Naomi Eliane Rocillo Rangel
11/12/2025

Modelo cinético.

Reacción:

$$A + B \rightarrow 2B$$

La formación del producto se describe por medio de esta ecuación:

$$\frac{dC}{dt} = k\ C(t)(C_{max} - C(t))$$

- **C(t):** Concentración del producto (mol/L).
- **K:** constante cinética.
- C_{max}: Concentración máxima alcanzada.

Condición inicial y parámetros.

C (0) = 0.02 mol/L

k = 0.45 L$mol^{-1} \cdot min^{-1}$

C_{max}= 1 mol/L

Intervalo de integración.

0 ≤ t ≤ 25 min

Δt=0.1 min

Función f (t, C).

$$\frac{dC}{dt} = f(t, C) = K\ C(C_{max} - C)$$

Esquema RK4 con Δt = 0.1.

$$k_1 = f(t_{n,}, C_n)$$

$$k_2 = f(t_n + \frac{\Delta t}{2}, C_n + \frac{\Delta t}{2} k_1)$$

$$k_3 = f(t_n + \frac{\Delta t}{2}, C_n + \frac{\Delta t}{2} k_2)$$

$$k_4 = f(t_n + \Delta t, C_n + \Delta t\ k_3)$$

$$C_{n+1} = C_n + \frac{\Delta t}{6}(\ k_1 + 2k_2 + 2k_3 + k_4\ )$$

Tabla

#	t(min)	C_RK4(mol/L)	C_RK2(mol/L)
	0.000	0.020000	0.020000
	0.100	0.020901	0.020901
	0.200	0.021842	0.021842
	0.300	0.022825	0.022824
	0.400	0.023850	0.023849
	0.500	0.024921	0.024919
	0.600	0.026038	0.026036
	0.700	0.027204	0.027201
	0.800	0.028420	0.028417
	0.900	0.029690	0.029686
	1.000	0.031014	0.031010
	1.100	0.032395	0.032390
	1.200	0.033836	0.033830
	1.300	0.035338	0.035332
	1.400	0.036904	0.036898
	1.500	0.038538	0.038530
	1.600	0.040240	0.040232
	1.700	0.042014	0.042005

1.800	0.043863	0.043853
1.900	0.045790	0.045779
2.000	0.047797	0.047785
2.100	0.049887	0.049874
2.200	0.052064	0.052049
2.300	0.054330	0.054314
2.400	0.056689	0.056672
2.500	0.059144	0.059125
2.600	0.061698	0.061678
2.700	0.064355	0.064334
2.800	0.067118	0.067096
2.900	0.069991	0.069967
3.000	0.072978	0.072952
3.100	0.076081	0.076053
3.200	0.079306	0.079275
3.300	0.082654	0.082622
3.400	0.086131	0.086097
3.500	0.089739	0.089703
3.600	0.093484	0.093445
3.700	0.097368	0.097327
3.800	0.101395	0.101351
3.900	0.105569	0.105523
4.000	0.109894	0.109845
4.100	0.114374	0.114322
4.200	0.119012	0.118957
4.300	0.123812	0.123754

4.400	**0.128776**	**0.128716**
4.500	**0.133910**	**0.133846**
4.600	**0.139216**	**0.139149**
4.700	**0.144696**	**0.144626**
4.800	**0.150355**	**0.150281**
4.900	**0.156194**	**0.156117**
5.000	**0.162218**	**0.162136**
5.100	**0.168426**	**0.168342**
5.200	**0.174824**	**0.174735**
5.300	**0.181410**	**0.181318**
5.400	**0.188189**	**0.188093**
5.500	**0.195161**	**0.195060**
5.600	**0.202326**	**0.202222**
5.700	**0.209686**	**0.209578**
5.800	**0.217241**	**0.217128**
5.900	**0.224990**	**0.224874**
6.000	**0.232934**	**0.232813**
6.100	**0.241070**	**0.240946**
6.200	**0.249399**	**0.249270**
6.300	**0.257918**	**0.257785**
6.400	**0.266624**	**0.266487**
6.500	**0.275515**	**0.275374**
6.600	**0.284587**	**0.284442**
6.700	**0.293837**	**0.293688**
6.800	**0.303260**	**0.303107**
6.900	**0.312852**	**0.312695**

7.000	**0.322606**	**0.322446**
7.100	**0.332518**	**0.332354**
7.200	**0.342579**	**0.342412**
7.300	**0.352785**	**0.352614**
7.400	**0.363126**	**0.362952**
7.500	**0.373596**	**0.373419**
7.600	**0.384185**	**0.384005**
7.700	**0.394886**	**0.394703**
7.800	**0.405688**	**0.405502**
7.900	**0.416582**	**0.416394**
8.000	**0.427558**	**0.427368**
8.100	**0.438606**	**0.438413**
8.200	**0.449715**	**0.449521**
8.300	**0.460875**	**0.460679**
8.400	**0.472074**	**0.471876**
8.500	**0.483301**	**0.483102**
8.600	**0.494545**	**0.494345**
8.700	**0.505795**	**0.505593**
8.800	**0.517038**	**0.516836**
8.900	**0.528265**	**0.528062**
9.000	**0.539463**	**0.539260**
9.100	**0.550621**	**0.550418**
9.200	**0.561728**	**0.561525**
9.300	**0.572774**	**0.572571**
9.400	**0.583748**	**0.583546**
9.500	**0.594640**	**0.594438**

9.600	0.605439	0.605238
9.700	0.616136	0.615936
9.800	0.626722	0.626523
9.900	0.637188	0.636990
10.000	0.647525	0.647329
10.100	0.657727	0.657532
10.200	0.667784	0.667591
10.300	0.677691	0.677499
10.400	0.687440	0.687251
10.500	0.697027	0.696840
10.600	0.706445	0.706260
10.700	0.715690	0.715507
10.800	0.724757	0.724576
10.900	0.733642	0.733464
11.000	0.742343	0.742167
11.100	0.750855	0.750682
11.200	0.759178	0.759008
11.300	0.767309	0.767142
11.400	0.775247	0.775082
11.500	0.782991	0.782829
11.600	0.790539	0.790380
11.700	0.797893	0.797737
11.800	0.805053	0.804899
11.900	0.812019	0.811868
12.000	0.818791	0.818644
12.100	0.825372	0.825228

12.200	0.831764	0.831622
12.300	0.837967	0.837828
12.400	0.843985	0.843849
12.500	0.849819	0.849686
12.600	0.855472	0.855342
12.700	0.860947	0.860820
12.800	0.866248	0.866124
12.900	0.871376	0.871255
13.000	0.876336	0.876218
13.100	0.881131	0.881015
13.200	0.885764	0.885651
13.300	0.890239	0.890129
13.400	0.894559	0.894452
13.500	0.898729	0.898625
13.600	0.902752	0.902650
13.700	0.906631	0.906532
13.800	0.910372	0.910275
13.900	0.913976	0.913882
14.000	0.917449	0.917358
14.100	0.920794	0.920705
14.200	0.924014	0.923928
14.300	0.927114	0.927030
14.400	0.930097	0.930015
14.500	0.932967	0.932887
14.600	0.935727	0.935650
14.700	0.938381	0.938306

14.800	**0.940932**	**0.940859**
14.900	**0.943384**	**0.943313**
15.000	**0.945740**	**0.945672**
15.100	**0.948003**	**0.947937**
15.200	**0.950177**	**0.950113**
15.300	**0.952265**	**0.952203**
15.400	**0.954269**	**0.954209**
15.500	**0.956194**	**0.956135**
15.600	**0.958040**	**0.957983**
15.700	**0.959812**	**0.959757**
15.800	**0.961513**	**0.961459**
15.900	**0.963144**	**0.963092**
16.000	**0.964708**	**0.964658**
16.100	**0.966209**	**0.966160**
16.200	**0.967648**	**0.967601**
16.300	**0.969027**	**0.968982**
16.400	**0.970350**	**0.970306**
16.500	**0.971617**	**0.971575**
16.600	**0.972832**	**0.972791**
16.700	**0.973997**	**0.973957**
16.800	**0.975112**	**0.975074**
16.900	**0.976181**	**0.976144**
17.000	**0.977206**	**0.977170**
17.100	**0.978187**	**0.978152**
17.200	**0.979126**	**0.979093**
17.300	**0.980027**	**0.979994**

17.400	0.980889	0.980857
17.500	0.981714	0.981684
17.600	0.982505	0.982476
17.700	0.983262	0.983234
17.800	0.983986	0.983959
17.900	0.984680	0.984654
18.000	0.985345	0.985319
18.100	0.985980	0.985956
18.200	0.986589	0.986565
18.300	0.987172	0.987149
18.400	0.987729	0.987707
18.500	0.988263	0.988241
18.600	0.988773	0.988753
18.700	0.989262	0.989242
18.800	0.989730	0.989711
18.900	0.990177	0.990159
19.000	0.990605	0.990588
19.100	0.991015	0.990998
19.200	0.991407	0.991390
19.300	0.991782	0.991766
19.400	0.992141	0.992125
19.500	0.992484	0.992469
19.600	0.992812	0.992798
19.700	0.993126	0.993113
19.800	0.993427	0.993414
19.900	0.993714	0.993702

20.000	**0.993989**	**0.993977**
20.100	**0.994252**	**0.994240**
20.200	**0.994504**	**0.994492**
20.300	**0.994744**	**0.994733**
20.400	**0.994974**	**0.994964**
20.500	**0.995195**	**0.995184**
20.600	**0.995405**	**0.995395**
20.700	**0.995606**	**0.995597**
20.800	**0.995799**	**0.995790**
20.900	**0.995983**	**0.995974**
21.000	**0.996159**	**0.996151**
21.100	**0.996327**	**0.996319**
21.200	**0.996488**	**0.996481**
21.300	**0.996642**	**0.996635**
21.400	**0.996790**	**0.996782**
21.500	**0.996931**	**0.996924**
21.600	**0.997065**	**0.997058**
21.700	**0.997194**	**0.997187**
21.800	**0.997317**	**0.997311**
21.900	**0.997435**	**0.997429**
22.000	**0.997547**	**0.997542**
22.100	**0.997655**	**0.997650**
22.200	**0.997758**	**0.997753**
22.300	**0.997857**	**0.997851**
22.400	**0.997951**	**0.997946**
22.500	**0.998041**	**0.998036**

22.600	**0.998127**	**0.998122**
22.700	**0.998209**	**0.998205**
22.800	**0.998288**	**0.998283**
22.900	**0.998363**	**0.998359**
23.000	**0.998435**	**0.998431**
23.100	**0.998504**	**0.998500**
23.200	**0.998569**	**0.998566**
23.300	**0.998632**	**0.998629**
23.400	**0.998692**	**0.998689**
23.500	**0.998750**	**0.998747**
23.600	**0.998805**	**0.998802**
23.700	**0.998857**	**0.998854**
23.800	**0.998907**	**0.998905**
23.900	**0.998956**	**0.998953**
24.000	**0.999001**	**0.998999**
24.100	**0.999045**	**0.999043**
24.200	**0.999087**	**0.999085**
24.300	**0.999127**	**0.999125**
24.400	**0.999166**	**0.999163**
24.500	**0.999202**	**0.999200**
24.600	**0.999238**	**0.999235**
24.700	**0.999271**	**0.999269**
24.800	**0.999303**	**0.999301**
24.900	**0.999334**	**0.999332**
25.000	**0.999363**	**0.999361**

Comparación RK4 vs RK2 (con Δt = 0.1)

$$\frac{dC}{dt} = k\ C(t)(C_{max} - C(t))$$

Con k = 0.45 · $mol^{-1} \cdot min^{-1}$, C_{max}= 1 mol/L y C(0) = 0.02 mol/L en el intervalo de 0 a 25 min utilizando los métodos de Runge- Kutta de segundo y cuarto orden, con un paso Δt = 0.1 min.

La tabla de resultados muestra que ambos métodos predicen concentraciones muy similares, t = 5 min se C_{RK4} = 0.162218 y C_{RK2} = 0.162136, mientras que a t= 25 min se tiene C_{RK4}= 0.999363 y C_{RK2} = 0.999361. Las diferencias son del orden de 10^{-5} − $10^{-5}10^{-6}$, por lo que para este problema y este tamaño de paso los dos métodos dan prácticamente la misma curva.

El método de cuarto orden es más preciso: para un mismo Δt, RK4 presenta errores globales menores que RK2, cerca del valor asintótico C_{max}.

¿De qué tamaño debe ser Δt para que RK2 dé el mismo resultado que RK4 con Δt = 0.1?

El error global de RK2 es proporcional a $(\Delta t)^2$, mientras que el de RK4 es proporcional a $(\Delta t)^4$. El RK2 tiene un error del mismo orden que RK4 con Δt = 0.1, se iguala:

$$(\Delta t_{RK2})^2 = (0.1)^4 = 0.0001$$

$$\Delta t_{RK2} = \sqrt{0.0001} = 0.01\ min$$

el método de segundo orden necesitaría un paso aproximadamente diez veces más pequeño (Δt = 0.01 min) para alcanzar una precisión similar a la obtenida con RK4 usando Δt=0.1 min.