“Mixing processes in enhanced and natural attenuation”

Phil Ham

Bodem Diep 2003, Zeist.

Phil Ham

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Delft University of Technology

Status Report!

Begun Oct. 2001

Literature Review

Draft version, but not corrected

Pure Analytical/Numerical Modelling

Keijzer *et al.* (2000) – soln. Of 2-D PDE's with coupled Monod kinetic term ⇒Conference paper

Gramling *et al.* (2002) – soln. Of 2-D PDE's with instantaneous reaction term ⇒Journal paper

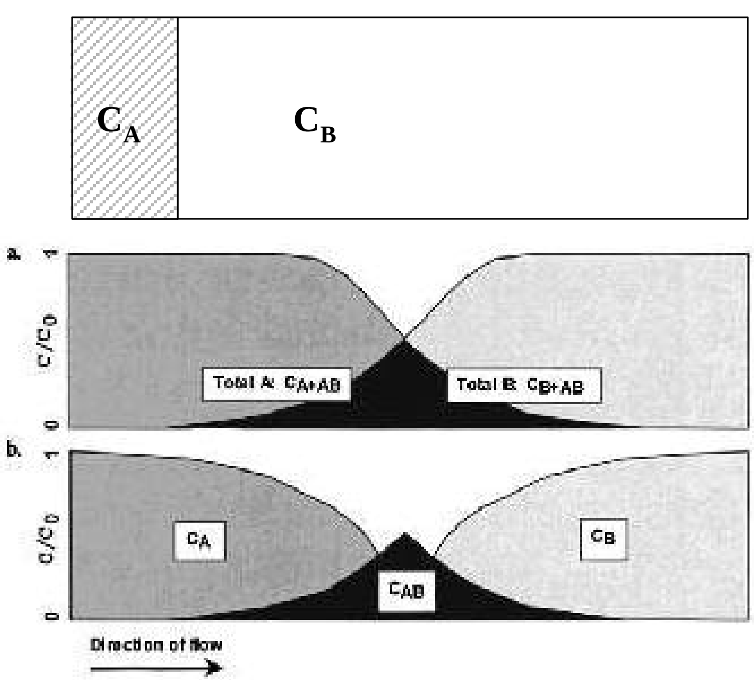
Huang *et al.* (2003) – comp. of analytical soln. with real data ⇒Joint article

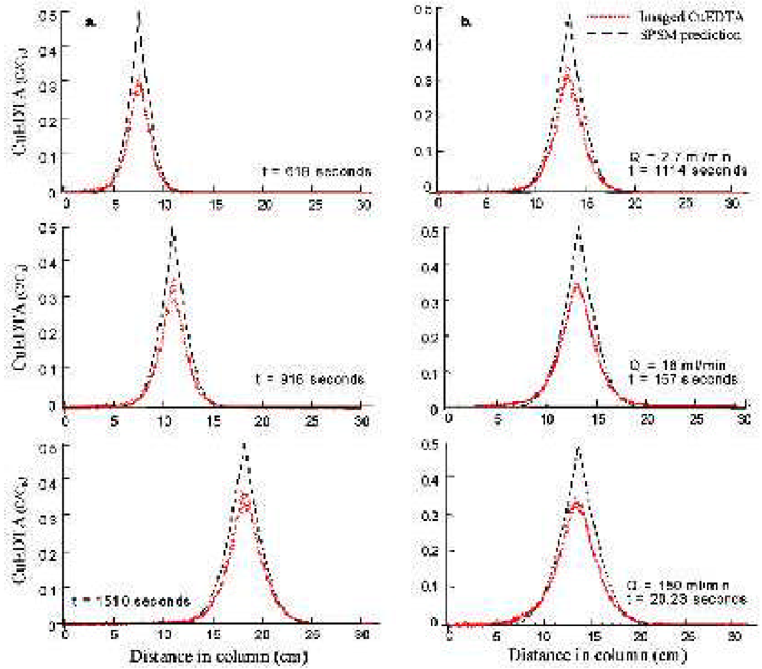
CORONA

New data, modelling imminent

Gramling *et al.* (2002)

Gramling *et al.* consider 1-D, instantaneous colourimetric reactions between solutions of aqueous Na_2EDTA^{4-} and $CuSO_4$ (both experimental and analytical solution).





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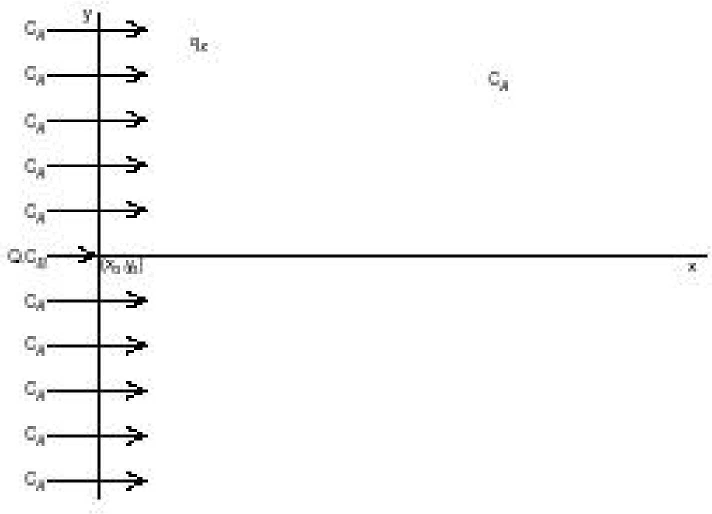
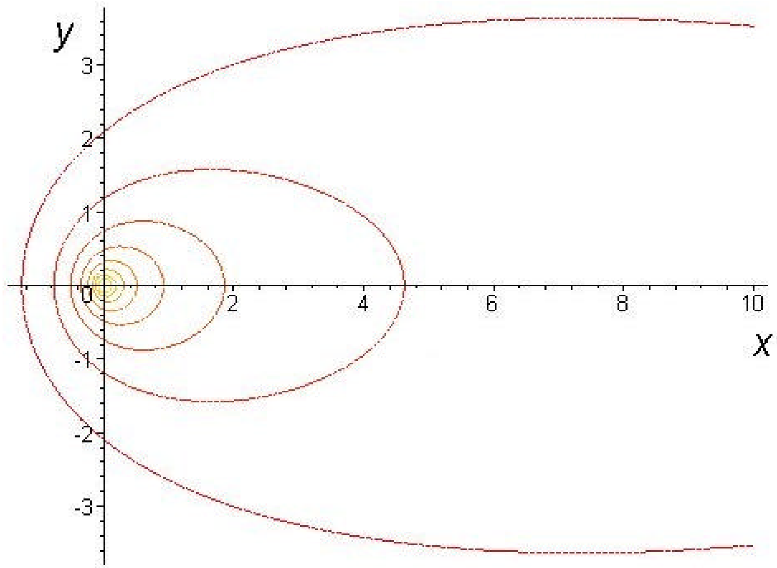
Introduction (1)

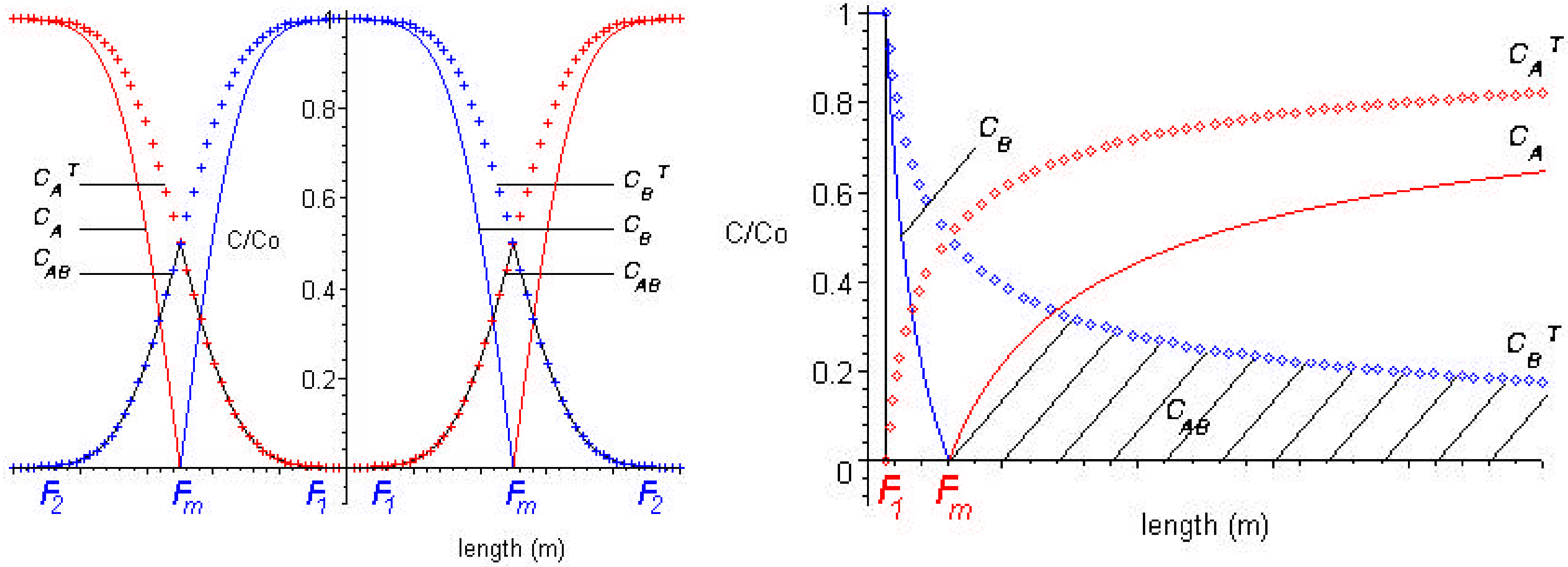
- 2-D Extension of the work by Gramling *et al*. (2002)
- Reaction of the form A + B $\rightarrow$ AB, where $r_{AB} = -r_A = -r_B$
- Contour distribution:





Introduction (2)

Reactant/Product distributions:



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Mass balance equations

Reactant A and B:

$$n\frac{\partial C_A}{\partial t} + \text{[illegible]} - \alpha_L q_x \frac{\partial^2 C_A}{\partial x^2} - \text{[illegible]} \frac{\partial^2 C_A}{\partial y^2} + r_{AB} = 0,$$

$$n\frac{\partial C_B}{\partial t} + q_x \frac{\partial C_B}{\partial x} - \text{[illegible]} \alpha_T q_x \frac{\partial^2 C_B}{\partial y^2} + r_{AB} = 0,$$

Product AB:

$$n\frac{\partial C_{AB}}{\partial t} + q_x \frac{\partial C_{AB}}{\partial x} - \text{[illegible]} - \alpha_T q_x \frac{\partial^2 C_{AB}}{\partial y^2} - r_{AB} = 0.$$

Adding [illegible]nd C_{AB} y[illegible]

$$n\frac{\partial C_B{}^T}{\partial t} + \text{[illegible]} \frac{\partial C_B{}^T}{\partial x} - \alpha_L q_x \frac{\partial^2 C_B{}^T}{\partial x^2} - \text{[illegible]} \frac{\partial^2 C_B{}^T}{\partial y^2} = 0,$$

Mass balance equations

Introducing the dimensionless parameters

$$x^* = \frac{x}{\alpha_L}, \quad y^* = \frac{y}{\alpha_L}, \quad \text{and} \quad q^* = \frac{q_x}{q_o}, \tag{7}$$

and substituting these into (6) gives

$$n\frac{\partial {C_B}^T}{\partial t} + \frac{q_o q^*}{\alpha_L}\frac{\partial {C_B}^T}{\partial x^*} - \frac{q_o q^*}{\alpha_L}\frac{\partial^2 {C_B}^T}{\partial x^{*2}} - \frac{q_o q^* \alpha_T}{{\alpha_L}^2}\frac{\partial^2 {C_B}^T}{\partial y^{*2}} = 0. \tag{8}$$

Multiplying (8) by α_L/q_o, introducing the dimensionless parameter $t^* = tq_o/n\alpha_L$ and the new variable $\beta = \alpha_T/\alpha_L$, and dropping the * notation for convenience yields

$$\frac{\partial {C_B}^T}{\partial t} + q\frac{\partial {C_B}^T}{\partial x} - q\frac{\partial^2 {C_B}^T}{\partial x^2} - \beta q {\alpha_L}^2 \frac{\partial^2 {C_B}^T}{\partial y^2} = 0, \tag{9}$$

i.e., the mass balance equation for ${C_B}^T$ in dimensionless notation. Let $q_o = q_x = 1$ and ${C_B}^T(x, y, t) = {C_B}^T(s(x, t), y, t)$; the application of the *Chain Rule* gives

$$\frac{\partial {C_B}^T}{\partial t} = \frac{\partial^2 {C_B}^T}{\partial s} + \beta\frac{\partial^2 {C_B}^T}{\partial y^2}, \tag{10}$$

which will be the starting point for further analysis.

Plume Length (1)

$$s^{\frac{1}{2}}\, e^{s}\, K_0(s) = 1.25331414 - 0.07832358\left(\frac{2}{s}\right) + 0.02189568\left(\frac{2}{s}\right)^2 - 0.01062446\left(\frac{2}{s}\right)^3$$
$$+0.00587872\left(\frac{2}{s}\right)^4 - 0.00251540\left(\frac{2}{s}\right)^5 + 0.00053208\left(\frac{2}{s}\right)^6 + \varepsilon,$$

where $|\varepsilon| < 1.9\ 10^{-7}$. As a first approximation only the first term on the right-hand side of the series expansion is included, i.e.

$$s^{\frac{1}{2}}\, e^{s}\, K_0(s) \approx 1.25331414.$$

Substitution of this approximation in (25) yields

$$L \approx 2\,\frac{F1.25331414}{0.1}\frac{1}{\alpha_T} \approx (2(1.25331414))\,.100F^2\,\frac{1}{\alpha_T} = 100\pi F^2\frac{1}{\alpha_T}.$$

$L = f(a_T)$ not $f(a_L)$

Plume Length (2)

As a next, more accurate approximation, the second term at the right-hand side of the series expansion for K_0 is also included, i.e.

$$s^{\frac{1}{2}}\, e^{s}\, K_0(s) \approx 1.25331414 - 0.07832358 \left(\frac{2}{s}\right).$$

Substitution of this approximation in (25) gives

$$\frac{F}{\sqrt{\alpha_T}}\sqrt{\frac{2}{L}}\left(1.25331414 - 0.07832358 \left(\frac{4\alpha_L}{L}\right)\right) = 0.1,$$

or

$$\frac{0.01\alpha_T}{F^2}\, L^3 - \pi\, L^2 + \frac{\pi\alpha_L}{2}\, L + \frac{\pi\alpha_L^2}{16} \approx 0.$$

$$\mathbf{L = \mathit{f}\,(a_T, a_L)}$$

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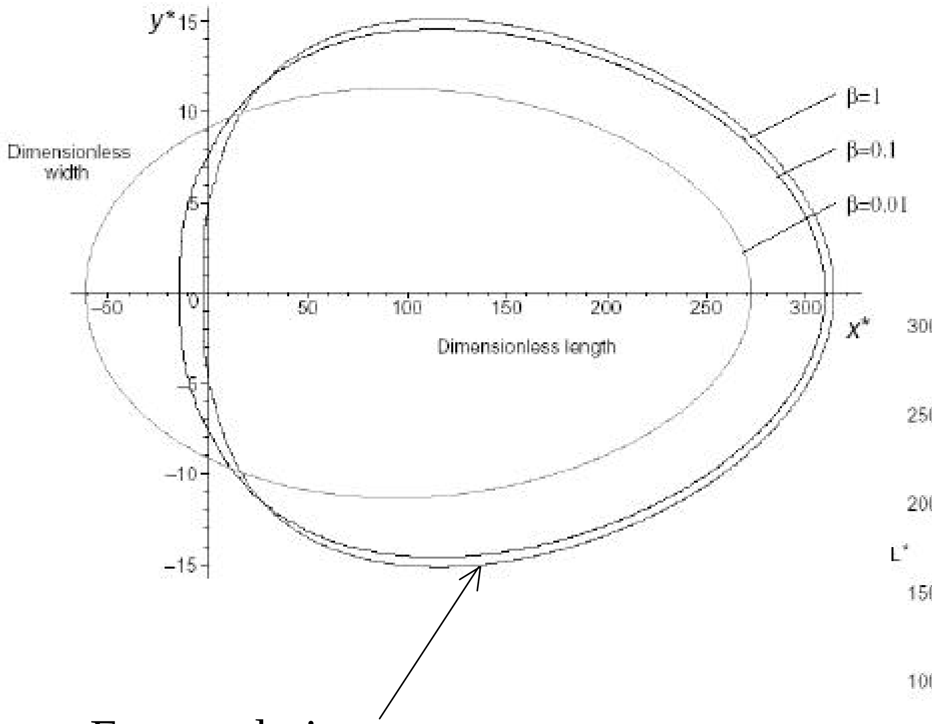
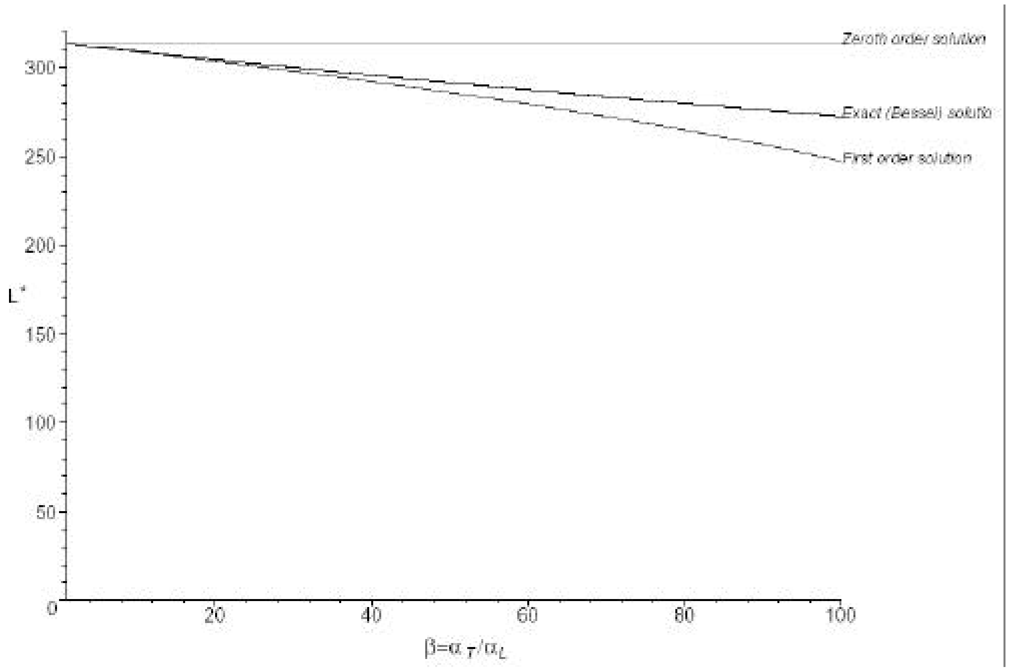
Results (1)



Exact solution
AND zeroth order
approximation



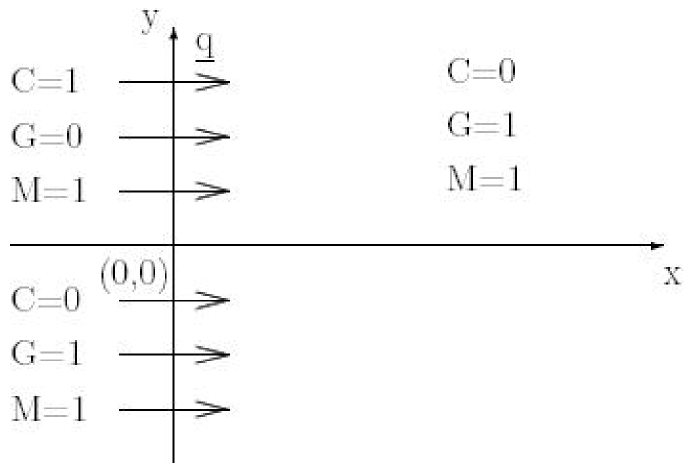
Keijzer *et al.* (2000)

Keijzer *et al.* consider a 1-D traveling wave solution for transport and biodegradation of a contaminant (electron donor) and electron acceptor controlled (coupled) by Monod reactions.

$$\frac{\partial C}{\partial t} = \frac{1}{Pe^L}\frac{\partial^2 C}{\partial x^2} + \frac{1}{Pe^T}\frac{\partial^2 C}{\partial y^2} - \frac{\partial C}{\partial x} - \frac{\partial C}{\partial y} - M_C\frac{\partial M}{\partial t} - M_C L_d(M-1),$$

$$R\frac{\partial G}{\partial t} = \frac{1}{Pe^L}\frac{\partial^2 G}{\partial x^2} + \frac{1}{Pe^T}\frac{\partial^2 G}{\partial y^2} - \frac{\partial G}{\partial x} - \frac{\partial G}{\partial y} - M_G\frac{\partial M}{\partial t} - M_G L_d(M-1),$$

$$\frac{\partial M}{\partial t} = L_\mu\left[\frac{C}{K_C + C}\right]\left[\frac{G}{K_G + G}\right] M - L_d(M-1).$$



Initial and boundary conditions

Solution

Multiplication of (14) by M_G and (15) by M_C, subtraction of the resulting equations and introduction of the parameter $\beta = M_C/M_G$ yields

$$\frac{\partial}{\partial t}[C - R\beta G] = \frac{1}{Pe^T}\frac{\partial^2}{\partial y^2}[C - \beta G] - \frac{\partial}{\partial x}[C - \beta G]\,. \qquad (17)$$

Disregarding contaminant retardation, i.e. $R = 1$ in (17), allows the introduction of the new variable

$$w(x, y, t) = C(x, y, t) - \beta G(x, y, t). \qquad (18)$$

After introduction of w, (17) reduces to

$$\frac{\partial w}{\partial t} = \frac{1}{Pe^T}\frac{\partial^2 w}{\partial y^2} - \frac{\partial w}{\partial x}, \qquad (19)$$

subject to (13),

$$w(x, y, 0) = w_0(x, y) = -\beta \;\text{ for }\; x > 0 \;\text{ and }\; y \in \mathbf{R} \qquad (20)$$

and the BC (Fig.2)

$$w(0, y, t) = +1 \;\text{ for }\; y > 0 \;\text{ and }\; t \geq 0, \qquad (21)$$

$$w(0, y, t) = -\beta \;\text{ for }\; y < 0 \;\text{ and }\; t \geq 0. \qquad (22)$$

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Results

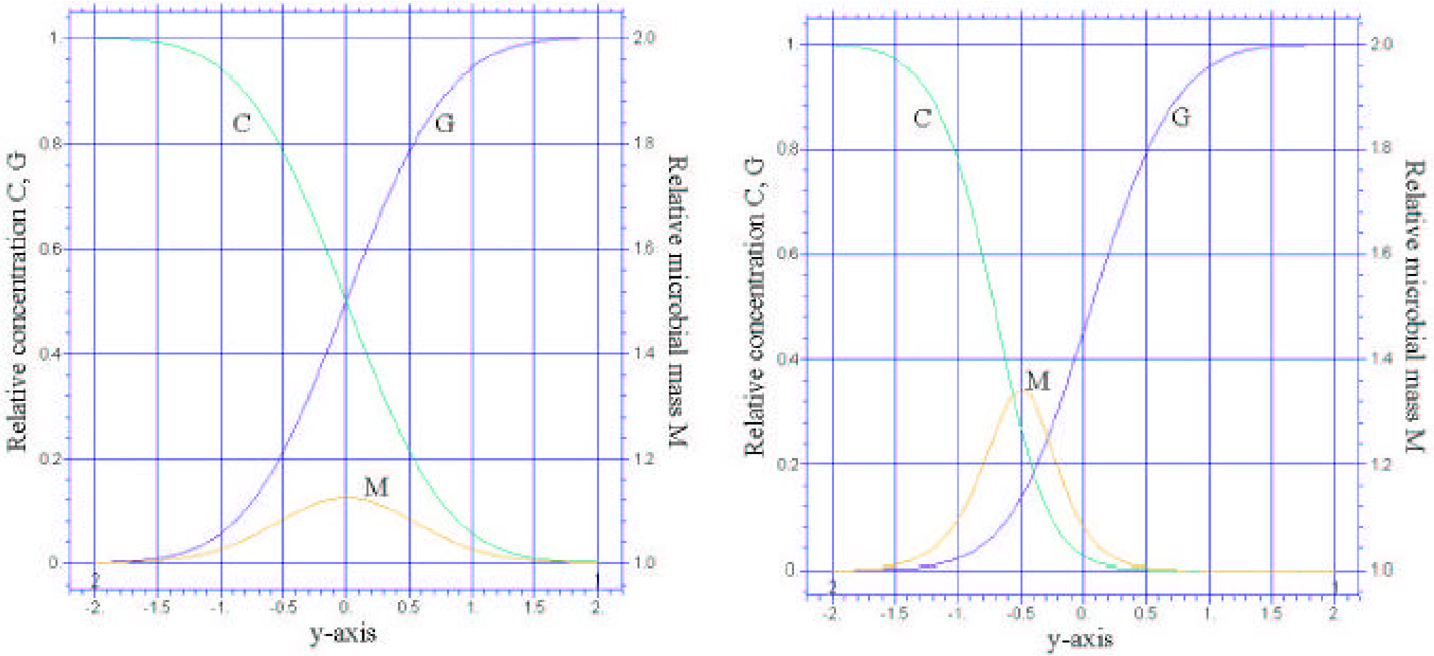

Figure 3. Electron acceptor C, contaminant G and microbial mass M distribution for $Pe^T = 5$ and, left, $M_C = 0$, $M_G = 0$, $L_\mu = 1$ and $L_d = 1$; right, $M_C = 0.5$, $M_G = 5$, $L_\mu = 5$ and $L_d = 0.5$. K_C and K_G equal unity in both cases.

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Compare...

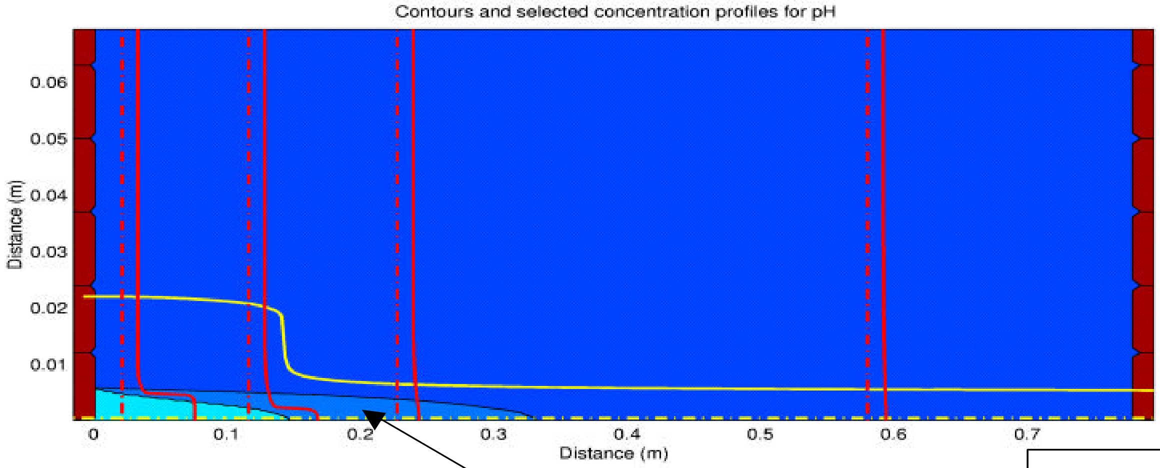
Solution of $\frac{\partial {C_B}^T}{\partial t} = \frac{\partial^2 {C_B}^T}{\partial s} + \beta \frac{\partial^2 {C_B}^T}{\partial y^2}$

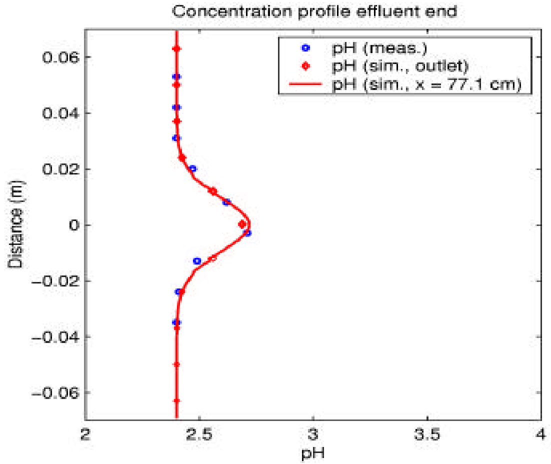
at stationary case is the same as $\frac{\partial w}{\partial t} = \frac{1}{Pe^T} \frac{\partial^2 w}{\partial y^2} - \frac{\partial w}{\partial x}$

→ provides similar solution

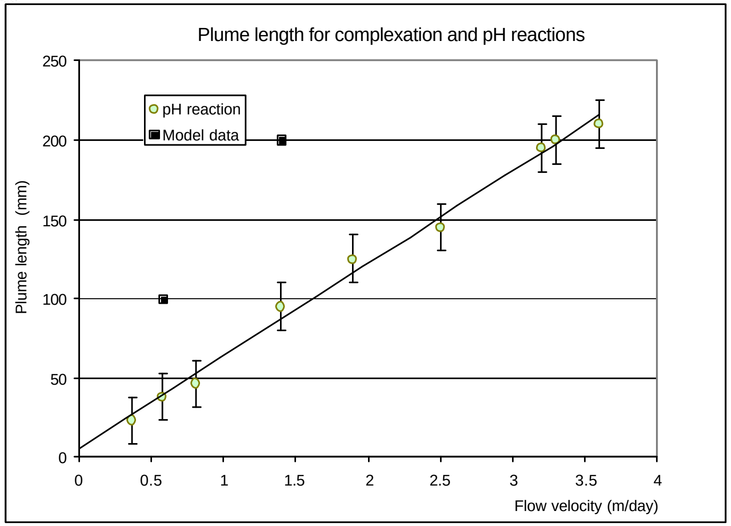
Huang *et al.* (2003) use imaging to study a steady-state plume resulting from (instantaneous) aerobic degradation. They compare real data to an MT3D solution (instantaneous and Monod kinetic reactions).

Tank Experiments





3>pH>4.6



Analysis

- Diffusion plays an important role on laboratory scale - diffusion has an influence on the result for the velocities that we have in the tankl, e.g. `Dzz_0.81 = 0.000175 m^2/d + 0.81 m/d * 0.000048 m`

```
                    = 0.000175       + 0.0000388
                    = 0.0002138
```

- Does transversal dispersivity depend on reactions???

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