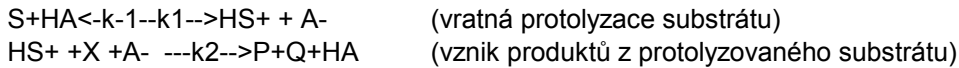


Kyselá katalýza - protonizace substrátu



koncentrace: S= 100 A= 1 konstanty: k1=
 výchozí HA= 5 X= 100 k-1=
 HS+= 0 P= 0 k2
 Q= 0
 první časový krok= 1
 k-1*A- 1.00E-04 <<
 1.00E-04 >> k2*X 1.00E-02 Je-li pravda
 1.00E-02 Je-li pravda
 expanze času 1.03

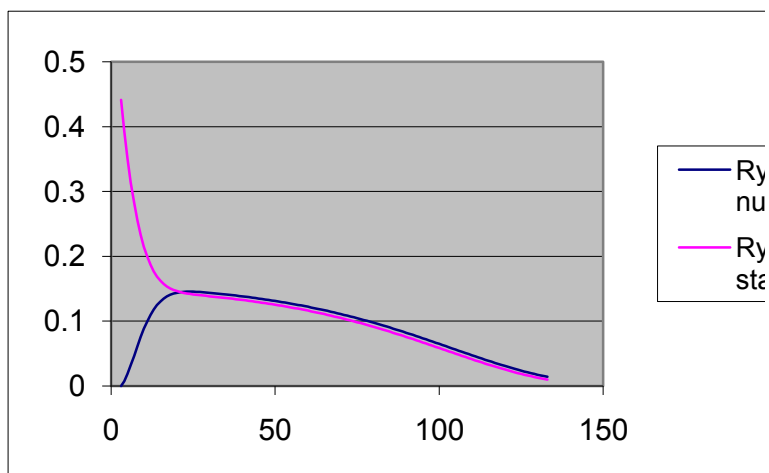
t/ s	substrát				produkty			katalyzátor	
	S	HA	HS+	A-	X	P (Q)	HA+A-		
0	100		5	0	1	100	0	6	
1	9.95E+01	4.50E+00	5.00E-01	1.50E+00	1.00E+02	0.00E+00	6.00E+00		
2.03	9.90E+01	4.05E+00	9.53E-01	1.95E+00	1.00E+02	7.73E-03	6.00E+00		
3.0909	9.86E+01	3.64E+00	1.36E+00	2.36E+00	1.00E+02	2.75E-02	6.00E+00		
4.183627	9.82E+01	3.28E+00	1.72E+00	2.72E+00	9.99E+01	6.25E-02	6.00E+00		
5.309136	9.79E+01	2.97E+00	2.03E+00	3.03E+00	9.99E+01	1.15E-01	6.00E+00		
6.46841	9.75E+01	2.71E+00	2.29E+00	3.29E+00	9.98E+01	1.86E-01	6.00E+00		
7.662462	9.72E+01	2.48E+00	2.52E+00	3.52E+00	9.97E+01	2.76E-01	6.00E+00		
8.892336	9.69E+01	2.30E+00	2.70E+00	3.70E+00	9.96E+01	3.84E-01	6.00E+00		
10.15911	9.66E+01	2.14E+00	2.86E+00	3.86E+00	9.95E+01	5.11E-01	6.00E+00		
11.46388	9.64E+01	2.02E+00	2.98E+00	3.98E+00	9.93E+01	6.54E-01	6.00E+00		
12.8078	9.61E+01	1.92E+00	3.08E+00	4.08E+00	9.92E+01	8.12E-01	6.00E+00		
14.19203	9.59E+01	1.84E+00	3.16E+00	4.16E+00	9.90E+01	9.85E-01	6.00E+00		
15.61779	9.56E+01	1.77E+00	3.23E+00	4.23E+00	9.88E+01	1.17E+00	6.00E+00		
17.08632	9.54E+01	1.72E+00	3.28E+00	4.28E+00	9.86E+01	1.37E+00	6.00E+00		
18.59891	9.51E+01	1.69E+00	3.31E+00	4.31E+00	9.84E+01	1.58E+00	6.00E+00		
20.15688	9.49E+01	1.66E+00	3.34E+00	4.34E+00	9.82E+01	1.80E+00	6.00E+00		
21.76159	9.46E+01	1.64E+00	3.36E+00	4.36E+00	9.80E+01	2.03E+00	6.00E+00		
23.41444	9.44E+01	1.62E+00	3.38E+00	4.38E+00	9.77E+01	2.26E+00	6.00E+00		
25.11687	9.41E+01	1.61E+00	3.39E+00	4.39E+00	9.75E+01	2.51E+00	6.00E+00		
26.87037	9.38E+01	1.60E+00	3.40E+00	4.40E+00	9.72E+01	2.76E+00	6.00E+00		
28.67649	9.36E+01	1.59E+00	3.41E+00	4.41E+00	9.70E+01	3.03E+00	6.00E+00		
30.53678	9.33E+01	1.59E+00	3.41E+00	4.41E+00	9.67E+01	3.30E+00	6.00E+00		
32.45288	9.30E+01	1.59E+00	3.41E+00	4.41E+00	9.64E+01	3.58E+00	6.00E+00		
34.42647	9.27E+01	1.59E+00	3.41E+00	4.41E+00	9.61E+01	3.86E+00	6.00E+00		
36.45926	9.24E+01	1.58E+00	3.42E+00	4.42E+00	9.58E+01	4.16E+00	6.00E+00		
38.55304	9.21E+01	1.58E+00	3.42E+00	4.42E+00	9.55E+01	4.46E+00	6.00E+00		
40.70963	9.18E+01	1.58E+00	3.42E+00	4.42E+00	9.52E+01	4.77E+00	6.00E+00		
42.93092	9.15E+01	1.58E+00	3.42E+00	4.42E+00	9.49E+01	5.09E+00	6.00E+00		
45.21885	9.12E+01	1.58E+00	3.42E+00	4.42E+00	9.46E+01	5.42E+00	6.00E+00		
47.57542	9.08E+01	1.58E+00	3.42E+00	4.42E+00	9.42E+01	5.75E+00	6.00E+00		
50.00268	9.05E+01	1.58E+00	3.42E+00	4.42E+00	9.39E+01	6.10E+00	6.00E+00		
52.50276	9.01E+01	1.58E+00	3.42E+00	4.42E+00	9.35E+01	6.45E+00	6.00E+00		
55.07784	8.98E+01	1.58E+00	3.42E+00	4.42E+00	9.32E+01	6.82E+00	6.00E+00		
57.73018	8.94E+01	1.58E+00	3.42E+00	4.42E+00	9.28E+01	7.19E+00	6.00E+00		

60.46208	8.90E+01	1.58E+00	3.42E+00	4.42E+00	9.24E+01	7.57E+00	6.00E+00
63.27594	8.86E+01	1.58E+00	3.42E+00	4.42E+00	9.20E+01	7.97E+00	6.00E+00
66.17422	8.82E+01	1.58E+00	3.42E+00	4.42E+00	9.16E+01	8.37E+00	6.00E+00
69.15945	8.78E+01	1.58E+00	3.42E+00	4.42E+00	9.12E+01	8.78E+00	6.00E+00
72.23423	8.74E+01	1.58E+00	3.42E+00	4.42E+00	9.08E+01	9.20E+00	6.00E+00
75.40126	8.69E+01	1.58E+00	3.42E+00	4.42E+00	9.04E+01	9.64E+00	6.00E+00
78.6633	8.65E+01	1.58E+00	3.42E+00	4.42E+00	8.99E+01	1.01E+01	6.00E+00
82.0232	8.60E+01	1.58E+00	3.42E+00	4.42E+00	8.95E+01	1.05E+01	6.00E+00
85.48389	8.56E+01	1.58E+00	3.42E+00	4.42E+00	8.90E+01	1.10E+01	6.00E+00
89.04841	8.51E+01	1.59E+00	3.41E+00	4.41E+00	8.85E+01	1.15E+01	6.00E+00
92.71986	8.46E+01	1.59E+00	3.41E+00	4.41E+00	8.80E+01	1.20E+01	6.00E+00
96.50146	8.41E+01	1.59E+00	3.41E+00	4.41E+00	8.75E+01	1.25E+01	6.00E+00
100.3965	8.36E+01	1.59E+00	3.41E+00	4.41E+00	8.70E+01	1.30E+01	6.00E+00
104.4084	8.31E+01	1.59E+00	3.41E+00	4.41E+00	8.65E+01	1.35E+01	6.00E+00
108.5406	8.25E+01	1.59E+00	3.41E+00	4.41E+00	8.59E+01	1.41E+01	6.00E+00
112.7969	8.20E+01	1.59E+00	3.41E+00	4.41E+00	8.54E+01	1.46E+01	6.00E+00
117.1808	8.14E+01	1.59E+00	3.41E+00	4.41E+00	8.48E+01	1.52E+01	6.00E+00
121.6962	8.08E+01	1.59E+00	3.41E+00	4.41E+00	8.43E+01	1.57E+01	6.00E+00
126.3471	8.03E+01	1.59E+00	3.41E+00	4.41E+00	8.37E+01	1.63E+01	6.00E+00
131.1375	7.96E+01	1.59E+00	3.41E+00	4.41E+00	8.31E+01	1.69E+01	6.00E+00
136.0716	7.90E+01	1.59E+00	3.41E+00	4.41E+00	8.24E+01	1.76E+01	6.00E+00
141.1538	7.84E+01	1.59E+00	3.41E+00	4.41E+00	8.18E+01	1.82E+01	6.00E+00
146.3884	7.78E+01	1.59E+00	3.41E+00	4.41E+00	8.12E+01	1.88E+01	6.00E+00
151.78	7.71E+01	1.59E+00	3.41E+00	4.41E+00	8.05E+01	1.95E+01	6.00E+00
157.3334	7.64E+01	1.59E+00	3.41E+00	4.41E+00	7.98E+01	2.02E+01	6.00E+00
163.0534	7.57E+01	1.59E+00	3.41E+00	4.41E+00	7.92E+01	2.08E+01	6.00E+00
168.945	7.50E+01	1.59E+00	3.41E+00	4.41E+00	7.84E+01	2.16E+01	6.00E+00
175.0134	7.43E+01	1.59E+00	3.41E+00	4.41E+00	7.77E+01	2.23E+01	6.00E+00
181.2638	7.36E+01	1.59E+00	3.41E+00	4.41E+00	7.70E+01	2.30E+01	6.00E+00
187.7017	7.29E+01	1.59E+00	3.41E+00	4.41E+00	7.63E+01	2.37E+01	6.00E+00
194.3328	7.21E+01	1.59E+00	3.41E+00	4.41E+00	7.55E+01	2.45E+01	6.00E+00
201.1627	7.13E+01	1.59E+00	3.41E+00	4.41E+00	7.47E+01	2.53E+01	6.00E+00
208.1976	7.05E+01	1.59E+00	3.41E+00	4.41E+00	7.39E+01	2.61E+01	6.00E+00
215.4436	6.97E+01	1.59E+00	3.41E+00	4.41E+00	7.31E+01	2.69E+01	6.00E+00
222.9069	6.89E+01	1.59E+00	3.41E+00	4.41E+00	7.23E+01	2.77E+01	6.00E+00
230.5941	6.81E+01	1.60E+00	3.40E+00	4.40E+00	7.15E+01	2.85E+01	6.00E+00
238.5119	6.72E+01	1.60E+00	3.40E+00	4.40E+00	7.06E+01	2.94E+01	6.00E+00
246.6672	6.64E+01	1.60E+00	3.40E+00	4.40E+00	6.98E+01	3.02E+01	6.00E+00
255.0673	6.55E+01	1.60E+00	3.40E+00	4.40E+00	6.89E+01	3.11E+01	6.00E+00
263.7193	6.46E+01	1.60E+00	3.40E+00	4.40E+00	6.80E+01	3.20E+01	6.00E+00
272.6309	6.37E+01	1.60E+00	3.40E+00	4.40E+00	6.71E+01	3.29E+01	6.00E+00
281.8098	6.28E+01	1.60E+00	3.40E+00	4.40E+00	6.62E+01	3.38E+01	6.00E+00
291.2641	6.18E+01	1.60E+00	3.40E+00	4.40E+00	6.52E+01	3.48E+01	6.00E+00
301.002	6.09E+01	1.60E+00	3.40E+00	4.40E+00	6.43E+01	3.57E+01	6.00E+00
311.0321	5.99E+01	1.60E+00	3.40E+00	4.40E+00	6.33E+01	3.67E+01	6.00E+00
321.363	5.89E+01	1.60E+00	3.40E+00	4.40E+00	6.23E+01	3.77E+01	6.00E+00
332.0039	5.80E+01	1.60E+00	3.40E+00	4.40E+00	6.13E+01	3.87E+01	6.00E+00
342.964	5.69E+01	1.61E+00	3.39E+00	4.39E+00	6.03E+01	3.97E+01	6.00E+00
354.2529	5.59E+01	1.61E+00	3.39E+00	4.39E+00	5.93E+01	4.07E+01	6.00E+00
365.8805	5.49E+01	1.61E+00	3.39E+00	4.39E+00	5.83E+01	4.17E+01	6.00E+00
377.857	5.39E+01	1.61E+00	3.39E+00	4.39E+00	5.73E+01	4.27E+01	6.00E+00
390.1927	5.28E+01	1.61E+00	3.39E+00	4.39E+00	5.62E+01	4.38E+01	6.00E+00

402.8984	5.18E+01	1.61E+00	3.39E+00	4.39E+00	5.51E+01	4.49E+01	6.00E+00
415.9854	5.07E+01	1.61E+00	3.39E+00	4.39E+00	5.41E+01	4.59E+01	6.00E+00
429.465	4.96E+01	1.61E+00	3.39E+00	4.39E+00	5.30E+01	4.70E+01	6.00E+00
443.3489	4.85E+01	1.62E+00	3.38E+00	4.38E+00	5.19E+01	4.81E+01	6.00E+00
457.6494	4.74E+01	1.62E+00	3.38E+00	4.38E+00	5.08E+01	4.92E+01	6.00E+00
472.3789	4.63E+01	1.62E+00	3.38E+00	4.38E+00	4.97E+01	5.03E+01	6.00E+00
487.5502	4.52E+01	1.62E+00	3.38E+00	4.38E+00	4.86E+01	5.14E+01	6.00E+00
503.1767	4.41E+01	1.62E+00	3.38E+00	4.38E+00	4.74E+01	5.26E+01	6.00E+00
519.272	4.29E+01	1.62E+00	3.38E+00	4.38E+00	4.63E+01	5.37E+01	6.00E+00
535.8502	4.18E+01	1.63E+00	3.37E+00	4.37E+00	4.52E+01	5.48E+01	6.00E+00
552.9257	4.07E+01	1.63E+00	3.37E+00	4.37E+00	4.40E+01	5.60E+01	6.00E+00
570.5135	3.95E+01	1.63E+00	3.37E+00	4.37E+00	4.29E+01	5.71E+01	6.00E+00
588.6289	3.84E+01	1.63E+00	3.37E+00	4.37E+00	4.18E+01	5.82E+01	6.00E+00
607.2877	3.72E+01	1.64E+00	3.36E+00	4.36E+00	4.06E+01	5.94E+01	6.00E+00
626.5064	3.61E+01	1.64E+00	3.36E+00	4.36E+00	3.95E+01	6.05E+01	6.00E+00
646.3016	3.50E+01	1.64E+00	3.36E+00	4.36E+00	3.83E+01	6.17E+01	6.00E+00
666.6906	3.38E+01	1.64E+00	3.36E+00	4.36E+00	3.72E+01	6.28E+01	6.00E+00
687.6913	3.27E+01	1.65E+00	3.35E+00	4.35E+00	3.60E+01	6.40E+01	6.00E+00
709.3221	3.16E+01	1.65E+00	3.35E+00	4.35E+00	3.49E+01	6.51E+01	6.00E+00
731.6017	3.04E+01	1.66E+00	3.34E+00	4.34E+00	3.38E+01	6.62E+01	6.00E+00
754.5498	2.93E+01	1.66E+00	3.34E+00	4.34E+00	3.26E+01	6.74E+01	6.00E+00
778.1863	2.82E+01	1.66E+00	3.34E+00	4.34E+00	3.15E+01	6.85E+01	6.00E+00
802.5319	2.71E+01	1.67E+00	3.33E+00	4.33E+00	3.04E+01	6.96E+01	6.00E+00
827.6078	2.60E+01	1.67E+00	3.33E+00	4.33E+00	2.93E+01	7.07E+01	6.00E+00
853.436	2.49E+01	1.68E+00	3.32E+00	4.32E+00	2.82E+01	7.18E+01	6.00E+00
880.0391	2.38E+01	1.68E+00	3.32E+00	4.32E+00	2.71E+01	7.29E+01	6.00E+00
907.4403	2.28E+01	1.69E+00	3.31E+00	4.31E+00	2.61E+01	7.39E+01	6.00E+00
935.6635	2.17E+01	1.69E+00	3.31E+00	4.31E+00	2.50E+01	7.50E+01	6.00E+00
964.7334	2.07E+01	1.70E+00	3.30E+00	4.30E+00	2.40E+01	7.60E+01	6.00E+00
994.6754	1.97E+01	1.71E+00	3.29E+00	4.29E+00	2.30E+01	7.70E+01	6.00E+00
1025.516	1.87E+01	1.72E+00	3.28E+00	4.28E+00	2.20E+01	7.80E+01	6.00E+00
1057.281	1.77E+01	1.72E+00	3.28E+00	4.28E+00	2.10E+01	7.90E+01	6.00E+00
1090	1.68E+01	1.73E+00	3.27E+00	4.27E+00	2.00E+01	8.00E+01	6.00E+00
1123.7	1.58E+01	1.74E+00	3.26E+00	4.26E+00	1.91E+01	8.09E+01	6.00E+00
1158.411	1.49E+01	1.75E+00	3.25E+00	4.25E+00	1.82E+01	8.18E+01	6.00E+00
1194.163	1.40E+01	1.76E+00	3.24E+00	4.24E+00	1.73E+01	8.27E+01	6.00E+00
1230.988	1.32E+01	1.77E+00	3.23E+00	4.23E+00	1.64E+01	8.36E+01	6.00E+00
1268.917	1.23E+01	1.79E+00	3.21E+00	4.21E+00	1.56E+01	8.44E+01	6.00E+00
1307.985	1.15E+01	1.80E+00	3.20E+00	4.20E+00	1.47E+01	8.53E+01	6.00E+00
1348.224	1.07E+01	1.82E+00	3.18E+00	4.18E+00	1.39E+01	8.61E+01	6.00E+00
1389.671	1.00E+01	1.83E+00	3.17E+00	4.17E+00	1.32E+01	8.68E+01	6.00E+00
1432.361	9.27E+00	1.85E+00	3.15E+00	4.15E+00	1.24E+01	8.76E+01	6.00E+00
1476.332	8.57E+00	1.87E+00	3.13E+00	4.13E+00	1.17E+01	8.83E+01	6.00E+00
1521.622	7.91E+00	1.89E+00	3.11E+00	4.11E+00	1.10E+01	8.90E+01	6.00E+00
1568.271	7.27E+00	1.91E+00	3.09E+00	4.09E+00	1.04E+01	8.96E+01	6.00E+00

	default		
	1.00E-03	1.00E-03	1.00E-03
	1.00E-04	1.00E-04	1.00E-04
	1.00E-04	1.00E-04	1.00E-08
	obecná	specifická kat.	

1.00E-04 pak obecná kyselá katalýza
 1.00E-08 pak specifická kyselá katalýza



rychlost numerická	rychlost stacionární
$v = dP/dt$	$v = (k_1 \cdot k_2 \cdot HA \cdot X \cdot S) / (k_1 \cdot A + k_2 \cdot S)$

0	4.41E-01
0.0075	3.93E-01
0.018622	3.51E-01
0.032035	3.14E-01
0.046562	2.82E-01
0.061226	2.56E-01
0.075286	2.33E-01
0.088226	2.15E-01
0.099738	1.99E-01
0.109685	1.87E-01
0.11806	1.77E-01
0.124945	1.69E-01
0.13048	1.63E-01
0.134833	1.58E-01
0.138179	1.54E-01
0.140687	1.51E-01
0.142513	1.48E-01
0.143792	1.46E-01
0.14464	1.45E-01
0.145153	1.44E-01
0.145408	1.43E-01
0.145467	1.42E-01
0.145378	1.41E-01
0.145177	1.41E-01
0.144893	1.40E-01
0.144545	1.39E-01
0.14415	1.39E-01
0.143718	1.38E-01
0.143257	1.38E-01
0.142771	1.37E-01
0.142265	1.37E-01
0.14174	1.36E-01
0.141198	1.36E-01
0.140641	1.35E-01

0.140067	1.34E-01
0.139478	1.34E-01
0.138874	1.33E-01
0.138254	1.33E-01
0.137618	1.32E-01
0.136965	1.31E-01
0.136297	1.31E-01
0.135611	1.30E-01
0.134909	1.29E-01
0.134189	1.28E-01
0.133452	1.28E-01
0.132697	1.27E-01
0.131923	1.26E-01
0.131131	1.25E-01
0.13032	1.25E-01
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0.12864	1.23E-01
0.127771	1.22E-01
0.126881	1.21E-01
0.125972	1.20E-01
0.125042	1.19E-01
0.12409	1.18E-01
0.123118	1.17E-01
0.122125	1.16E-01
0.12111	1.15E-01
0.120073	1.14E-01
0.119014	1.13E-01
0.117933	1.12E-01
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0.115705	1.10E-01
0.114556	1.08E-01
0.113385	1.07E-01
0.112192	1.06E-01
0.110975	1.05E-01
0.109736	1.04E-01
0.108473	1.02E-01
0.107188	1.01E-01
0.10588	9.97E-02
0.104549	9.83E-02
0.103195	9.70E-02
0.101819	9.56E-02
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0.098999	9.27E-02
0.097557	9.13E-02
0.096092	8.98E-02
0.094607	8.83E-02
0.0931	8.68E-02
0.091573	8.52E-02
0.090026	8.37E-02
0.08846	8.21E-02
0.086875	8.05E-02
0.085271	7.89E-02

0.08365	7.72E-02
0.082012	7.56E-02
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0.078688	7.23E-02
0.077004	7.06E-02
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0.070146	6.37E-02
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0.066659	6.03E-02
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0.061383	5.50E-02
0.059619	5.33E-02
0.057853	5.15E-02
0.056089	4.98E-02
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0.04734	4.12E-02
0.045616	3.95E-02
0.043906	3.79E-02
0.042211	3.62E-02
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0.037232	3.14E-02
0.035615	2.99E-02
0.034022	2.83E-02
0.032454	2.68E-02
0.030915	2.54E-02
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0.027925	2.25E-02
0.026478	2.12E-02
0.025066	1.99E-02
0.023689	1.86E-02
0.02235	1.74E-02
0.021049	1.62E-02
0.019787	1.50E-02
0.018566	1.39E-02
0.017387	1.28E-02
0.016251	1.18E-02
0.015158	1.09E-02
0.014109	9.95E-03

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