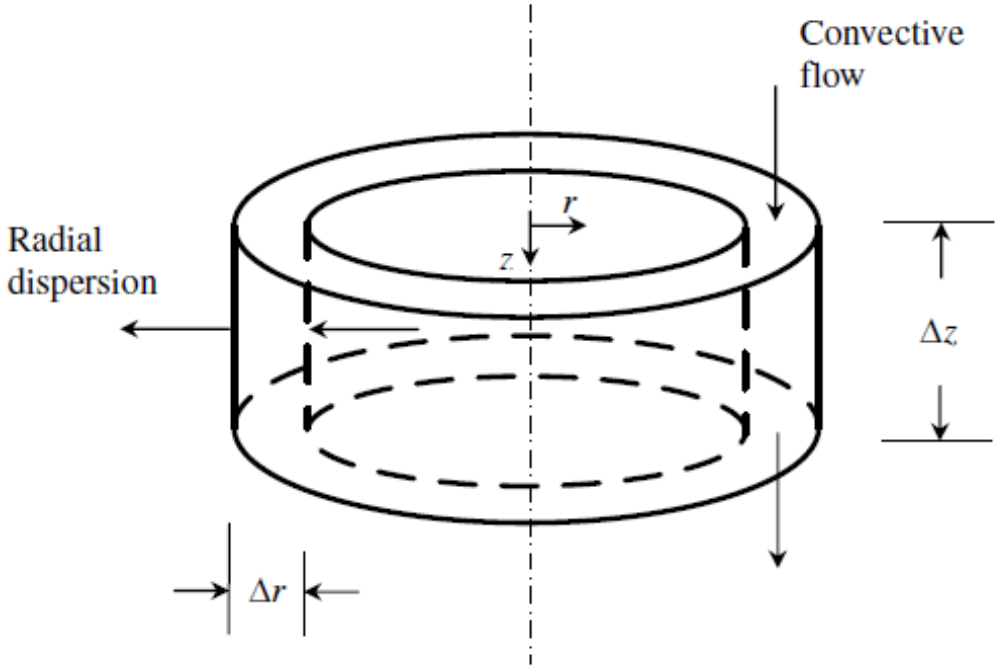
CHE 611
Advanced Chemical Reaction Engineering



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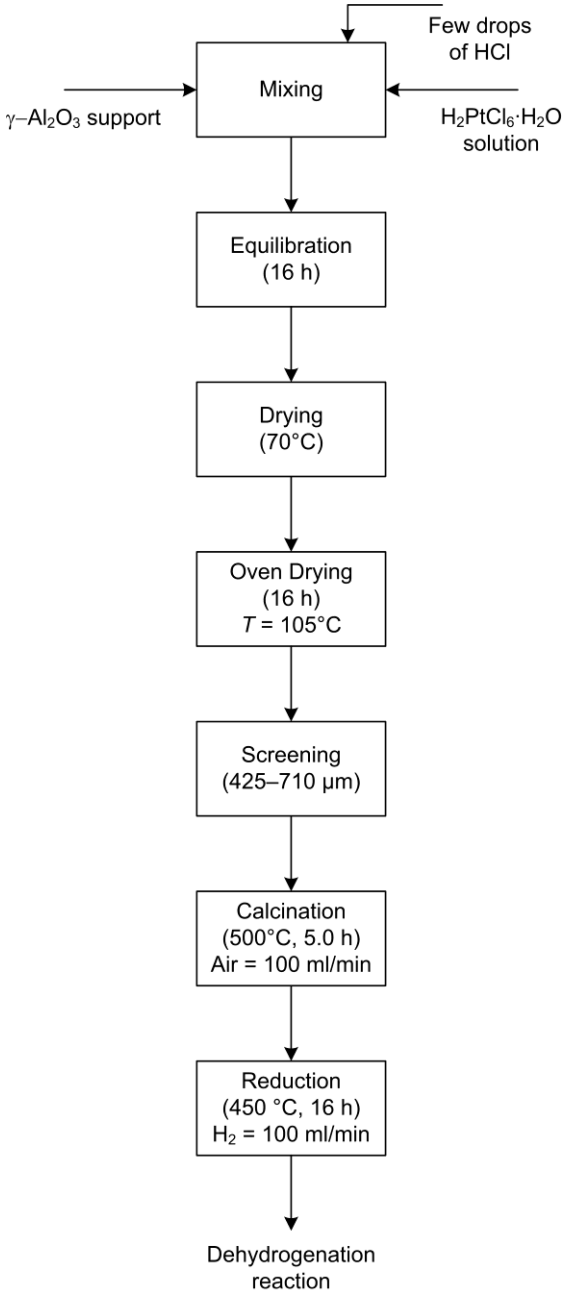
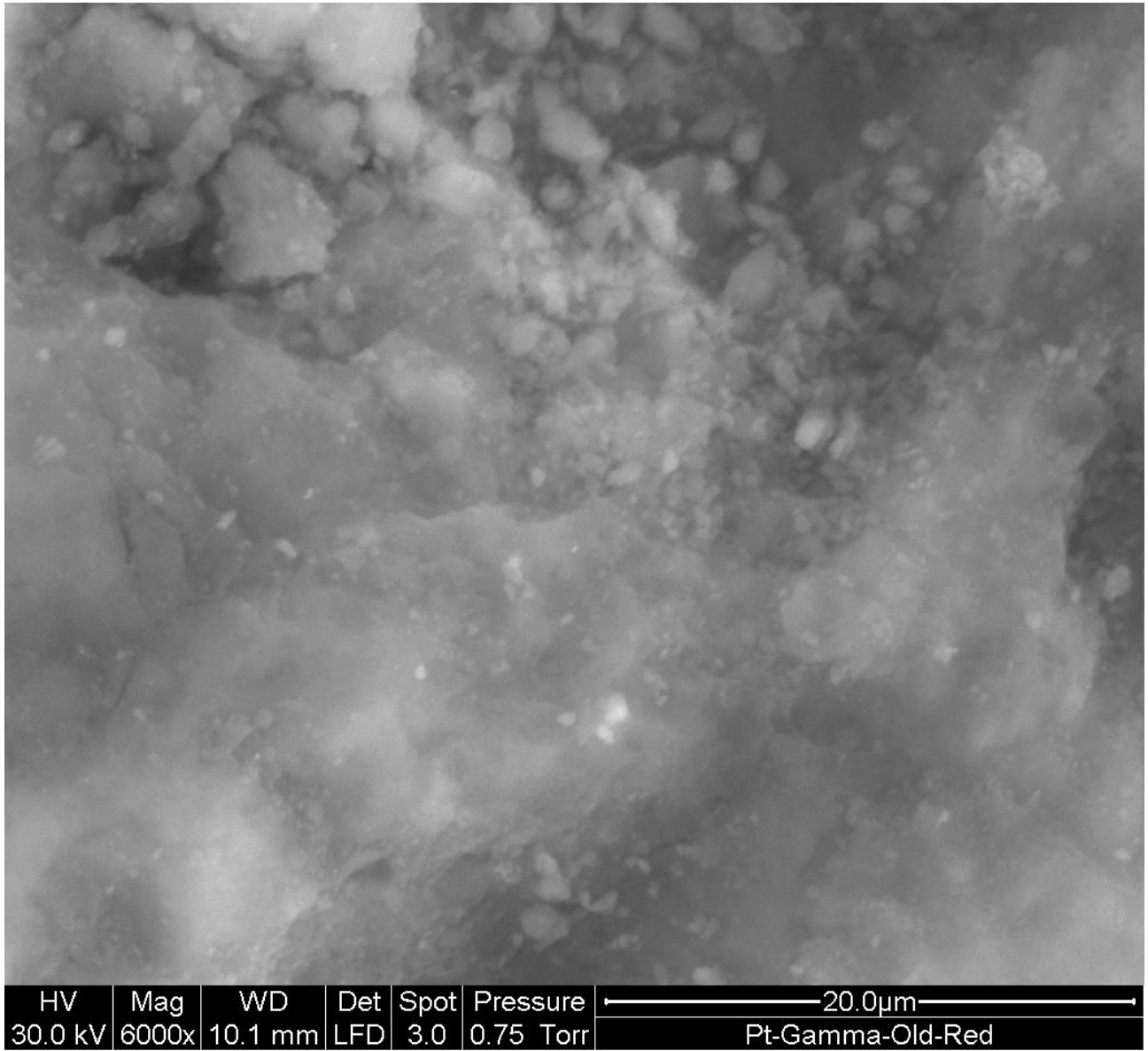
Catalyst preparation (1.0 wt% Pt/γ-Al2O3)



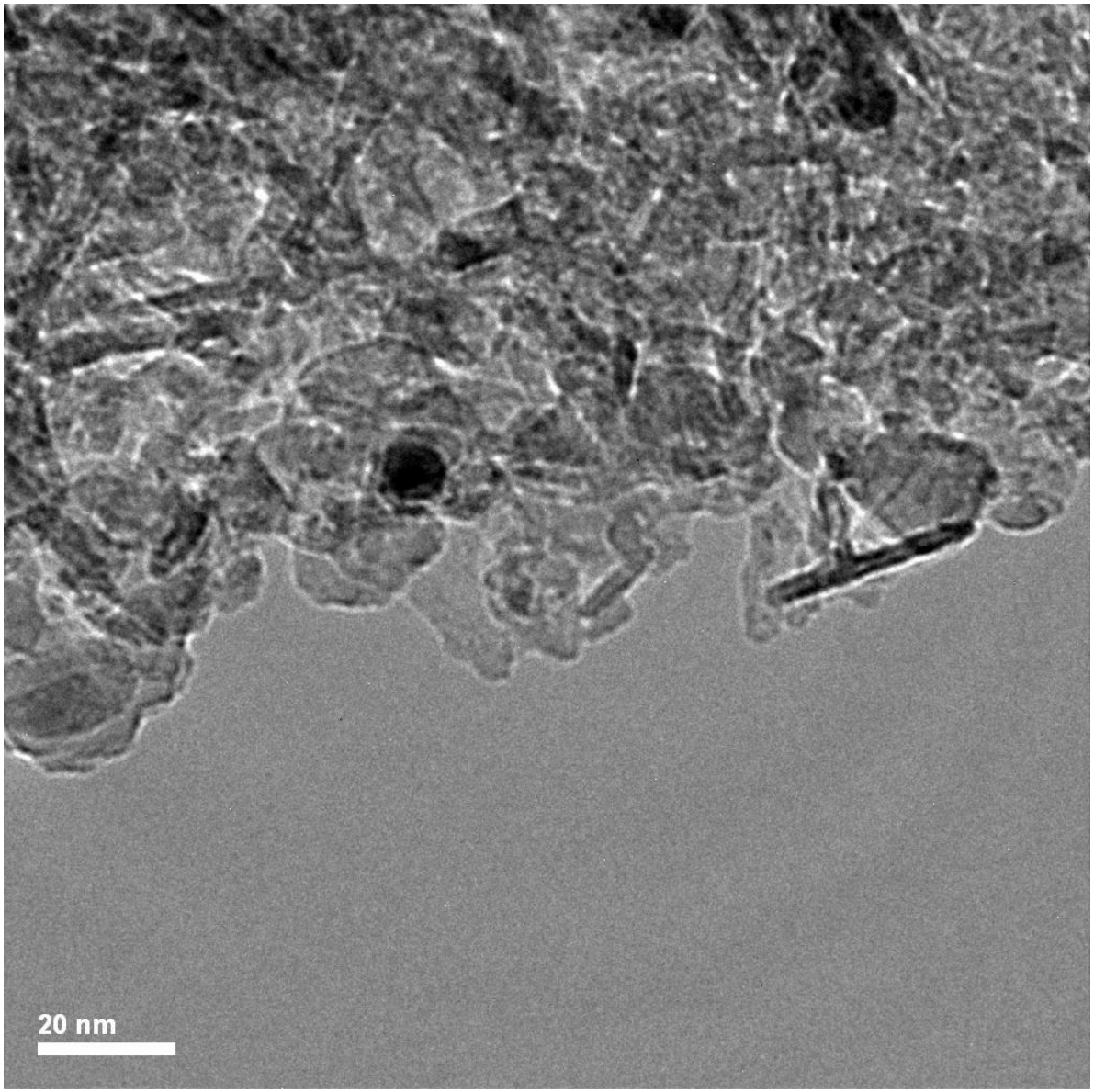
Catalyst characterization [4]

Technique	Acronym	Type of Information
Low-energy electron diffraction	LEED	Two-dimensional structure and registry with metal surface
Auger electron spectroscopy	AES	Elemental analysis
X-ray photoelectron spectroscopy	XPS	Elemental analysis and valence state
Ion scattering spectroscopy	ISS	Elemental analysis
Ultraviolet photoelectron spectroscopy	UPS	Electronic structure
Electron energy loss spectroscopy	EELS	Molecular structure
Infrared spectroscopy	IRS	Molecular structure
Laser Raman spectroscopy	LRS	Molecular structure
X-ray diffraction	XRD	Bulk crystal structure
Extended x-ray absorption fine structure	EXAFS	Bond distance and coordination number
Transmission electron microscopy	TEM	Crystal size, shape, morphology, and structure
Scanning transmission electron microscopy	STEM	Microstructure and composition
Scanning tunneling microscopy	STM	Microstructure
Ultraviolet spectroscopy	—	Electronic state
Mössbauer spectroscopy	—	Ionic state
Nuclear magnetic resonance spectroscopy	NMR	Molecular structure and motion

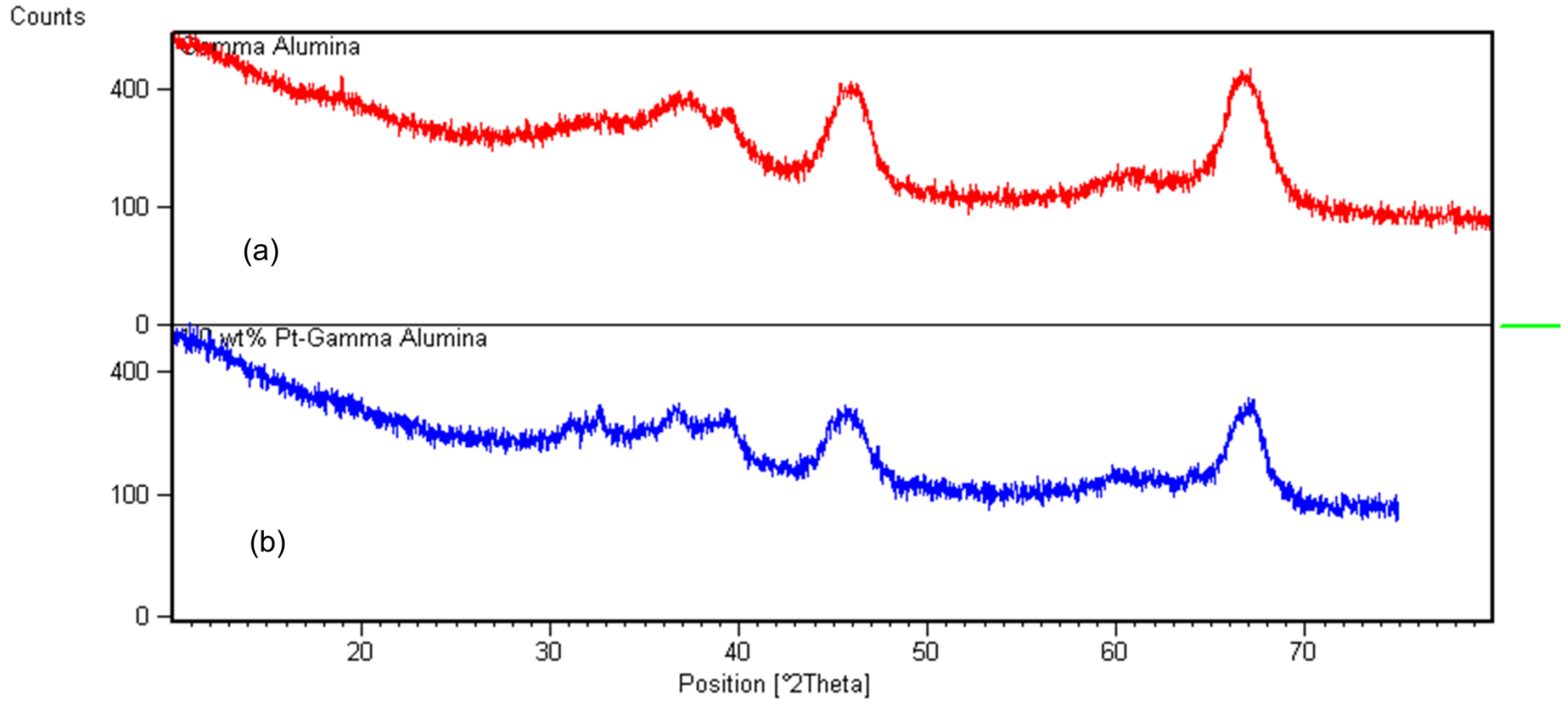
Catalyst characterization (SEM for 1.0 wt% Pt/γ-Al2O3)



Catalyst characterization (TEM for 1.0 wt% Pt/γ-Al2O3)



Catalyst characterization (XRD for 1.0 wt% Pt/γ-Al2O3)



Laboratory experimental setup

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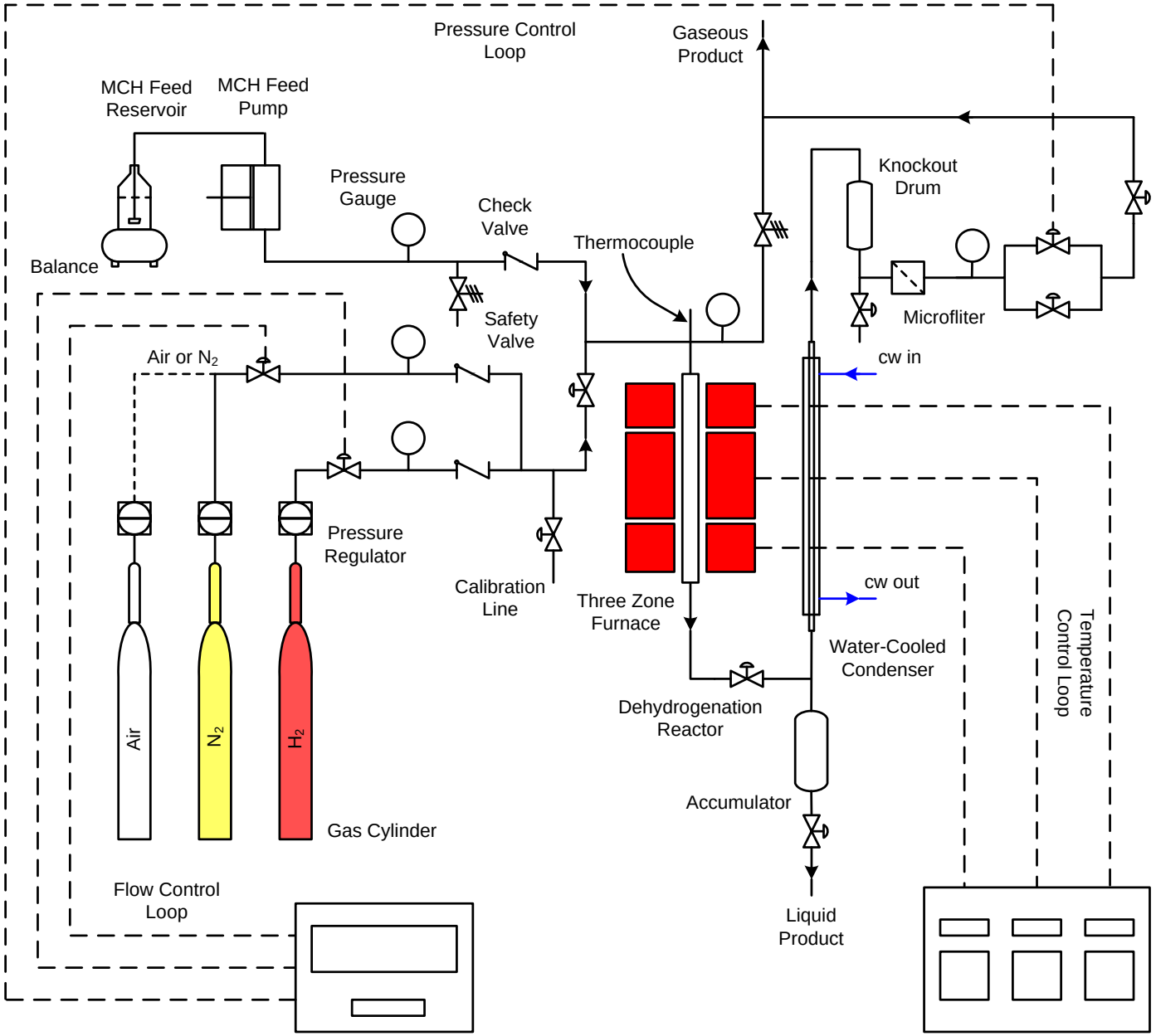

Laboratory experimental data

RUN No.	Fmch,0	Fhyd,0	Fhyd,0/Fmch,0	W/Fmch,0	(W/Fmch,0) ×10^{-5}	Target T	Tave	Tave	Xave
	ml/min	mol/s	—	(g·s)/mol	(g·s)/mol	°C	°C	K	—
1	0.25	2.74E-04	8.3774	61875.8	0.6187584	380	377.72	650.87	0.119
2	0.125	1.37E-04	8.3774	123752	1.2375168	380	378.93	652.08	0.2005
3	0.5	5.47E-04	8.3774	30937.9	0.3093792	380	374.53	647.68	0.032
4	0.25	2.74E-04	8.3774	61875.8	0.6187584	380	378.73	651.88	0.063
5	0.25	0	0	61875.8	0.6187584	380	369.46	642.61	0.3405
6	0.125	0	0	123752	1.2375168	380	373.54	646.69	0.4895
7	0.5	0	0	30937.9	0.3093792	380	366.11	639.26	0.2135
8	0.063	0	0	245539	2.4553906	380	376.28	649.43	0.644
9	0.25	0	0	61875.8	0.6187584	430	412.57	685.72	0.6145
10	0.125	0	0	123752	1.2375168	430	418.44	691.59	0.855
11	0.5	0	0	30937.9	0.3093792	430	407.61	680.76	0.3845
12	0.063	0	0	245539	2.4553906	430	423.87	697.02	0.9745

Continuous stirred tank reactor (CSTR)

We will discuss flow reactors only.

For a CSTR reactor system:

$$\frac{W}{F_{A0}} = \frac{X_A}{(-r_A)} \qquad (17)$$

Where,

W = weight of catalyst, kg

F_{A0} = initial molar flowrate of component A, mol·s^{-1}

X = fractional conversion

$(-r_A)$ = rate of chemical reaction, mol·kg-cat^{-1}·s^{-1}

Differential and integral forms: Plug flow reactor

- The differential form of the one-dimensional pseudo-homogeneous model for the catalytic plug flow reactor is shown below:

$$\frac{dX_A}{d\left(\frac{W}{F_{A0}}\right)} = (-r_A) \qquad (18)$$

- Upon integration between the limits when $X = 0$ at $\frac{W}{F_{A0}} = 0$ and $X = X$ at $\frac{W}{F_{A0}} = \frac{W}{F_{A0}}$, we may write that the integral form

$$\frac{W}{F_{A0}} = \int_0^{X_A} \frac{dX_A}{(-r_A)} \qquad (19)$$

Example 1: Fitting of experimental data

The experimental data given below for the dehydrogenation of methylcyclohexane (MCH) is generated in a catalytic continuous stirred tank reactor (CSTR) under integral conditions. Using power law kinetics for the irreversible reaction, fit the experimental data and find the kinetic parameters.

Experimental data

Twall (°C)	*Tave* (°C)	*Tave* (K)	*p* (bar)	*Fmch* (mol/s)	*Fhyd* (mol/s)	*Fhyd/ Fmch*	*W/Fmch* (s.g/gmol)	*ymch*	*yhyd*	*yimp*	*Xe*	%*X*MCH
360.6	324.6	597.786	1.013	3.23E-05	2.72E-04	8.428431	62185.22	0.106	0.893	0.0011	0.992	93.676
360.6	321.7	594.864	1.013	6.46E-05	5.45E-04	8.428431	31092.61	0.106	0.893	0.0011	0.991	62.878
360.6	338.1	611.2	1.013	1.62E-05	1.36E-04	8.428431	124370.4	0.106	0.893	0.0011	0.997	98.349
360.6	328.3	601.457	2	3.23E-05	3.41E-05	1.053554	62185.22	0.485	0.5105	0.0049	0.972	87.802
360.6	323	596.121	2	6.46E-05	6.81E-05	1.053554	31092.61	0.485	0.5105	0.0049	0.959	50.802
340.49	312.4	585.571	1.013	3.23E-05	2.72E-04	8.428431	62185.22	0.106	0.893	0.0011	0.982	78.1895
340.5	307.7	580.814	1.013	3.23E-05	3.41E-05	1.053554	62185.22	0.485	0.5105	0.0049	0.983	79.211
360.6	341.5	614.6	2	1.62E-05	1.70E-05	1.053554	124370.4	0.485	0.5105	0.0049	0.989	97.699
360.6	322.5	595.614	1.013	3.23E-05	3.41E-05	1.053554	62185.22	0.485	0.5105	0.0049	0.994	90.57
360.6	337.2	610.329	1.013	1.62E-05	1.70E-05	1.053554	124370.4	0.485	0.5105	0.0049	0.998	99.217
380.44	342.4	615.5	1.013	3.23E-05	2.72E-04	8.428431	62185.22	0.106	0.893	0.0011	0.998	97.622
340.5	312	585.143	1.013	3.23E-05	2.72E-04	8.428431	62185.22	0.106	0.893	0.0011	0.981	78.37
340.5	308.2	581.386	1.013	3.23E-05	3.41E-05	1.053554	62185.22	0.485	0.5105	0.0049	0.983	77.549
360.6	320.1	593.214	1.013	6.46E-05	6.81E-05	1.053554	31092.61	0.485	0.5105	0.0049	0.993	55.609
340.5	307	580.121	1.013	3.23E-05	0	0	62185.22	0.99	0	0.01	0.985	77.653
360.6	318.6	591.793	1.013	6.46E-05	0	0	31092.61	0.99	0	0.01	0.994	54.001
360.6	322.2	595.321	1.013	3.23E-05	0	0	62185.22	0.99	0	0.01	0.995	87.951
360.6	336.4	609.507	1.013	1.62E-05	0	0	124370.4	0.99	0	0.01	0.998	98.507
380.44	339.8	612.979	1.013	3.23E-05	3.41E-05	1.053554	62185.22	0.485	0.5105	0.0049	0.998	97.371
380.44	339.5	612.614	1.013	3.23E-05	0	0	62185.22	0.99	0	0.01	0.999	96.204
340.69	317.1	590.271	1.013	1.62E-05	1.70E-05	1.053554	124370.4	0.485	0.5105	0.0049	0.9914	98.241
340.69	307.9	581.093	1.013	6.46E-05	6.81E-05	1.053554	31092.61	0.485	0.5105	0.0049	0.9828	44.015
319.76	290.1	563.279	1.013	6.46E-05	0	0	31092.61	0.99	0	0.01	0.9453	35.4
340.69	304.5	577.621	1.013	6.46E-05	0	0	31092.61	0.99	0	0.01	0.9817	44.3

Fitting of experimental data and discrimination among the various rate models

For the irreversible reaction, using power law of the form

$$(-r) = k \cdot p_A^n \tag{20}$$

$$k = k_r \cdot \exp\left(B \cdot \left(1 - \frac{T_r}{T} \right) \right) \tag{21}$$

$$B = \frac{E}{R \cdot T_r} \tag{22}$$

Mole fractions in the vapor phase (reaction mixture) at conversion X

Component	Representation	Mole fraction
MCH	A	$\frac{y_{A0} \cdot (1 - X)}{1 + 3 \cdot y_{A0} \cdot X}$
Tol	B	$\frac{y_{B0} + y_{A0} \cdot X}{1 + 3 \cdot y_{A0} \cdot X}$
H_2	C	$\frac{y_{C0} + 3 \cdot y_{A0} \cdot X}{1 + 3 \cdot y_{A0} \cdot X}$
Inert	I	$\frac{y_{I0}}{1 + 3 \cdot y_{A0} \cdot X}$

Non-linear regression

Examples of non-linear regression software tools:

- Excel using the Solver tool.
- Polymath (available in a CD with book of Elements of Chemical Reaction Engineering, by H. S. Fogler, 3rd ed., Prentice-Hall, 1999)
- TableCurve 2D
- SigmaPlot