Chemical Reactor Design II

Lecture (1) :
Importance of understanding multiple reactions in CRD.

Chemical and Petrochemical Engineering Department

6th Semester

Salahaddin University

Importance of understanding multiple reactions

Understanding multiple reactions is crucial in the field of chemical engineering and reactor design. Multiple reactions refer to situations where *more than one chemical reaction* occurs simultaneously within a system. This complexity introduces challenges and opportunities that significantly impact the design, optimization, and operation of chemical reactors.

Importance of understanding multiple reactions

Here are some key reasons highlighting the importance of understanding multiple reactions:

1.Product Selectivity:

- Different reactions often lead to the formation of various products.
- Understanding the kinetics and thermodynamics of each reaction helps optimize conditions for desired product formation.
- Achieving high selectivity ensures efficient use of resources and minimizes waste.

Importance of understanding multiple reactions

2.Reaction Kinetics:

- Each reaction in a multiple reaction system *has its own kinetics*.
- The rate of each reaction *influences the overall system behavior*.
- Accurate knowledge of reaction kinetics aids in predicting the conversion of reactants and *the evolution of product concentrations over time*.

Importance of understanding multiple reactions

3.Energy Considerations:

- Multiple reactions can have different energy requirements.
- Balancing energy input and removal is essential for maintaining temperature control and preventing undesired side reactions.
- Understanding the heat generated or absorbed by each reaction is critical for reactor safety and efficiency.

Importance of understanding multiple reactions

4.Optimization of Yield:

- Some reactions may compete for the same set of reactants, affecting the overall yield of desired products.
- Balancing reaction rates and concentrations is essential for optimizing the yield of the target product while minimizing the formation of by-products.

Importance of understanding multiple reactions

5.Reactor Design:

- Different types of reactors are suitable for different types of reactions.
- Understanding the nature of multiple reactions helps in selecting an appropriate reactor design that maximizes efficiency and minimizes costs.

Importance of understanding multiple reactions

6.Process Economics:

- The economic feasibility of a chemical process is influenced by the efficiency of the reactor system.
- Knowledge of multiple reactions allows for the design of cost-effective processes with minimal energy consumption and raw material waste.

Importance of understanding multiple reactions

7.Environmental Impact:

- Optimizing reactions to reduce by-products and waste is crucial for sustainable and environmentally friendly manufacturing.

Importance of understanding multiple reactions

8.Process Control:

- Multiple reactions introduce additional variables that need to be controlled for stable operation.
- Understanding the interplay between reactions aids in developing effective control strategies for maintaining product quality and consistency.

Importance of understanding multiple reactions

In conclusion, a deep understanding of multiple reactions is essential for achieving optimal performance in chemical reactors. It not only enhances the efficiency of chemical processes but also contributes to sustainability, cost-effectiveness, and safety in the chemical industry.

Polymath Software

Polymath™ is an easy-to-use numerical computation package that allows students and professionals to use personal computers to solve the following types of problems:

Polymath Software

- Simultaneous Linear Algebraic Equations
- Simultaneous Nonlinear Algebraic Equations
- Simultaneous Ordinary Differential Equations

Polymath Software

- Data Regressions (including the following)

  - ❖ Curve Fitting by Polynomials and Splines
  - ❖ Multiple Linear Regression with Statistics
  - ❖ Nonlinear Regression with Statistics

Polymath Software

- Polymath™ is unique in that the problems are entered just like their mathematical equations, and there is a minimal learning curve. Problem solutions are easily found with robust algorithms. This allows very convenient problem solving to be used in chemical reaction engineering and other areas of chemical engineering, leading to an enhanced educational experience for students.

Example-1

The elementary gas phase reaction

$$3A+2B \xrightarrow{k1} 3C+5D$$

is carried out in a flow reactor operated isothermally at 427°C and 28.7 atmospheres. Pressure drop can be neglected. The entering volumetric flow rate is 10 dm^3/s and the reaction rate constant (k_1) is 200 $dm^{12}/mol^4.s$. The feed is equal molar in A and B.

a) *Express the rate law and the concentration of each species*

b) *Calculate the required CSTR volume for 50% conversion.*

Example-1-solution

```
d(cd) / d(t) = rd
d(cc) / d(t) = rc
d(cb) / d(t) = rb
d(ca) / d(t) = ra
rd = -(5/3)*ra
rc = -ra
rb = 0.66667*ra
ra = -k*(0.25*(1-X)/(1+0.5*X))^3*(0.25*(1-0.6667*X)/(1+0.5*X))^2
X=(0.25-ca)/0.25
k=200
cd(0) = 0
cc(0) = 0
cb(0) = 0.25
ca(0) = 0.25
t(0) = 0
t(f) = 500
VCSTR=X*2.5/(-ra)
```

POLYMATH 6.10 Professional Release - [Ordinary Differential Equations Solver]

File Program Edit Format Problem Examples Window Help

RKF45 ☑ Table ☑ Graph ☑ Report

Differential Equations: 4 Auxiliary Equations: 7 ✔ Ready for solution

```
#example 1 solution
d(cd) / d(t) = rd
d(cc) / d(t) = rc
d(cb) / d(t) = rb
d(ca) / d(t) = ra
rd = -(5/3)*ra
rc = -ra
rb = 0.66667*ra
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X=(0.25-ca)/0.25
k=200
cd(0) = 0
cc(0) = 0
cb(0) = 0.25
ca(0) = 0.25
t(0) = 0
t(f) = 500
VCSTR=X*2.5/(-ra)
```

POLYMATH 6.10 Professional Release - [Differential Equations Solution #12]

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POLYMATH Report

Ordinary Differential Equations

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	ca	0.25	0.03981	0.25	0.03981
2	cb	0.25	0.1098727	0.25	0.1098727
3	cc	0	0	0.21019	0.21019
4	cd	0	0	0.3503166	0.3503166
5	k	200.	200.	200.	200.
6	ra	-0.1953125	-0.1953125	-2.635E-05	-2.635E-05
7	rb	-0.130209	-0.130209	-1.756E-05	-1.756E-05
8	rc	0.1953125	2.635E-05	0.1953125	2.635E-05
9	rd	0.3255208	4.391E-05	0.3255208	4.391E-05
10	t	0	0	500.	500.
11	VCSTR	0	0	7.978E+04	7.978E+04
12	X	0	0	0.8407598	0.8407598

Differential equations

1 d(cd)/d(t) = rd

2 d(cc)/d(t) = rc

3 d(cb)/d(t) = rb

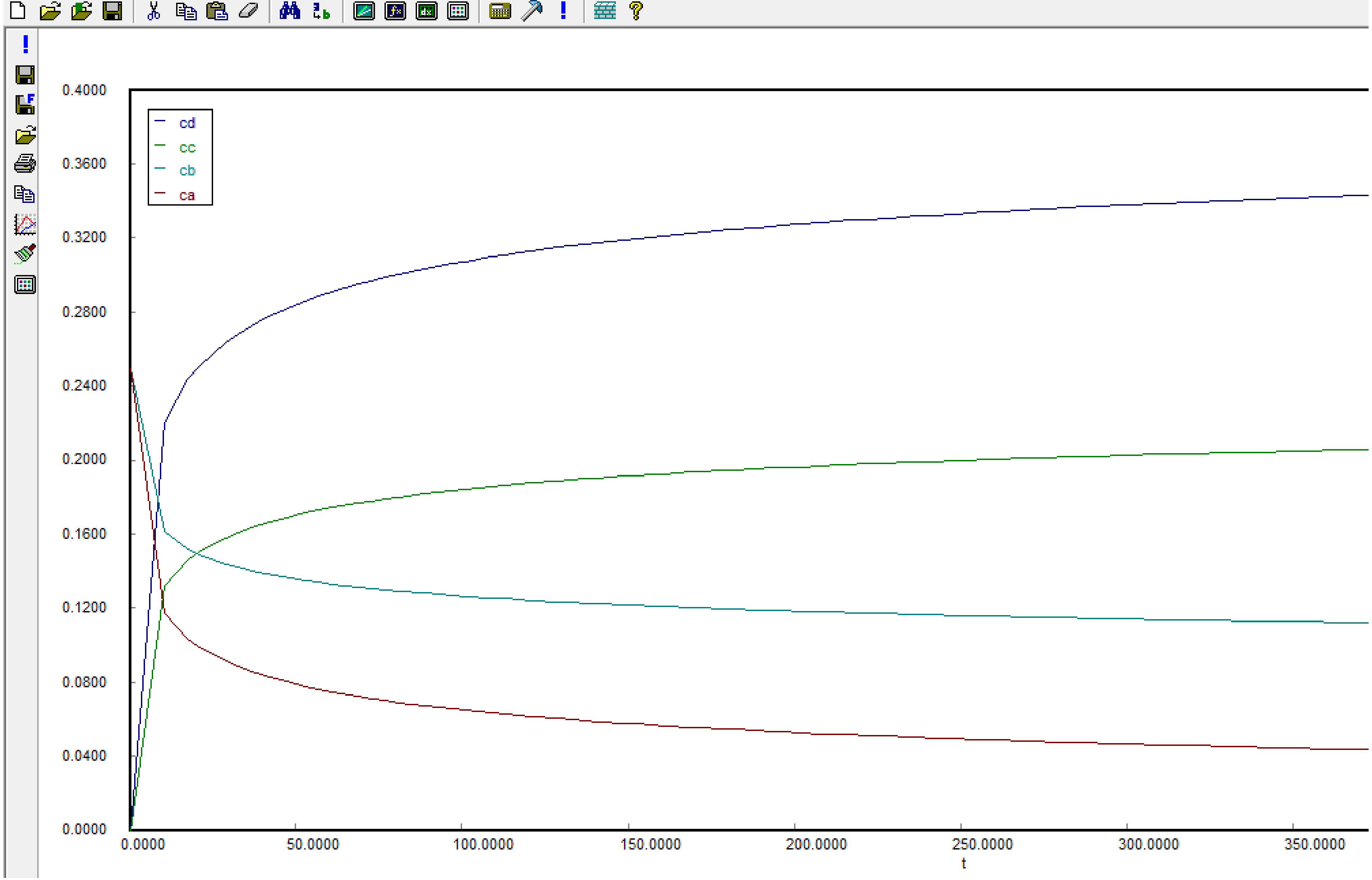
4 d(ca)/d(t) = ra

Explicit equations

1 X = (0.25-ca)/0.25

2 k = 200

3 ra = -k*(0.25*(1-X)/(1+0.5*X))^3*(0.25*(1-0.6667*X)/(1+0.5*X))^2


0.4000
0.3600
0.3200
0.2800
0.2400
0.2000
0.1600
0.1200
0.0800
0.0400
0.0000
cd
cc
cb
ca
0.0000
50.0000
100.0000
150.0000
200.0000
250.0000
300.0000
350.0000
t

POLYMATH 6.10 Professional Release - [ODE Results: RKF45, Solution #12]

File Program Edit Row Column Format Analysis Examples Window Help

R001 : C001 C01

	t	cd	cc	cb	ca	X	k	ra	rd	rc	rb	VCSTR
1	0	0	0	0.25	0.25	0	200.	-0.1953125	0.3255208	0.1953125	-0.130209	0
2	10.2143	0.2209472	0.1325683	0.1616207	0.1174317	0.5302733	200.	-0.0026102	0.0043503	0.0026102	-0.0017401	507.8891
3	17.40908	0.2439012	0.1463407	0.152439	0.1036593	0.5853628	200.	-0.0014341	0.0023901	0.0014341	-0.000956	1020.471
4	20.71334	0.2510473	0.1506284	0.1495806	0.0993716	0.6025136	200.	-0.0011769	0.0019614	0.0011769	-0.0007846	1279.915
5	28.60062	0.2638552	0.1583131	0.1444574	0.0916869	0.6332525	200.	-0.000813	0.001355	0.000813	-0.000542	1947.273
6	32.60062	0.2688775	0.1613265	0.1424484	0.0886735	0.6453061	200.	-0.000699	0.001165	0.000699	-0.000466	2308.013
7	36.60062	0.2732331	0.1639398	0.1407062	0.0860602	0.6557594	200.	-0.0006113	0.0010188	0.0006113	-0.0004075	2681.918
8	40.60062	0.2770684	0.166241	0.1391721	0.083759	0.664964	200.	-0.0005419	0.0009031	0.0005419	-0.0003612	3067.944
9	48.60062	0.2835656	0.1701394	0.1365732	0.0798606	0.6805574	200.	-0.0004393	0.0007321	0.0004393	-0.0002929	3873.054
10	52.60062	0.286361	0.1718166	0.135455	0.0781834	0.6872664	200.	-0.0004004	0.0006674	0.0004004	-0.000267	4290.797
11	56.60062	0.2889177	0.1733506	0.1344324	0.0766494	0.6934024	200.	-0.0003674	0.0006124	0.0003674	-0.000245	4717.926
12	60.60062	0.2912704	0.1747622	0.1334913	0.0752378	0.6990489	200.	-0.0003391	0.0005651	0.0003391	-0.0002261	5153.973
13	68.60062	0.2954704	0.1772822	0.1318112	0.0727178	0.709129	200.	-0.000293	0.0004883	0.000293	-0.0001953	6051.212
14	72.60062	0.297359	0.1784154	0.1310558	0.0715846	0.7136616	200.	-0.000274	0.0004567	0.000274	-0.0001827	6511.706
15	76.60062	0.2991284	0.179477	0.1303481	0.070523	0.717908	200.	-0.0002571	0.0004286	0.0002571	-0.0001714	6979.708
16	80.60062	0.3007915	0.1804749	0.1296828	0.0695251	0.7218997	200.	-0.0002421	0.0004035	0.0002421	-0.0001614	7454.946
17	88.60062	0.303842	0.1823052	0.1284626	0.0676948	0.7292207	200.	-0.0002164	0.0003606	0.0002164	-0.0001442	8426.16
18	92.60062	0.3052469	0.1831481	0.1279006	0.0668519	0.7325925	200.	-0.0002053	0.0003421	0.0002053	-0.0001369	8921.7
19	96.60062	0.3065813	0.1839488	0.1273669	0.0660512	0.7357951	200.	-0.0001952	0.0003253	0.0001952	-0.0001301	9423.598
20	100.6006	0.3078514	0.1847109	0.1268588	0.0652891	0.7388435	200.	-0.000186	0.00031	0.000186	-0.000124	9931.676
21	108.6006	0.3102199	0.186132	0.1259114	0.063868	0.7445278	200.	-0.0001697	0.0002829	0.0001697	-0.0001132	1.097E+04
22	112.6006	0.3113273	0.1867964	0.1254685	0.0632036	0.7471854	200.	-0.0001626	0.0002709	0.0001626	-0.0001084	1.149E+04
23	116.6006	0.3123885	0.1874331	0.125044	0.0625669	0.7497324	200.	-0.0001559	0.0002598	0.0001559	-0.0001039	1.202E+04
24	120.6006	0.313407	0.1880442	0.1246366	0.0619558	0.7521768	200.	-0.0001497	0.0002495	0.0001497	-9.982E-05	1.256E+04
25	128.6006	0.3153276	0.1891966	0.1238683	0.0608034	0.7567862	200.	-0.0001386	0.000231	0.0001386	-9.241E-05	1.365E+04
26	132.6006	0.3162349	0.1897409	0.1235054	0.0602591	0.7589636	200.	-0.0001336	0.0002227	0.0001336	-8.908E-05	1.42E+04
27	136.6006	0.3171098	0.1902659	0.1231554	0.0597341	0.7610635	200.	-0.0001289	0.0002149	0.0001289	-8.595E-05	1.476E+04
28	140.6006	0.3179545	0.1907727	0.1228176	0.0592273	0.7630907	200.	-0.0001245	0.0002075	0.0001245	-8.302E-05	1.532E+04
29	148.6006	0.3195602	0.1917361	0.1221753	0.0582639	0.7669444	200.	-0.0001165	0.0001942	0.0001165	-7.766E-05	1.646E+04
30	152.6006	0.3203244	0.1921947	0.1218696	0.0578053	0.7687787	200.	-0.0001128	0.000188	0.0001128	-7.521E-05	1.704E+04

Regression | Analysis | Graph

Graph Residuals

Report Store Model

Linear & Polynomial | Multiple linear | Nonlinear

Dependent Variable: cd

Independent Variable: t

Polynomial Degree: 1 Linear, 2, 3, 4, 5, 6, 7, 8

Through origin

Polynomial Integration

Polynomial Derivative

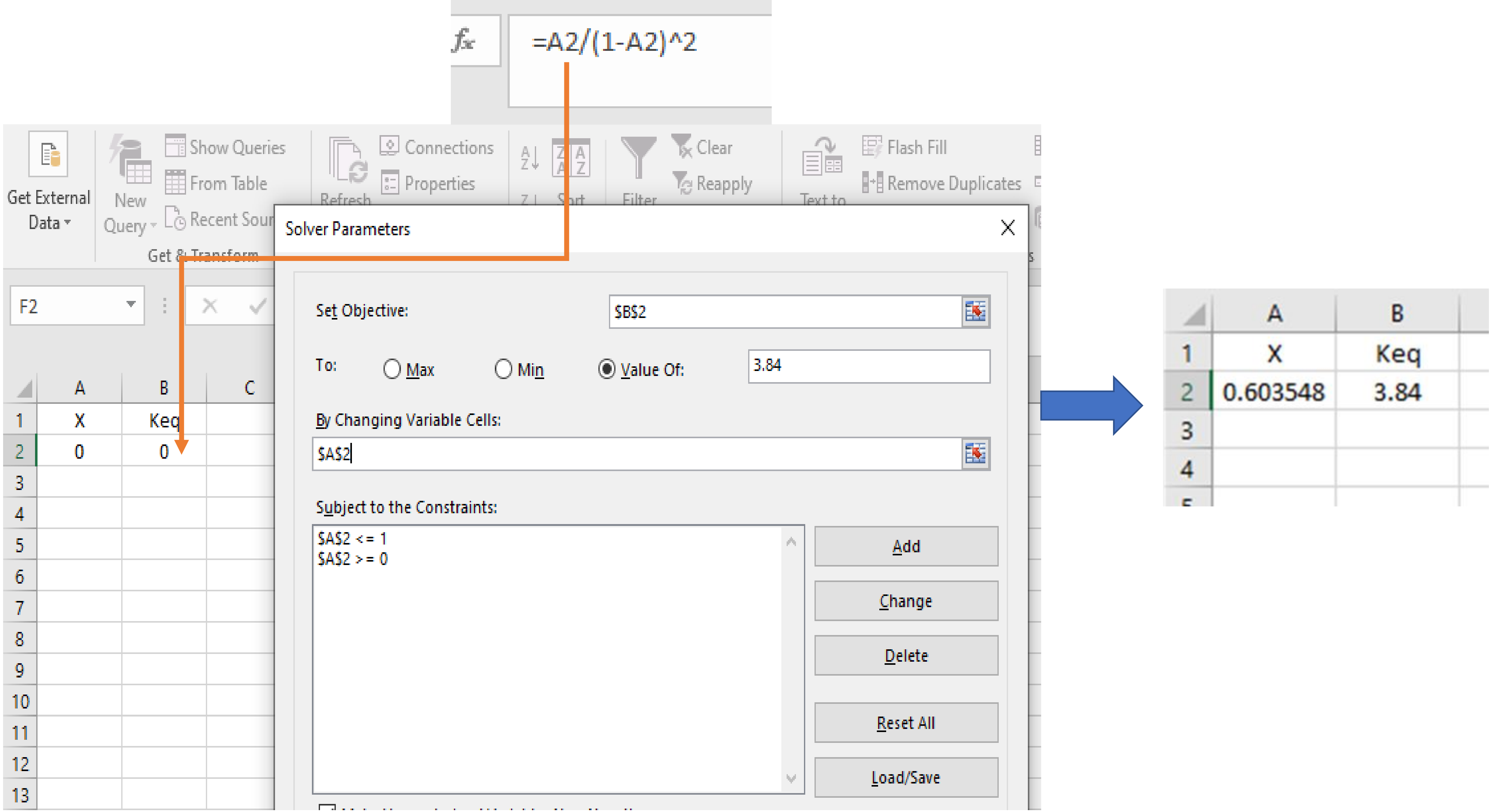
Example-2(by Microsoft Excel)

The elementary reversible reaction:

$$2A \rightleftarrows B$$

is carried out isothermally and isobarically in a flow reactor where pure A is fed at a concentration of 4.0 mol/dm^3.

What is the equilibrium conversion (X_e), for a liquid-phase reaction and the equilibrium constant = 0.48 dm^3/mol?



=A2/(1-A2)^2
Solver Parameters
Set Objective: B2
To: Max Min Value Of: 3.84
By Changing Variable Cells: A2
Subject to the Constraints:
A2 <= 1
A2 >= 0
Add
Change
Delete
Reset All
Load/Save
X Keq
0 0
X Keq
0.603548 3.84

End od 1st week –part 1 lecture