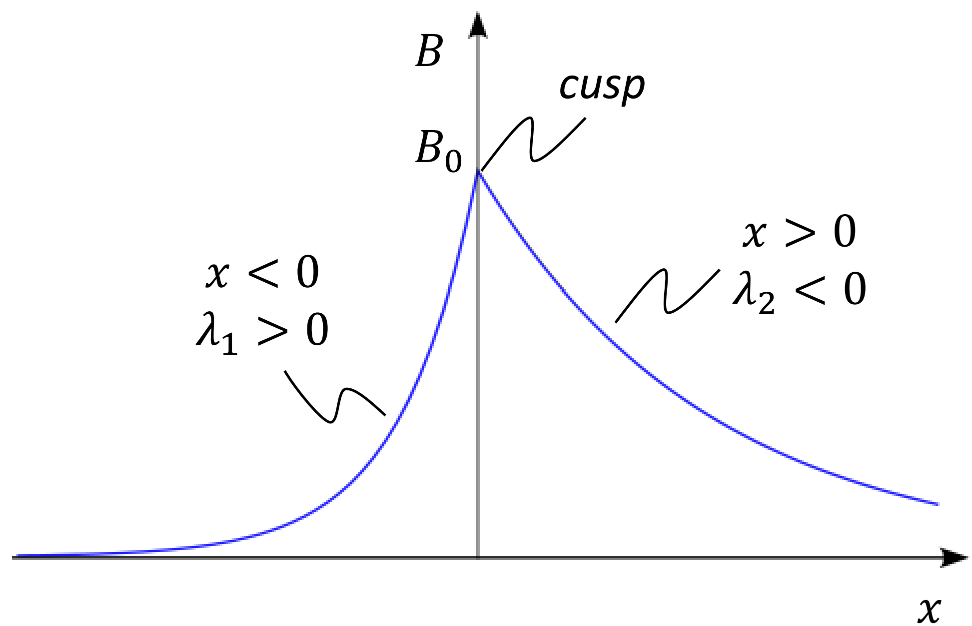
$$B = c_1 \cancelto{0}{e^{-\lambda_1 \infty}} + c_2 e^{-\lambda_2 \infty} = 0 \quad \longrightarrow \quad c_2 = 0 \ \text{for } x < 0$$

We must split the solution:

$$\begin{cases} B = c_2 e^{\lambda_2 x} & x \geq 0 \\ B = c_1 e^{\lambda_1 x} & x < 0 \end{cases}$$

Considering the condition (a) and expanding the equations:

$$\begin{cases} B = B_0 e^{\frac{U}{2K_x}(1-m_d)x} & x \geq 0 \\ B = B_0 e^{\frac{U}{2K_x}(1+m_d)x} & x < 0 \end{cases}$$



It is worth noting that, being $|\lambda_1| > |\lambda_2|$, the upstream concentration decays faster!

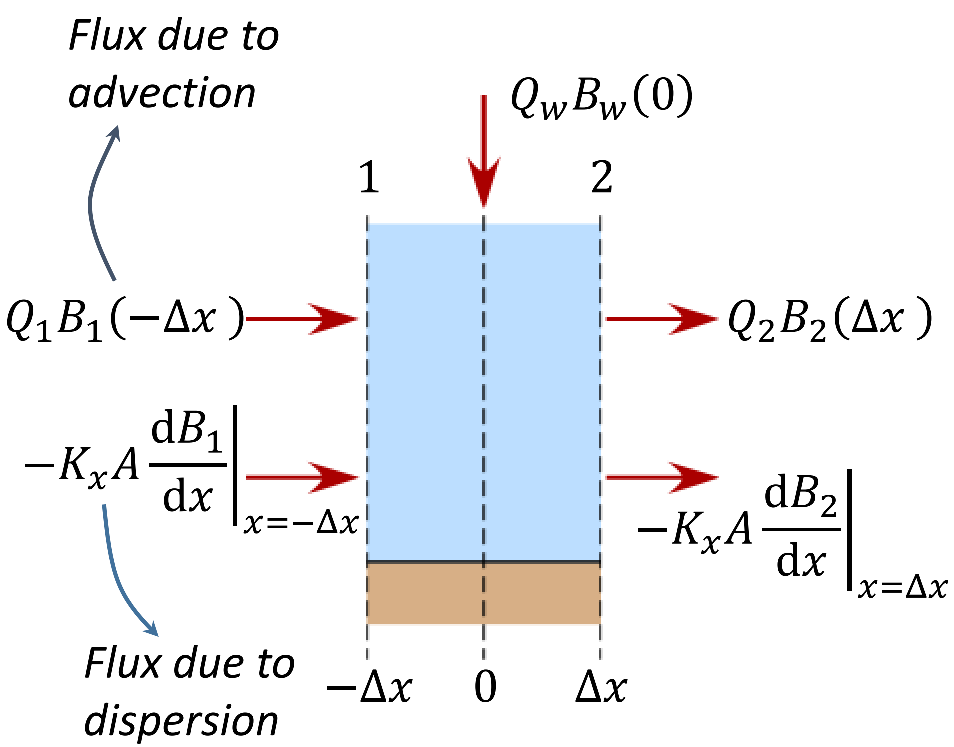
EVALUATION OF B_0

B_0 is calculated by the following mass balance:

$$QB_1(-\Delta x) - K_x A \left.\frac{\mathrm{d}B_1}{\mathrm{d}x}\right|_{x=-\Delta x} + Q_w B_w(0) = QB_2(\Delta x) - K_x A \left.\frac{\mathrm{d}B_2}{\mathrm{d}x}\right|_{x=\Delta x}$$

If $\Delta x \to 0$, we can use the Taylor's expansion series till 1st factor:

- $B_1(-\Delta x) \cong B_1(0) - \cancel{\Delta x \left.\frac{\mathrm{d}B_1}{\mathrm{d}x}\right|_{x=0}} + \cdots$
- $B_2(\Delta x) \cong B_2(0) + \cancel{\Delta x \left.\frac{\mathrm{d}B_2}{\mathrm{d}x}\right|_{x=0}} + \cdots$
- $\left.\frac{\mathrm{d}B_1}{\mathrm{d}x}\right|_{x=-\Delta x} \cong \left.\frac{\mathrm{d}B_1}{\mathrm{d}x}\right|_{x=0} - \cancel{\Delta x \left.\frac{\mathrm{d}^2B_1}{\mathrm{d}x^2}\right|_{x=0}} + \cdots$
- $\left.\frac{\mathrm{d}B_2}{\mathrm{d}x}\right|_{x=\Delta x} \cong \left.\frac{\mathrm{d}B_2}{\mathrm{d}x}\right|_{x=0} + \cancel{\Delta x \left.\frac{\mathrm{d}^2B_2}{\mathrm{d}x^2}\right|_{x=0}} + \cdots$



EVALUATION OF B_0

Noting that $B_1(0) = B_2(0) = B_0$. By replacing:

$$\left.\frac{\mathrm{d}B_1}{\mathrm{d}x}\right|_{x=0} = \left.B_0\lambda_1 e^{\lambda_1 x}\right|_{x=0} = B_0\lambda_1$$

$$\cancel{QB_0} - K_x A \left.\frac{\mathrm{d}B_1}{\mathrm{d}x}\right|_{x=0} + Q_w B_w = \cancel{QB_0} + Q_w B_0 - K_x A \left.\frac{\mathrm{d}B_2}{\mathrm{d}x}\right|_{x=0}$$

$$\left.\frac{\mathrm{d}B_2}{\mathrm{d}x}\right|_{x=0} = \left.B_0\lambda_2 e^{\lambda_2 x}\right|_{x=0} = B_0\lambda_2$$

$$Q_w B_w - K_x A B_0 \lambda_1 = Q_w B_0 - K_x A B_0 \lambda_2$$

$$Q_w B_w = Q_w B_0 + K_x A(\lambda_1 - \lambda_2)B_0 = B_0[Q_w + K_x A(\lambda_1 - \lambda_2)]$$

$$\lambda_1 - \lambda_2 = \frac{U}{2K_x}(1 + m_d - 1 + m_d) = \frac{U}{K_x} m_d$$

$$B_0 = B_w \frac{Q_w}{Q_w + \cancel{K_x} A \frac{U}{\cancel{K_x}} m_d}$$

$$B_0 = B_w \frac{Q_w}{Q_w + Q m_d}$$

It is worth noting that for pure advection $K_x = 0$, i.e. $m_d = 1$, the solution is the same determined in the standard S-P model:

$$B_0 = B_w \frac{Q_w}{Q_w + Q}$$

DEFICIT OF OXYGEN DISTRIBUTION

The eq. (1) in the most general form reads:

$$\frac{\mathrm{d}^2\tilde{O}}{\mathrm{d}x^2}-\frac{U}{K_x}\frac{\mathrm{d}\tilde{O}}{\mathrm{d}x}-\frac{r_a}{K_x}\tilde{O}+\frac{r_d}{K_x}B=0 \longrightarrow \frac{\mathrm{d}^2y}{\mathrm{d}x^2}+a_1\frac{\mathrm{d}y}{\mathrm{d}x}-a_0y=c$$

The solution is the sum of the solution of the homogeneous eq. and a particular solution:

$$\frac{\mathrm{d}^2y}{\mathrm{d}x^2}+a_1\frac{\mathrm{d}y}{\mathrm{d}x}-a_0y=0 \quad + \quad \tilde{O}_p=kx^me^{\lambda x}$$

The procedure to derive the solution of homegenous eq. is the same of the one developed for BOD:

$$\tilde{O}=c_1e^{\lambda_1 x}+c_2e^{\lambda_2 x} \qquad \text{with} \qquad \lambda_{1,2}=\frac{U}{2K_x}(1\pm m_a)$$

$$m_a=\sqrt{1+\frac{4r_aK_x}{U^2}}>1$$

And the particular solution is:

$$\tilde{O}_p=\frac{r_dB_0}{r_a-r_d}e^{\frac{U}{2K_x}(1\pm m_d)x}$$

The particular integral changes when $x \geq 0$ or $x < 0$.

DEFICIT OF OXYGEN DISTRIBUTION

Also in this case: $c_1 = 0$ for $x > 0$

$c_2 = 0$ for $x < 0$

The last Boundary Condition is $\tilde{O}(0) = \tilde{O}_0$, thus:

$$\begin{cases} \tilde{O}(0) = c_2 \cancelto{1}{e^{\lambda_2 x}} + \dfrac{r_d B_0}{r_a - r_d} \cancelto{1}{e^{\frac{U}{2K_x}(1-m_d)x}} = \tilde{O}_0 & x \geq 0 \\ \tilde{O}(0) = c_1 \cancelto{1}{e^{\lambda_1 x}} + \dfrac{r_d B_0}{r_a - r_d} \cancelto{1}{e^{\frac{U}{2K_x}(1+m_d)x}} = \tilde{O}_0 & x < 0 \end{cases}$$

$$\begin{cases} \tilde{O}_0 = c_2 + \dfrac{r_d B_0}{r_a - r_d} & x \geq 0 \\ \tilde{O}_0 = c_1 + \dfrac{r_d B_0}{r_a - r_d} & x < 0 \end{cases}$$

$$\longrightarrow \quad c_1 = c_2 = \tilde{O}_0 - \tilde{O}_p = \tilde{O}_0 - \frac{r_d B_0}{r_a - r_d}$$

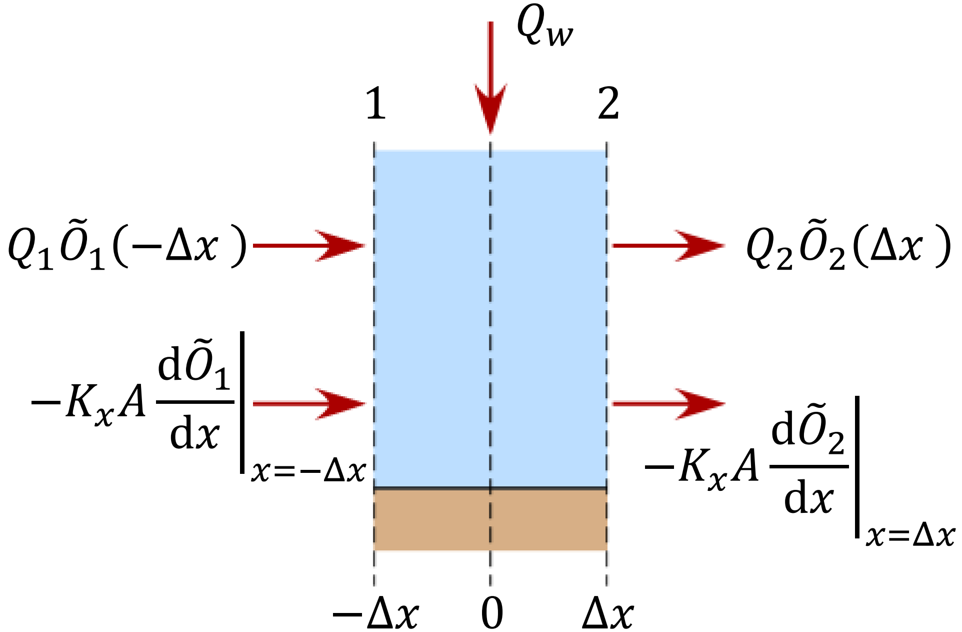
EVALUATION OF $\tilde{O}_0$

As in the previous case $\tilde{O}_0$ is calculated by the following mass balance:

$$Q\tilde{O}_1(-\Delta x) - K_x A \left.\frac{\mathrm{d}\tilde{O}_1}{\mathrm{d}x}\right|_{x=-\Delta x} = Q\tilde{O}_2(\Delta x) - K_x A \left.\frac{\mathrm{d}\tilde{O}_2}{\mathrm{d}x}\right|_{x=\Delta x}$$

By expanding the Taylor's series around the inflow:

- $\tilde{O}_1(-\Delta x) \cong \tilde{O}_1(0)$
- $\tilde{O}_2(\Delta x) \cong \tilde{O}_2(0)$
- $\left.\frac{\mathrm{d}\tilde{O}_1}{\mathrm{d}x}\right|_{x=-\Delta x} \cong \left.\frac{\mathrm{d}\tilde{O}_1}{\mathrm{d}x}\right|_{x=0}$
- $\left.\frac{\mathrm{d}\tilde{O}_2}{\mathrm{d}x}\right|_{x=\Delta x} \cong \left.\frac{\mathrm{d}\tilde{O}_2}{\mathrm{d}x}\right|_{x=0}$



By replacing and considering that $\tilde{O}_1(0) = \tilde{O}_2(0) = \tilde{O}_0$:

EVALUATION OF $\tilde{O}_0$

$$\cancel{Q\tilde{O}_0} - K_x A \left.\frac{\mathrm{d}\tilde{O}_1}{\mathrm{d}x}\right|_{x=0} = \cancel{Q\tilde{O}_0} + Q_w \tilde{O}_0 - K_x A \left.\frac{\mathrm{d}\tilde{O}_2}{\mathrm{d}x}\right|_{x=0}$$

Being generally $Q_w \tilde{O}_0 \ll 1$: $\left.\frac{\mathrm{d}\tilde{O}_1}{\mathrm{d}x}\right|_{x=0} = \left.\frac{\mathrm{d}\tilde{O}_2}{\mathrm{d}x}\right|_{x=0}$

The two derivative are equal, thus there is no cusp.

To calculate the latter we derive the following expression:

$$\tilde{O}_{1,2} = c_{1,2} e^{\lambda_{1,2} x} + \frac{r_d B_0}{r_a - r_d} e^{\frac{U}{2K_x}(1 \pm m_d)x} \quad \text{with} \quad \lambda_{1,2} = \frac{U}{2K_x}(1 \pm m_a)$$

That is:

$$\left.\frac{\mathrm{d}\tilde{O}_1}{\mathrm{d}x}\right|_{x=0} = c_1 \lambda_1 + \frac{r_d B_0}{r_a - r_d} \frac{U}{2K_x}(1 + m_d) = c_2 \lambda_2 + \frac{r_d B_0}{r_a - r_d} \frac{U}{2K_x}(1 - m_d) = \left.\frac{\mathrm{d}\tilde{O}_2}{\mathrm{d}x}\right|_{x=0}$$

$$c_1 \cancel{\frac{U}{2K_x}}(1 + m_a) + \frac{r_d B_0}{r_a - r_d} \cancel{\frac{U}{2K_x}}(1 + m_d) = c_2 \cancel{\frac{U}{2K_x}}(1 - m_a) + \frac{r_d B_0}{r_a - r_d} \cancel{\frac{U}{2K_x}}(1 - m_d)$$

EVALUATION OF $\tilde{O}_0$

But $c_1 = c_2 = c$:

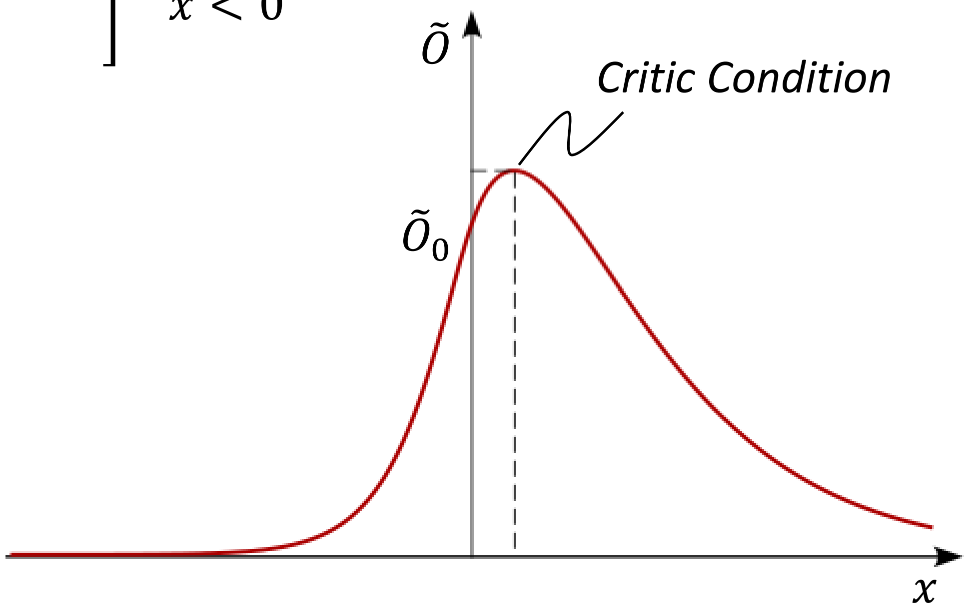
$$c(1 + \overset{\cancel{2}m_a}{m_a - 1 + m_a}) = \frac{r_d B_0}{r_a - r_d}(1 - \overset{-\cancel{2}m_d}{m_d - 1 - m_d}) \longrightarrow c_{1,2} = -\frac{r_d B_0}{r_a - r_d}\frac{m_d}{m_a}$$

By replacing the coefficients into the expression of $\tilde{O}_0$, finally we find:

$$\begin{cases} \tilde{O} = \dfrac{r_d B_0}{r_a - r_d}\left[e^{\frac{U}{2K_x}(1-m_d)x} - \dfrac{m_d}{m_a} e^{\frac{U}{2K_x}(1-m_a)x}\right] & x \geq 0 \\ \tilde{O} = \dfrac{r_d B_0}{r_a - r_d}\left[e^{\frac{U}{2K_x}(1+m_d)x} - \dfrac{m_d}{m_a} e^{\frac{U}{2K_x}(1+m_a)x}\right] & x < 0 \end{cases}$$

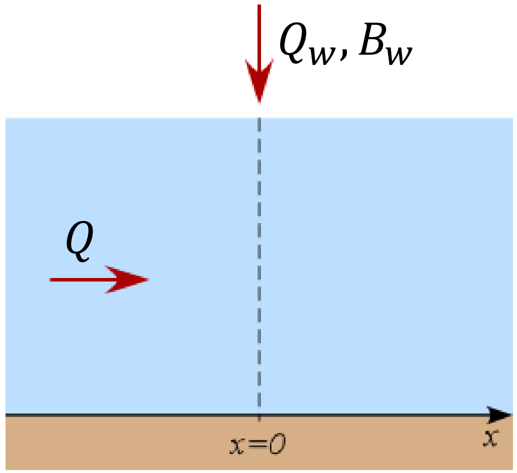
The parameters m_d and m_a determine the regime of $\tilde{O}$ dinamycs:

- $\dfrac{r_{a,d} K_x}{U^2} > 20$ <u>Dispersion prevailing</u>
- $\dfrac{r_{a,d} K_x}{U^2} < 0.05$ <u>Advection prevailing</u> (S-P Model)



EXERCISE: $\widetilde{O}$ IN ESTUARY

Let's study the BOD and DO distribution of the following scenario.



Data:

- $Q = 30$ m³/s
- $Q_w = 5$ m³/s
- $B_w = 50$ mg/l
- $U = 0.15$ m/s $\longrightarrow U = 12.96$ km/d
- $K_x = 380$ m²/s $\longrightarrow K_x = 32.83$ km²/d
- $r_d = 0.5$ d⁻¹
- $r_a = 0.9$ d⁻¹
- $O_s = 7.5$ mg/l

The regime of O is determined by the values of the following parameter:

$$\frac{r_d K_x}{U^2} = \frac{0.5 \cdot 32.83}{12.96^2} = 0.098 \qquad \frac{r_a K_x}{U^2} = \frac{0.9 \cdot 32.83}{12.96^2} = 0.176$$

The two parameters are within the range [0.05, 20], thus we have to take into account both advection and dispersion.

The equations describing the dynamics of B and $\tilde{O}$ depend on the parameter m_d and m_a:

$$m_d = \sqrt{1 + \frac{4 r_d K_x}{U^2}} = \sqrt{1 + 4 \cdot 0.098} = 1.18$$

$$m_a = \sqrt{1 + \frac{4 r_a K_x}{U^2}} = \sqrt{1 + 4 \cdot 0.176} = 1.31$$

The BOD distribution is given by:

$$\begin{cases} B = B_0 e^{\frac{U}{2K_x}(1-m_d)x} & x \geq 0 \\ B = B_0 e^{\frac{U}{2K_x}(1+m_d)x} & x < 0 \end{cases}$$

where the value of B_0 is equal to:

$$B_0 = B_w \frac{Q_w}{Q_w + Q m_d} = 80 \frac{5}{5 + 30 \cdot 1.18} = 9.9 \quad \text{mg/l}$$

By replacing all the parameters into the system, we find:

$$\begin{cases} B^+ = 9.9 \cdot e^{-0.035 \cdot x} \\ B^- = 9.9 \cdot e^{+0.430 \cdot x} \end{cases}$$

Similarly the $\tilde{O}$ distribution is described by the following system:

$$\begin{cases} \tilde{O}^{+} = \dfrac{r_d B_0}{r_a - r_d}\left[e^{\frac{U}{2K_x}(1-m_d)x} - \dfrac{m_d}{m_a}\, e^{\frac{U}{2K_x}(1-m_a)x}\right] = 12.38[e^{-0.035\cdot x} - 0.903e^{-0.060\cdot x}] \\ \tilde{O}^{-} = \dfrac{r_d B_0}{r_a - r_d}\left[e^{\frac{U}{2K_x}(1+m_d)x} - \dfrac{m_d}{m_a}\, e^{\frac{U}{2K_x}(1+m_a)x}\right] = 12.38[e^{+0.430\cdot x} - 0.903e^{+0.455\cdot x}] \end{cases}$$

Finally, the DO distribution can be trivially determined by: $O = O_s - \tilde{O}$

The numerical analysis of $\tilde{O}$ shows that the critic condition is:

$x_c = 17.3$ km

$\tilde{O}_c = 2.8$ mg/l $\longrightarrow$ $O_c = 7.5 - 2.8 = 4.7 > 4.0$ mg/l

The critic condition shows accettable concentration of DO.

EXERCISE: O IN ESTUARY