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~\OneDrive\python folder\Reaction rate project 1.py

1 """
2 Reaction Rate Calculator
3 Calculates rate for Zero order,First order,Second order reactions
4 """
5 print("Reaction Rate Calculation")
6 print("1 Zero order reaction")
7 print("2 First order reaction")
8 print("3 Second order reaction")
9
10 #Choice input with validation
11 while True:
12     try:
13         choice =int(input("Select reaction type(1/2/3):"))
14         if choice in [1,2,3]:
15             break
16         else:
17             print("Invalid choice.Enter 1,2 or 3.")
18     except:
19         print("Enter number only!")
20
21 #K value input
22 while True:
23     try:
24         k=float(input("Enter rate constant(k):"))
25         break
26     except:
27         print("Enter a valid number!")
28
29 #Calculation
30 if choice==1:
31     rate=k
32 elif choice==2:
33     while True:
34         try:
35             A=float(input("Enter concentration [A]:"))
36             break
37         except:
38             print("Enter a valid number!")
39     rate=k*A
40 elif choice==3:
41     while True:
42         try:
43             A=float(input("Enter concentration [A]:"))
44             break
45         except:
46             print("Enter a valid number!")
47     rate=k* (A**2)
48
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49 #Output
50 print("Reaction rate=",rate)
51
52 #Graph plot
53 plot=input("Do you want graph? (yes/no):")
54 import matplotlib.pyplot as plt
55 import numpy as np
56 if plot.lower()=='yes':
57     t_max=float(input("Enter time limit:"))
58     points=int(input("How many points for graph:"))
59     t=np.linspace(0,t_max,points)
60     if choice==1:
61         A_values =A-k*t
62     elif choice==2:
63         A_values=A*np.exp(-k*t)
64     elif choice==3:
65         A_values=A/(1+k*A*t)
66     else:
67         print("Invalid choice")
68         exit()
69     plt.plot(t,A_values,marker='o')
70     plt.xlabel("concentration[A]")
71     plt.ylabel("rates")
72     plt.title("rate vs concentration graph")
73     plt.grid(True)
74     plt.show()
75 else:
76     print("graph not displayed")
77
78
79
80
81
82
83
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