Applications of mathematical software packages for modelling and simulations in environmental engineering education

Asher Brenner[a], Mordechai Shacham[b] and Michael B. Cutlip[c]

[a]Dept. Env. Eng., Ben-Gurion University, Beer-Sheva, Israel
[b]Dept. Chem. Eng., Ben-Gurion University, Beer-Sheva, Israel
[c]Dept. Chem. Eng, University of Connecticut,
Storrs, CT, USA

Simulation of the oxygen sag model

- The oxygen-sag model is a classical problem, used for demonstration of various subjects in the basic course of "Water Pollution Control".
- It is used to predict the oxygen concentration and deficit in a river, caused by a discharge of a sewage containing BOD consuming oxygen.
- The model consists of a system of differential equations that describe the processes of de-oxygenation and re-oxygenation as a function of time or distance (related to the river velocity), assuming ideal plug-flow conditions in the flowing river.
- The natural oxygen balance in the river is disturbed by de-oxygenation due to the sewage BOD which is biodegraded aerobically by natural bacteria. Re-oxygenation is caused by absorption of atmospheric oxygen stimulated by the turbulent flow.

The Oxygen Sag Model (1)

The change of ultimate BOD in the river as a function of hydraulic detention time (actual time of flow) can be described by a first order reaction:

$$\frac{dL}{dt} = -kL$$

L – Ultimate BOD [mg/L]

k – First order BOD degradation rate coefficient (de-oxygenation constant) [d^{-1}]

The integrated form of this equation is:

$$L_t = L_a \exp(-kt)$$

(Index a – Dilution point)

The resulting change of oxygen concentration due to the biochemical reaction is:

$$\frac{dC_{de}}{dt} = \frac{dL}{dt} = -kL = -kL_a \exp(-kt)$$

Index de – de-oxydation

The Oxygen Sag Model (2)

The rate of re-oxygenation is described

$$\frac{dC_{re}}{dt} = r(C_s - C)$$

r – Atmospheric oxygen dissolution rate coefficient (re-oxygenation constant) [d^{-1}]

C_s – Oxygen saturation concentration [mg/L]

Index re – re-oxygenation

The complete oxygen balance along the river

$$\frac{dC}{dt} = \frac{dC_{re}}{dt} + \frac{dC_{de}}{dt} = r(C_s - C) - kL_a \exp(-kt)$$

Rewriting in terms of ***deficit $D = (C_s$-$C)$*** yields

$$\frac{dD}{dt} = kL_a \exp(-kt) - rD$$

The Oxygen Sag Model (3)

To find the maximal deficit the integrated form of the equation is needed:

$$D_t = \frac{kL_a}{(r-k)}\left[\exp(-kt) - \exp(-rt)\right] + D_a \exp(-rt)$$

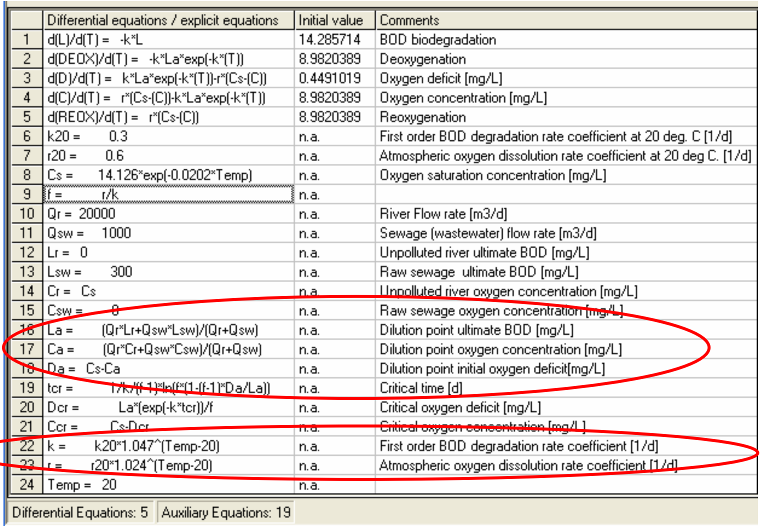
Differentiating this equation with respect to t and solving for d*D*/d*t* = 0 yields:

$$D_{cr} = \frac{L_a \exp(-kt_{cr})}{f}$$

where

$$t_{cr} = \frac{1}{k(f-1)}\ln\left\{f\left[1 - \frac{(f-1)D_a}{L_a}\right]\right\} \quad \text{and} \quad f = \frac{r}{k}$$

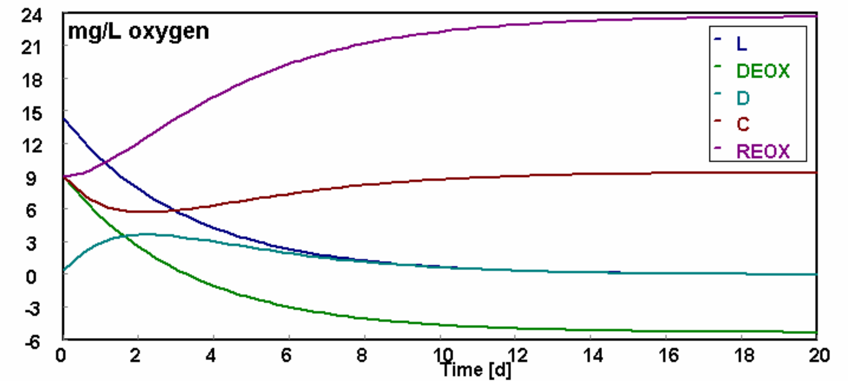
Definition of the Parameters of the Problem: ultimate BOD (*L*), oxygen concentration and oxygen deficit at the discharge (dilution) point (*C*,*D*)



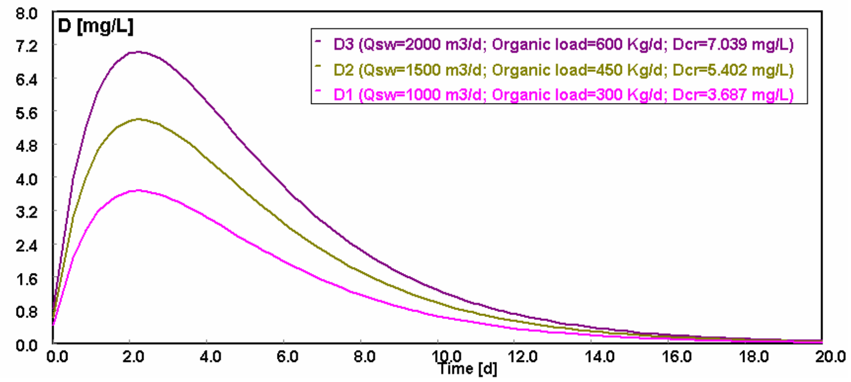
	Differential equations / explicit equations	Initial value	Comments
1	d(L)/d(T) = -k*L	14.285714	BOD biodegradation
2	d(DEOX)/d(T) = -k*La*exp(-k*(T))	8.9820389	Deoxygenation
3	d(D)/d(T) = k*La*exp(-k*(T))-r*(Cs-(C))	0.4491019	Oxygen deficit [mg/L]
4	d(C)/d(T) = r*(Cs-(C))-k*La*exp(-k*(T))	8.9820389	Oxygen concentration [mg/L]
5	d(REOX)/d(T) = r*(Cs-(C))	8.9820389	Reoxygenation
6	k20 = 0.3	n.a.	First order BOD degradation rate coefficient at 20 deg. C [1/d]
7	r20 = 0.6	n.a.	Atmospheric oxygen dissolution rate coefficient at 20 deg C. [1/d]
8	Cs = 14.126*exp(-0.0202*Temp)	n.a.	Oxygen saturation concentration [mg/L]
9	f = r/k	n.a.	
10	Qr = 20000	n.a.	River Flow rate [m3/d]
11	Qsw = 1000	n.a.	Sewage (wastewater) flow rate [m3/d]
12	Lr = 0	n.a.	Unpolluted river ultimate BOD [mg/L]
13	Lsw = 300	n.a.	Raw sewage ultimate BOD [mg/L]
14	Cr = Cs	n.a.	Unpolluted river oxygen concentration [mg/L]
15	Csw = 0	n.a.	Raw sewage oxygen concentration [mg/L]
16	La = (Qr*Lr+Qsw*Lsw)/(Qr+Qsw)	n.a.	Dilution point ultimate BOD [mg/L]
17	Ca = (Qr*Cr+Qsw*Csw)/(Qr+Qsw)	n.a.	Dilution point oxygen concentration [mg/L]
18	Da = Cs-Ca	n.a.	Dilution point initial oxygen deficit[mg/L]
19	tcr = 1/k/(f-1)*ln(f*(1-(f-1)*Da/La))	n.a.	Critical time [d]
20	Dcr = La*(exp(-k*tcr))/f	n.a.	Critical oxygen deficit [mg/L]
21	Ccr = Cs-Dcr	n.a.	Critical oxygen concentration [mg/L]
22	k = k20*1.047^(Temp-20)	n.a.	First order BOD degradation rate coefficient [1/d]
23	r = r20*1.024^(Temp-20)	n.a.	Atmospheric oxygen dissolution rate coefficient [1/d]
24	Temp = 20	n.a.	

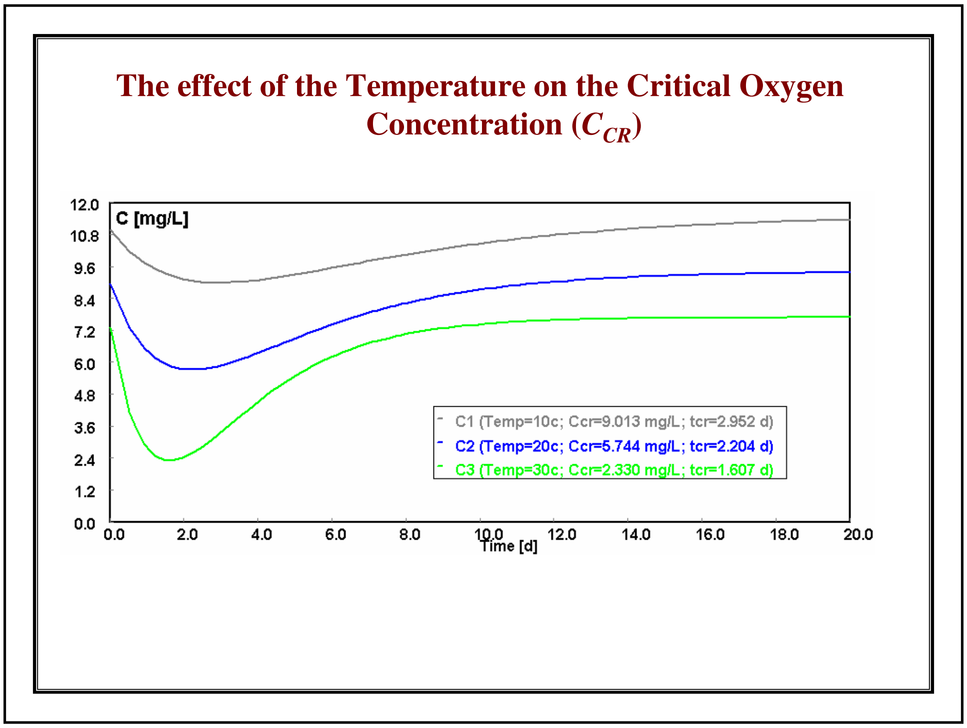
Differential Equations: 5 Auxiliary Equations: 19

Ultimate BOD (*L*), oxygen concentration (C) and oxygen deficit (*D*) profiles



The effect of the Organic Load on the Maximal Deficit (D_{CR})





The effect of the Temperature on the Critical Oxygen Concentration (C_{CR})