Homework #2

Due: Oct 15, 23:59

Construct an Excel spreadsheet to predict the substrate and biomass concentration (S and X_a) at time t for a batch-type bioreactor by numerical approach with the explicit method.

Use the following initial conditions and growth parameters:

$S^0 = 500\ mg\ COD/L$ $X_a^0 = 100\ mg\ VSS/L$ $\hat{q} = 20\ g\ VSS/g\ COD-d$

$K = 100\ mg\ COD/L$ $Y = 0.4\ g\ VSS/g\ COD$ $b = 0.1/d$

1) What are the substrate and biomass concentrations at $t = 0.1\,d$ calculated by setting the following values as Δt?

   i. $\Delta t = 0.0001\,d$; ii. $\Delta t = 0.001\,d$; iii. $\Delta t = 0.05\,d$

2) Compare the results for the numerical solution with different Δt values. Which one do you think will be the most accurate? Why? For $\Delta t = 0.05\,d$, obtain the solutions for substrate and biomass concentrations at $t = 0.5\,d$. What do you get? How would you describe the reason for getting that result?

Provide your answers in the Excel spreadsheet you have constructed and turn in the spreadsheet. Grading will be given based on the correctness of your employment of the numerical approach, the correctness of your numerical solution, and the reasonableness of your written answers.

(100 points)

Solution)

Following is an example spreadsheet (the structure and the extent of embedded calculations are up to the decision of each student)

	A	B	C	D	E	F	G	H
1	**Input parameters**					**Time (d)**	**S**	**X_a**
2	S^0	500	mg COD/L			0.000	500	100
3	X_a^0	100	mg VSS/L			0.001	498.3	100.7
4	q	20	g VSS/g COD-d			0.002	496.7	101.3
5	K	100	mg COD/L			0.003	495.0	102.0
6	Y	0.4	g VSS/g COD			0.004	493.3	102.7
7	b	0.1	1/d			0.005	491.6	103.3
8	Δt	0.001	d			0.006	489.8	104.0
9	t	0.1				0.007	488.1	104.7
10						0.008	486.4	105.4
11	**Solution**					0.009	484.6	106.1
12	S	**279.3**	mg COD/L			0.010	482.9	106.7
13	X_a	**186.9**	mg VSS/L			0.011	481.1	107.4
14						0.012	479.3	108.1
15						0.013	477.5	108.8
16						0.014	475.7	109.6
17						0.015	473.9	110.3
18						0.016	472.1	111.0
19						0.017	470.3	111.7
20						0.018	468.4	112.4
21						0.019	466.6	113.2
22						0.020	464.7	113.9
23						0.021	462.8	114.6
24						0.022	461.0	115.4
25						0.023	459.1	116.1
26						0.024	457.2	116.9
27						0.025	455.2	117.6
28						0.026	453.3	118.4
29						0.027	451.4	119.2
30						0.028	449.4	119.9
31						0.029	447.5	120.7
32						0.030	445.5	121.5
33						0.031	443.5	122.3
34						0.032	441.5	123.0
35						0.033	439.5	123.8
36						0.034	437.5	124.6

Results for 0.1 d:

Δt = 0.0001 d: S = 278.7 mg COD/L, X_a = 187.1 mg VSS/L
Δt = 0.001 d: S = 279.3 mg COD/L, X_a = 186.9 mg VSS/L
Δt = 0.05 d: S = 309.5 mg COD/L, X_a = 175.0 mg VSS/L

Results for 0.5 d using Δt = 0.05 d:
S = -26.8 mg COD/L, X_a = 299.0 mg VSS/L
(negative S value indicates that the numerical approximation failed)

The smaller the Δt, the higher the accuracy of numerical approximation. This is due to the nature of numerical approximation – the derivatives ($\Delta t \rightarrow 0$) are replaced with algebraic calculations (nonzero Δt). Therefore as Δt gets longer the calculation error will get larger. If Δt exceeds a certain value for an explicit method, the calculation error will be magnified with the progress of calculation such that we may get a stable solution as we see from Δt=0.05 d in this case.