UNIVERSIDAD TECNOLOGICA NACIONAL - FACULTAD REGIONAL ROSARIO
Departamento de Ingeniería Química

Cátedra: Integración IV

Tema: Resolución de Sistemas de Ecuaciones Diferenciales Ordinarias

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Año de cursado: 1999

Problema:

Sea un reactor tanque agitado continuo, cuya velocidad de alimentación es q = 20 lt/min de una solución que contiene 10 mol/lt de la sustancia *A*.

Antes de comenzar la reacción, el reactor se llena con una solución que contiene para el instante t_0 = 0: C_A = 10 mol/lt y $C_B = C_C = C_D$ = 0 mol/lt

El volumen del reactor es de 500 lt y en el mismo se producen las siguientes reacciones irreversibles:

$$A \xrightarrow{k_1} B$$
$$A + B \xrightarrow{k_2} C$$
$$A + C \xrightarrow{k_3} D$$

Asumiendo que el reactor es isotérmico, y que las reacciones elementales, los caudales de entrada y salida y el volumen del reactor son constantes; entonces la variación de la concentración desde el instante en que comienza la reacción hasta que el reactor entra en régimen estacionario, viene dado por:

$$\frac{\mathrm{d}C_A}{\mathrm{d}t} = \left(\frac{q}{V}C_A^F - \frac{q}{V}C_A\right) - k_1 C_A - k_2 C_A C_B - k_3 C_A C_C$$
$$\frac{\mathrm{d}C_B}{\mathrm{d}t} = -\frac{q}{V}C_B + k_1 C_A - k_2 C_A C_B$$
$$\frac{\mathrm{d}C_C}{\mathrm{d}t} = -\frac{q}{V}C_C + k_2 C_A C_B - k_3 C_A C_C$$
$$\frac{\mathrm{d}C_D}{\mathrm{d}t} = -\frac{q}{V}C_D + k_3 C_A C_C$$

donde C_A^F es la concentración del componente *A* en la alimentación, q el caudal volumétrico, V el volumen del reactor y C_i la concentración del componente *i* (a la salida del reactor).

Calcular la concentración de los componentes *A*, *B*, *C* y *D* en función del tiempo teniendo en cuenta que: k_1 = 0.20 lt/(mol min), k_2 = 0.05 lt^2/(mol^2 min) y k_3 = 0.08 lt^2/(mol^2 min). Determinar también el tiempo en el cual *C* alcanza la máxima concentración.

Resolución:

Para resolver el problema anteriormente planteado se utilizaron los dos métodos que se detallan a continuación:

1. Euler-Gauss:

$$\underline{y}_{i+1} = \underline{y}_i + h * \underline{f}(t_i, \underline{y}_i)$$
$$\underline{y}_{i+1}^{(c)} = \underline{y}_i + \frac{h}{2}\left(\underline{f}(t_{i+1}, \underline{y}_{i+1}) + \underline{f}(t_i, \underline{y}_i)\right)$$
$$\underline{y}_{i+1}^{(p)} = \underline{y}_i^{(c)} + h * \underline{f}(t_i, \underline{y}_i^{(c)})$$

2. Runge-Kutta de 4to orden:

$$\underline{y}_{i+1} = \underline{y}_i + \frac{h}{6}\left(\underline{k}_1 + 2\underline{k}_2 + 2\underline{k}_3 + \underline{k}_4\right)$$
$$\underline{k}_1 = \underline{f}(t_i, \underline{y}_i)$$
$$\underline{k}_2 = \underline{f}\left(t_i + \frac{h}{2}, \underline{y}_i + \frac{h}{2}\underline{k}_1\right)$$
$$\underline{k}_3 = \underline{f}\left(t_i + \frac{h}{2}, \underline{y}_i + \frac{h}{2}\underline{k}_2\right)$$
$$\underline{k}_4 = \underline{f}(t_i + h, \underline{y}_i + h\underline{k}_3)$$

1. Resultados obtenidos a través del método de Euler-Gauss:

t_i	C_{Ai}	C_{Bi}	C_{Ci}	C_{Di}	$f1(t_i,C_{Ai},C_{Bi},C_{Ci})$	$f2(t_i,C_{Ai},C_{Bi})$	$f3(t_i,C_{Ai},C_{Bi},C_{Ci})$	$f4(t_i,C_{Ai},C_{Ci},C_{Di})$	C_{Ai} ©	C_{Bi} ©	C_{Ci} ©	C_{Di} ©
0.0	10.00000	0.00000	0.00000	0.00000	-2.00000	2.00000	0.00000	0.00000	-	-	-	-
0.1	9.80000	0.20000	0.00000	0.00000	-2.05000	1.85400	0.09800	0.00000	9.79750	0.19270	0.00490	0.00000
0.2	9.59250	0.37810	0.01470	0.00000	-2.09483	1.72203	0.16948	0.01128	9.59276	0.37880	0.01337	0.00056
0.3	9.38328	0.55100	0.03032	0.00169	-2.13326	1.59610	0.23454	0.02269	9.38110	0.54401	0.03490	0.00170
0.4	9.16777	0.70362	0.05835	0.00397	-2.16559	1.48288	0.27740	0.04264	9.16833	0.70495	0.05592	0.00496
0.5	8.95177	0.85324	0.08366	0.00922	-2.19024	1.37432	0.31864	0.05954	8.94998	0.84648	0.08816	0.00908
0.6	8.73095	0.98391	0.12002	0.01503	-2.20878	1.27731	0.34089	0.08323	8.73182	0.98582	0.11663	0.01636
0.7	8.51094	1.11355	0.15072	0.02468	-2.21912	1.18378	0.36522	0.10164	8.50956	1.10696	0.15533	0.02427
0.8	8.28765	1.22534	0.19185	0.03444	-2.22399	1.10076	0.37289	0.12582	8.28879	1.22778	0.18763	0.03606
0.9	8.06639	1.33786	0.22492	0.04864	-2.22066	1.02018	0.38544	0.14320	8.06541	1.33139	0.22976	0.04789
1.0	7.84335	1.43341	0.26831	0.06221	-2.21289	0.94920	0.38305	0.16587	7.84471	1.43633	0.26334	0.06409
2.0	5.75991	2.11693	0.62483	0.29117	-1.87996	0.45764	0.29676	0.27627	5.76142	2.12172	0.61676	0.29444
3.0	4.11857	2.44739	0.86914	0.56525	-1.37881	0.22183	0.18285	0.26376	4.11902	2.45347	0.85842	0.57022
4.0	2.96087	2.60482	1.01544	0.80115	-0.93676	0.10235	0.10448	0.20848	2.95967	2.61190	1.00235	0.80791
5.0	2.19100	2.67253	1.09822	0.98001	-0.61111	0.03852	0.05635	0.15330	2.18787	2.68044	1.08306	0.98852
6.0	1.69547	2.69149	1.14241	1.10941	-0.39003	0.00327	0.02752	0.11058	1.69016	2.70019	1.12544	1.11959
7.0	1.38271	2.68334	1.16346	1.20234	-0.24606	-0.01631	0.01028	0.08060	1.37486	2.69283	1.14487	1.21419
8.0	1.18808	2.66021	1.17063	1.27015	-0.15443	-0.02682	-0.00006	0.06046	1.17720	2.67055	1.15056	1.28371
9.0	1.06869	2.62918	1.16944	1.32108	-0.09696	-0.03192	-0.00627	0.04714	1.05410	2.64050	1.14799	1.33648
10.0	0.99694	2.59449	1.16323	1.36070	-0.06137	-0.03372	-0.00998	0.03835	0.97773	2.60695	1.14046	1.37813
11.0	0.95537	2.55869	1.15404	1.39262	-0.03972	-0.03350	-0.01214	0.03250	0.93041	2.57252	1.13000	1.41236
12.0	0.93306	2.52328	1.14311	1.41915	-0.02698	-0.03204	-0.01333	0.02856	0.90090	2.53880	1.11784	1.44154
13.0	0.92324	2.48912	1.13123	1.44172	-0.02003	-0.02982	-0.01390	0.02588	0.88209	2.50672	1.10479	1.46720
14.0	0.92177	2.45666	1.11890	1.46126	-0.01696	-0.02714	-0.01404	0.02406	0.86939	2.47685	1.09135	1.49035
15.0	0.92615	2.42605	1.10644	1.47831	-0.01660	-0.02416	-0.01389	0.02285	0.85978	2.44949	1.07787	1.51166
16.0	0.93500	2.39730	1.09404	1.49320	-0.01831	-0.02097	-0.01352	0.02211	0.85122	2.42480	1.06458	1.53160
17.0	0.94763	2.37028	1.08184	1.50614	-0.02175	-0.01759	-0.01298	0.02177	0.84222	2.40288	1.05166	1.55052
18.0	0.96384	2.34479	1.06989	1.51720	-0.02682	-0.01402	-0.01229	0.02181	0.83160	2.38377	1.03924	1.56872
19.0	0.98381	2.32055	1.05822	1.52640	-0.03355	-0.01021	-0.01147	0.02223	0.81834	2.36754	1.02741	1.58644
20.0	1.00801	2.29724	1.04680	1.53371	-0.04212	-0.00607	-0.01050	0.02307	0.80143	2.35425	1.01625	1.60394

2. Resultados obtenidos a través del método de Runge-Kutta de 4to orden:

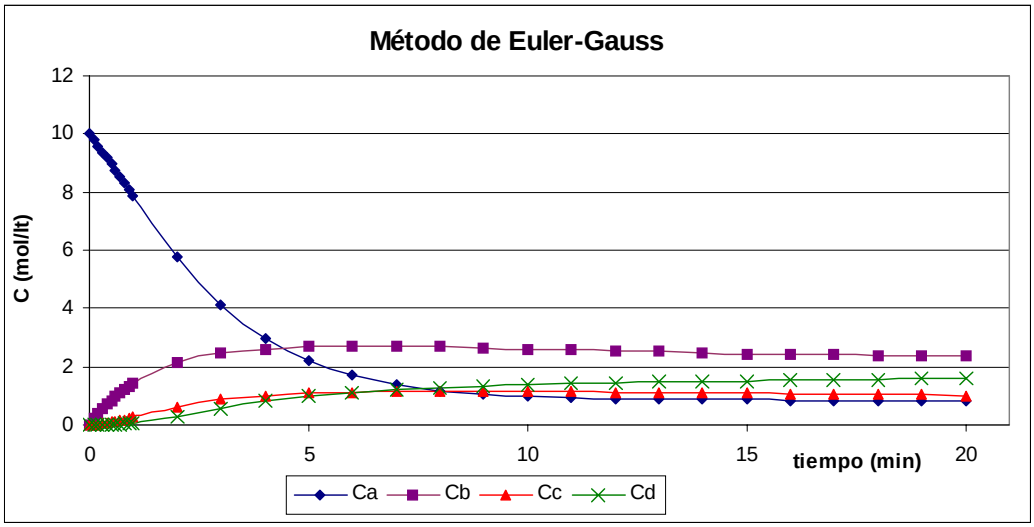
t_i	$hk_1(C_A)$	$hk_1(C_B)$	$hk_1(C_C)$	$hk_1(C_D)$	$hk_2(C_A)$	$hk_2(C_B)$	$hk_2(C_C)$	$hk_2(C_D)$	$hk_3(C_A)$	$hk_3(C_B)$	$hk_3(C_C)$	$hk_3(C_D)$	$hk_4(C_A)$	$hk_4(C_B)$	$hk_4(C_C)$	$hk_4(C_D)$	$C_A(i)$	$C_B(i)$	$C_C(i)$	$C_D(i)$
0.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	10.0000	0.00000	0.00000	0.00000
0.1	-0.20000	0.20000	0.00000	0.00000	-0.20255	0.19265	0.00495	0.00000	-0.20253	0.19282	0.00456	0.00020	-0.20494	0.18573	0.00907	0.00001	9.79748	0.19278	0.00468	0.00007
0.2	-0.20495	0.18573	0.00906	0.00037	-0.20724	0.17891	0.01310	0.00071	-0.20720	0.17907	0.01276	0.00087	-0.20934	0.17249	0.01642	0.00042	9.59029	0.37181	0.01755	0.00073
0.3	-0.20934	0.17249	0.01641	0.00134	-0.21133	0.16616	0.01967	0.00195	-0.21128	0.16630	0.01938	0.00207	-0.21310	0.16019	0.02232	0.00146	9.37901	0.53808	0.03702	0.00253
0.4	-0.21311	0.16019	0.02231	0.00277	-0.21477	0.15432	0.02489	0.00356	-0.21471	0.15445	0.02465	0.00365	-0.21620	0.14878	0.02696	0.00296	9.16430	0.69249	0.06175	0.00589
0.5	-0.21620	0.14878	0.02696	0.00450	-0.21752	0.14333	0.02897	0.00542	-0.21746	0.14345	0.02877	0.00549	-0.21860	0.13820	0.03055	0.00477	8.94684	0.83592	0.09058	0.01107
0.6	-0.21860	0.13820	0.03055	0.00644	-0.21958	0.13314	0.03208	0.00743	-0.21950	0.13325	0.03191	0.00748	-0.22030	0.12838	0.03325	0.00677	8.72733	0.96915	0.12255	0.01824
0.7	-0.22030	0.12838	0.03324	0.00848	-0.22093	0.12369	0.03437	0.00950	-0.22086	0.12379	0.03423	0.00954	-0.22131	0.11927	0.03519	0.00888	8.50646	1.09292	0.15682	0.02748
0.8	-0.22131	0.11927	0.03519	0.01056	-0.22160	0.11492	0.03597	0.01158	-0.22153	0.11502	0.03585	0.01161	-0.22165	0.11083	0.03650	0.01101	8.28493	1.20791	0.19271	0.03881
0.9	-0.22165	0.11083	0.03649	0.01262	-0.22161	0.10680	0.03699	0.01361	-0.22154	0.10689	0.03689	0.01363	-0.22134	0.10300	0.03728	0.01310	8.06338	1.31478	0.22963	0.05218
1.0	-0.22134	0.10300	0.03728	0.01460	-0.22099	0.09926	0.03754	0.01556	-0.22093	0.09935	0.03746	0.01556	-0.22043	0.09574	0.03763	0.01511	7.84245	1.41411	0.26711	0.06750
2.0	-0.19204	0.05004	0.03086	0.02677	-0.18976	0.04827	0.03028	0.02699	-0.18977	0.04831	0.03027	0.02698	-0.18745	0.04660	0.02968	0.02702	5.77437	2.09554	0.61403	0.29748
3.0	-0.14301	0.02455	0.01960	0.02643	-0.14055	0.02367	0.01911	0.02623	-0.14058	0.02369	0.01911	0.02623	-0.13813	0.02284	0.01863	0.02626	4.14527	2.42903	0.85347	0.57004
4.0	-0.09830	0.01162	0.01149	0.02124	-0.09632	0.01116	0.01117	0.02095	-0.09636	0.01117	0.01118	0.02095	-0.09441	0.01072	0.01087	0.02090	2.99119	2.59041	0.99808	0.80505
5.0	-0.06471	0.00469	0.00641	0.01574	-0.06331	0.00444	0.00621	0.01549	-0.06333	0.00444	0.00622	0.01549	-0.06196	0.00420	0.00603	0.01541	2.21877	2.66178	1.08056	0.98417
6.0	-0.04157	0.00084	0.00332	0.01137	-0.04063	0.00070	0.00321	0.01118	-0.04065	0.00071	0.00321	0.01118	-0.03974	0.00057	0.00309	0.01111	1.71776	2.68388	1.12493	1.11451
7.0	-0.02632	-0.00132	0.00146	0.00824	-0.02571	-0.00140	0.00139	0.00812	-0.02572	-0.00139	0.00139	0.00812	-0.02513	-0.00147	0.00132	0.00807	1.39870	2.67838	1.14626	1.20869
8.0	-0.01649	-0.00251	0.00033	0.00611	-0.01610	-0.00255	0.00029	0.00603	-0.01611	-0.00255	0.00029	0.00603	-0.01572	-0.00259	0.00025	0.00600	1.19795	2.65750	1.15365	1.27780
9.0	-0.01022	-0.00312	-0.00035	0.00469	-0.00998	-0.00314	-0.00038	0.00463	-0.00998	-0.00314	-0.00038	0.00463	-0.00974	-0.00316	-0.00040	0.00462	1.07288	2.62843	1.15259	1.33002
10.0	-0.00626	-0.00338	-0.00076	0.00373	-0.00611	-0.00338	-0.00078	0.00369	-0.00611	-0.00338	-0.00078	0.00369	-0.00596	-0.00339	-0.00080	0.00369	0.99583	2.59549	1.14643	1.37089
11.0	-0.00376	-0.00342	-0.00101	0.00307	-0.00366	-0.00342	-0.00102	0.00304	-0.00366	-0.00342	-0.00102	0.00305	-0.00357	-0.00342	-0.00103	0.00305	0.94912	2.56133	1.13721	1.40409
12.0	-0.00219	-0.00334	-0.00115	0.00261	-0.00212	-0.00333	-0.00116	0.00259	-0.00213	-0.00333	-0.00116	0.00259	-0.00207	-0.00333	-0.00116	0.00260	0.92153	2.52753	1.12619	1.43198
13.0	-0.00120	-0.00318	-0.00123	0.00228	-0.00116	-0.00317	-0.00123	0.00227	-0.00116	-0.00317	-0.00123	0.00227	-0.00112	-0.00316	-0.00123	0.00228	0.90597	2.49505	1.11419	1.45608
14.0	-0.00058	-0.00298	-0.00126	0.00203	-0.00055	-0.00297	-0.00126	0.00202	-0.00055	-0.00297	-0.00126	0.00202	-0.00053	-0.00296	-0.00126	0.00203	0.89795	2.46440	1.10173	1.47735
15.0	-0.00019	-0.00277	-0.00126	0.00183	-0.00018	-0.00276	-0.00126	0.00182	-0.00018	-0.00276	-0.00126	0.00182	-0.00016	-0.00275	-0.00126	0.00183	0.89463	2.43584	1.08915	1.49642
16.0	0.00005	-0.00255	-0.00124	0.00166	0.00005	-0.00254	-0.00124	0.00165	0.00005	-0.00254	-0.00124	0.00166	0.00006	-0.00253	-0.00124	0.00167	0.89423	2.40947	1.07668	1.51372
17.0	0.00019	-0.00233	-0.00121	0.00152	0.00019	-0.00232	-0.00121	0.00152	0.00019	-0.00232	-0.00121	0.00152	0.00020	-0.00231	-0.00120	0.00153	0.89559	2.38530	1.06447	1.52952
18.0	0.00027	-0.00212	-0.00117	0.00140	0.00027	-0.00211	-0.00116	0.00139	0.00027	-0.00211	-0.00116	0.00139	0.00028	-0.00210	-0.00116	0.00140	0.89800	2.36323	1.05264	1.54401
19.0	0.00031	-0.00193	-0.00112	0.00129	0.00031	-0.00192	-0.00112	0.00128	0.00031	-0.00192	-0.00112	0.00128	0.00032	-0.00191	-0.00111	0.00129	0.90097	2.34318	1.04126	1.55734
20.0	0.00033	-0.00174	-0.00107	0.00118	0.00033	-0.00174	-0.00107	0.00118	0.00033	-0.00174	-0.00107	0.00118	0.00033	-0.00173	-0.00106	0.00119	0.90423	2.32501	1.03037	1.56962

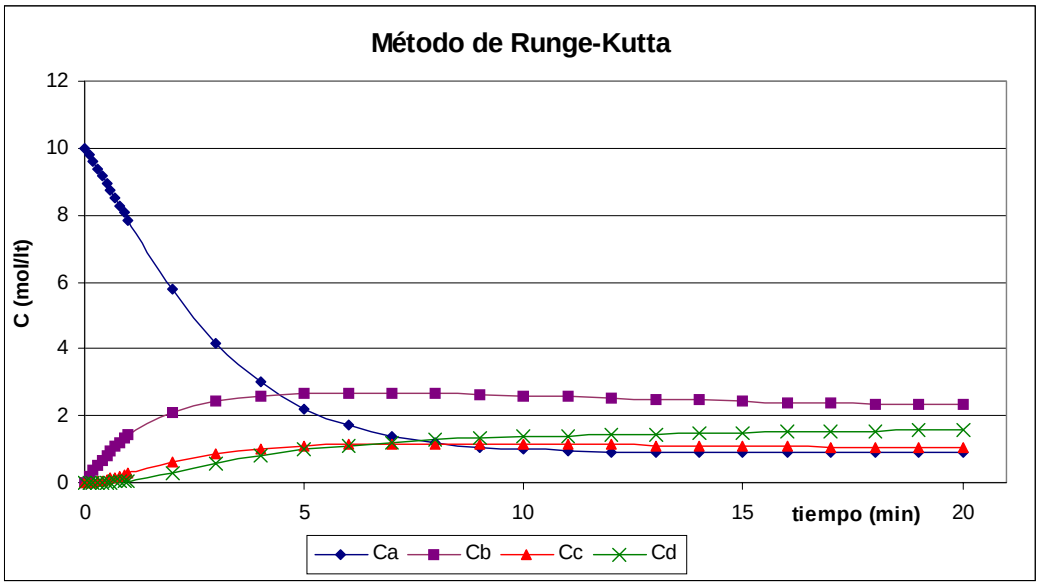
Comparación entre ambos métodos:

Comparando los métodos de E-G y R-K se puede concluir que ambos dan resultados muy similares. Por lo tanto, optar por uno u otro desde el punto de vista del error cometido debido al método utilizado, es indistinto.

La concentración del componente C, alcanza su máximo para el método de E-G en el tiempo t = 8 min, con un valor de Cc = 1.15056 mol/lt y para el método de R-K a t = 8.3 min, con Cc = 1.15403 mol/lt (Runge-Kutta).

	Euler-Gauss				**Runge-Kutta**			
t_i	$C_A(i)$	$C_B(i)$	$C_C(i)$	$C_D(i)$	$C_A(i)$	$C_B(i)$	$C_C(i)$	$C_D(i)$
0.0	10.00000	0.00000	0.00000	0.00000	10.00000	0.00000	0.00000	0.00000
0.1	9.80000	0.20000	0.00000	0.00000	9.79748	0.19278	0.00468	0.00007
0.2	9.59250	0.37810	0.01470	0.00000	9.59029	0.37181	0.01755	0.00073
0.3	9.38328	0.55100	0.03032	0.00169	9.37901	0.53808	0.03702	0.00253
0.4	9.16777	0.70362	0.05835	0.00397	9.16430	0.69249	0.06175	0.00589
0.5	8.95177	0.85324	0.08366	0.00922	8.94684	0.83592	0.09058	0.01107
0.6	8.73095	0.98391	0.12002	0.01503	8.72733	0.96915	0.12255	0.01824
0.7	8.51094	1.11355	0.15072	0.02468	8.50646	1.09292	0.15682	0.02748
0.8	8.28765	1.22534	0.19185	0.03444	8.28493	1.20791	0.19271	0.03881
0.9	8.06639	1.33786	0.22492	0.04864	8.06338	1.31478	0.22963	0.05218
1.0	7.84335	1.43341	0.26831	0.06221	7.84245	1.41411	0.26711	0.06750
2.0	5.75991	2.11693	0.62483	0.29117	5.77437	2.09554	0.61403	0.29748
3.0	4.11857	2.44739	0.86914	0.56525	4.14527	2.42903	0.85347	0.57004
4.0	2.96087	2.60482	1.01544	0.80115	2.99119	2.59041	0.99808	0.80505
5.0	2.19100	2.67253	1.09822	0.98001	2.21877	2.66178	1.08056	0.98417
6.0	1.69547	2.69149	1.14241	1.10941	1.71776	2.68388	1.12493	1.11451
7.0	1.38271	2.68334	1.16346	1.20234	1.39870	2.67838	1.14626	1.20869
8.0	1.18808	2.66021	1.17063	1.27015	1.19795	2.65750	1.15365	1.27780
9.0	1.06869	2.62918	1.16944	1.32108	1.07288	2.62843	1.15259	1.33002
10.0	0.99694	2.59449	1.16323	1.36070	0.99583	2.59549	1.14643	1.37089
11.0	0.95537	2.55869	1.15404	1.39262	0.94912	2.56133	1.13721	1.40409
12.0	0.93306	2.52328	1.14311	1.41915	0.92153	2.52753	1.12619	1.43198
13.0	0.92324	2.48912	1.13123	1.44172	0.90597	2.49505	1.11419	1.45608
14.0	0.92177	2.45666	1.11890	1.46126	0.89795	2.46440	1.10173	1.47735
15.0	0.92615	2.42605	1.10644	1.47831	0.89463	2.43584	1.08915	1.49642
16.0	0.93500	2.39730	1.09404	1.49320	0.89423	2.40947	1.07668	1.51372
17.0	0.94763	2.37028	1.08184	1.50614	0.89559	2.38530	1.06447	1.52952
18.0	0.96384	2.34479	1.06989	1.51720	0.89800	2.36323	1.05264	1.54401
19.0	0.98381	2.32055	1.05822	1.52640	0.90097	2.34318	1.04126	1.55734
20.0	1.00801	2.29724	1.04680	1.53371	0.90423	2.32501	1.03037	1.56962


Método de Euler-Gauss
C (mol/lt)
12
10
8
6
4
2
0
0
5
10
15
20
tiempo (min)
Ca
Cb
Cc
Cd


Método de Runge-Kutta
C (mol/lt)
12
10
8
6
4
2
0
0
5
10
15
20
tiempo (min)
Ca
Cb
Cc
Cd