

CH3 Tut 1

October 5, 2017

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At 500K the initial rate of a certain reaction occurring in a batch reactor is ten times the initial rate at 400K. Will the rate ratio of 10:1 stay constant as the composition changes in the reactor? What is the activation energy of this reaction? [38.29 kJ/mol]

```
In [7]: # with increasing reaction rate when T is lower indicates an exothermic
        # reaction
        # the rate ratio of 10:1 will NOT stay constant as the composition changes.
        # rate ratio is only valid at initial conditions.
        # (because when you divide the two rate equations, the initial concentrations cancel out)
        #
```

```
In [32]: from numpy import linspace, exp, log
        from scipy.integrate import odeint
        import matplotlib.pyplot as plt
```

```
In [39]: T1 = 500
        T2 = 400
        r2 = 1 # doesn't matter what value it is in this case
        r1 = 10*r2
        CA0n = 1 # also arbitrary
```

```
In [37]: R = 8.314e-3 #KJ/kmol.K
```

```
In [42]: k1= r1/CA0n
```

```
In [43]: k2 = r2/CA0n
```

```
In [44]: k1/k2
```

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Out[44]:
```

10.0

```
In [26]: # log (k1/k2) = (-Ea/R*T)*(1/T1 - 1/T2)
```

```
In [45]: Ea = -(R*log(k1/k2))/(1/T1 - 1/T2)
        Ea
```

```
Out[45]:
```

38.2873849263

```
In [ ]:
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