

CHEMICAL REACTORS

1. INTRODUCTION

The chemical processes are centered in chemical reactors. They are one of the main factors while determining industrial processes. There is not a theoretical exact model to design a reactor for any chemical reaction. The reactor should be designed keeping in mind all requirements of a specific system of reaction.

2. THEORY

2.1 Classification of Reactors

The chemical reactors used in industrial processes have different designs, depending on the reaction and the conditions. In general, the chemical reactors have been classified in two ways,

- depending on the type of operation and
- depending on the design of the reactor

The formal classification is done for homogeneous reactions according to the type of operation. These are discontinuous, continuous and semi-continuous reactors.

Discontinuous reactor (Batch): This type of reactors is filled with all reactives at the beginning of the process and it makes them react in a predetermined way of reaction. During the reaction, no material enters to or exits from the reactor. The reactor usually has the shape of a tank, stirred or not, and used for small scales.

The discontinuous reactor has the advantage of high conversions that can be obtained by leaving the reactants in the reactor for long periods of time. On the other hand, it has the disadvantage of high labor costs and difficulty of large-scale production.⁴

Continuous reactor: The reagents are introduced continuously and also the products leave the reactor in a continuous way. It can have the shape of a tank, but also can be tubular. They

can be applied to big productions with the purpose of reducing the operation costs and to make the quality control of the product easy.

Semi-continuous reactors: All reactors that do not adjust with continuous or discontinuous reactors are semi-continuous. Sometimes the reagents are introduced at the beginning of the process and then, the feeding of any reagent keeps existing during the reaction. Some other times most of the substances are introduced discontinuously, but there is no substance that is fed continuously.

According to their design, the reactors can be classified as:

Tank reactor: This is probably the most common type of reactor used in chemical industry. This type of reactor can develop discontinuous and also continuous processes in a wide range of pressure and temperature. *Perfect mixture approximation* can be used in stirred tank reactors, except for very viscose liquids. In a continuous process many reactors can be connected in series. It can also be a reactor divided in sections, in which each section corresponds to one stirred tank reactor.

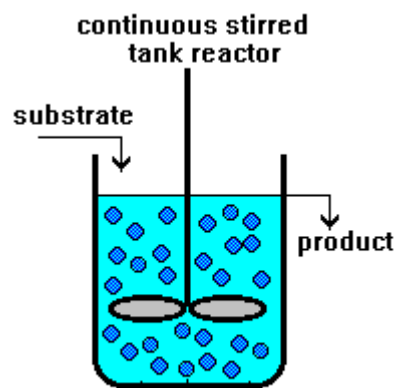


Fig. 1 Tank reactor

Tubular reactor: Many tubes in parallel or a single tube can constitute this type of reactor. The reagents enter in the reactor through one of the ends of the tube and the products leave the reactor through the other end of the tube. Inside the tube, the composition of the mixture always varies with length. ¹



Fig. 2 Tubular reactor¹

Tower reactor: It has a vertical cylindrical structure with a big diameter / height ratio, which is the main characteristic of this type of reactor.

Fluidized bed reactor: It consists of a vertical cylindrical tank that has some little solid particles of catalyst and also some reagents. The reacting fluid steam is introduced from the base of the reactor with a speed which is sufficient to suspend the solids in the steam without going out of the system.

Suspension combustible reactor: A vertical column that contains small solid particles suspended in a liquid characterizes this type of reactor. The liquid in which the particles are suspended can be any of the reagents. The reactive steam will bubble through the suspension.¹

2.2 Design Equations of Reactors

2.2.1 Discontinuous Reactor

If perfect mixture is assumed, the composition of the process can be considered constant in the whole reactor. Carrying out the mass balance of any reagent:

$$\text{INLET} - \text{OUTLET} - \text{REACTION} = \text{ACCUMULATION} \quad (1)$$

In the case of a discontinuous reactor there is neither inlet nor outlet of mass during the process, so this equation is simplified as:

$$-|\text{REACTION}| = |\text{ACCUMULATION}| \quad (2)$$

Each of these factors can be mathematically expressed for the A reagent as:

$$-|\text{REACTION}| = (-r_A)V \quad (3)$$

$$|\text{ACCUMULATION}| = \frac{dN_A}{dt} = \frac{d[N_{A0}(1-x_A)]}{dt} = -N_{A0} \frac{dx_A}{dt} \quad (4)$$

where N_{A0} represents the moles of the reagent A at the beginning of the process, x_A is the conversion factor, V is the volume occupied by the reaction mixture, t is the time and $(-r_A)$ is the disappearance velocity of the reagent A (reaction rate of A).

If we substitute the values of these two last equations in the Equation (2) we will obtain:

$$(-r_A)V = -N_{A0} \frac{dx_A}{dt} \quad (5)$$

The integration of the Equation (5) allows us to determine the time that is necessary to reach any conversion (x_A) under isothermal conditions.²

Clearing up the variables mathematically and integrating, finally the obtained equation is:

$$t = C_{A0} \int_0^{x_A} \frac{dx_A}{(-r_A)} \quad (6)$$

where t is the necessary time to reach any conversion x_A , C_{A0} is the concentration of the reagent A at the beginning and $(-r_A)$ is the disappearance velocity of the reagent A.

2.2.2 Perfect Mixture Continuous Reactors

In the case of perfect mixture continuous reactors there is a stationary regime, so the time is not a variable. Only the spatial time concept will be used (τ):

$$\tau = \frac{V}{Q} \quad (7)$$

where V is the volume of the mixture and Q is the volumetric flow rate of the reagent.

For this type of reactors, the Equation (1) varies as:

$$|\text{ACCUMULATION}| = 0 \quad (8)$$

$$|\text{INLET}| = QC_{A0} = F_{A0} \quad (9)$$

$$|\text{OUTLET}| = QC_A = QC_{A0}(1-x_A) = F_{A0}(1-x_A) \quad (10)$$

$$|\text{REACTION}| = (-r_A)V \quad (11)$$

where F_{A0} is the molar flow of the reagent A that is fed to the reactor, V is the volume of the mixture, C_{A0} is the concentration of the reagent A during the feeding.

x_A is the conversion factor, Q is the volumetric flow rate of the reagent A and $(-r_A)$ is the disappearance velocity of the reagent A .

If we substitute all these values in the Equation (1), the obtained equation will be:

$$F_{A0} - [F_{A0}(1-x_A)] - (-r_A)V = 0 \quad (12)$$

The previous equation can be also represented by:

$$\frac{V}{F_{A0}} = \frac{x_A}{(-r_A)} \quad (13)$$

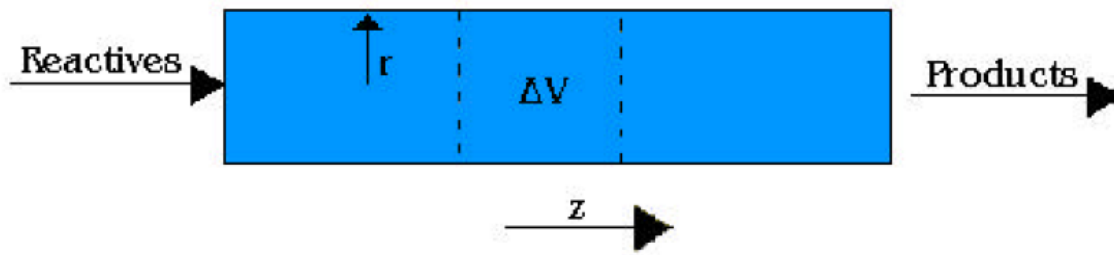
Therefore, expression of the spatial time (τ) will be:

$$\tau = C_{A0} \frac{x_A}{(-r_A)} \quad (14)$$

The conversion factor for each spatial time with known the reaction rate $(-r_A)$ will be calculated by using the Equation (14).

2.5 Tubular Reactor Design

A tubular reactor is the reactor that there is no mixing in the flux direction, but there is a mixing in the radial direction. Figure 3 shows a diagram about tubular reactor.

Fig. 3 Tubular reactor flow diagram³

The concentration changes through the z axis, but there is no change in r direction. When the reaction is going on isothermally, the temperature doesn't change in z direction. Because of that the length of the reactor is the single variable in the conversion of the reaction. The conditions of the systems are the same during the time. Tubular reactor is a steady-state system.

General equation of the mass conservation of component i in a volume element (ΔV) is:

$$|\text{INLET}| - |\text{OUTLET}| - |\text{REACTION}| = |\text{ACCUMULATION}| \quad (15)$$

This equation is applied to the volume element (ΔV) and it is used in stationary state conditions without accumulation.

$$QC_i|_V - QC_i|_{V+\Delta V} + r_i \Delta V = 0 \quad (16)$$

where:

Q : volumetric flow rate, (l/s).

C_i : concentration of i component, (mol/l).

ΔV : Differential element of volume, (l).

r_i : reaction rate of i component, (mol/l).

By taking the limit of $\Delta V \rightarrow 0$, Equation (17) is obtained:

$$\frac{d(QC_i)}{dV} = r_i \quad (17)$$

This equation could be written in the way of conversion of A (x_A) and its volumetric flow rate (Q):

$$x_A = \frac{QC_A - Q_0 C_{A0}}{QC_A} \quad (18)$$

It should be noted that the conversion of the reactive is negative and the conversion of the product is positive. Applying the equation of conversion the Equation (19) is obtained.

$$\frac{dx_A}{dV} = -\frac{r_A}{F_A} \quad (19)$$

where:

$F_A = QC_A$ and it is called molar flow of A (mol/s).

The integral of this equation is:

$$\frac{V}{F_A} = -\int_{x_A=0}^{x_A} \frac{dx_A}{r_A} \quad (20)$$

In case the flow is constant through the reactor (like reactions between liquids), the reaction can be simplified to:

$$r_i = \frac{dC_A}{d\theta} \quad (21)$$

In this equation θ is the resident time of the fluid in the reactor. When the flow is constant, it is possible to use the following equation:

$$\theta = V/Q \quad (22)$$

It is necessary to know that variations of temperature, pressure or number of moles (in gas state) produce changes in flow.³

2.5 Measurement Of Laboratory Interpretation

Starting from the Equations (17) – (19) it is supposed that the reactor is small and the change in the composition and temperature of the fluid is small, too. The reaction speed along the reactor is constant. With this hypothesis by integration of the equation it is obtained as:

$$\frac{\Delta(QC_i)}{\Delta V} = r_i \quad (23)$$

When the conditions of the reaction speed are not constant, the measure of conversion represents the integral value of the reaction speed in all points of the reactor. Then the equations should be integrated to a determinate reaction speed (Equation (20)) and compared with other values from experimental measures.

In the Table 2.1 the units for some orders of reaction are shown:

Table 2.1.¹ Rate equations for some orders of reaction.

Order	Expression of velocity	Equation of integrated velocity (V = constant)
0	$-r_A = k$	$kt = C_{A0} - C_A$
1/2	$-r_A = kC_A^{1/2}$	$kt = 2(C_{A0}^{1/2} - C_A^{1/2})$
1	$-r_A = kC_A$	$kt = \ln \frac{C_{A0}}{C_A}$
2	$-r_A = kC_A^2$	$kt = \frac{1}{C_A} - \frac{1}{C_{A0}}$
2	$-r_A = kC_A C_B$	$kt = \frac{1}{\Delta_{BA}^0} \ln C_{A0} (C_A + (C_{A0} - C_{B0}))$ $C_{A0} \neq C_{B0}$

r_A is equal to dC_A/dt when volume is constant, C_i is the concentration of i, C_{i0} is the initial

$$\Delta_{AB}^0 = C_{A0} - C_{B0}$$

concentration of i , t is the time, k is the reaction rate constant and .

For a reaction that requires two or more reagents, the reaction rate can be determined by measuring independently the dependence, regarding the concentration of each reagent. All reagents should have a constant concentration, except one of them. The reaction rate will be calculated as a function of the concentration of this reagent.

Assumptions:

- a) The reaction lapses at constant temperature. If T is a constant value, k is also constant.
- c) The reaction is <<irreversible>>, which means that the inverse reaction is insignificant. This is true if the value of the balance constant is very high or if only the initial velocity is studied.

2.5.1 Determination of the Kinetic Parameters

In this section we will study a method to obtain the reaction order, α and the specific reaction rate constant, k by using the kinetic equations starting from experimental data.

Discontinuous reactors are used primarily to determine rate law parameters for homogeneous reactions. This determination is usually achieved by measuring concentration as a function of time and then using either the differential, integral or nonlinear regression method of data analysis to determine α , k .

When a reaction is irreversible, it is possible in many cases to determine the reaction order and the specific rate constant by either nonlinear regression or by numerically differentiating concentration versus time data. This latter method is most applicable when reaction conditions are such that the rate is essentially a function of the concentration of only one reactant; for example, if, for the decomposition reaction,



Then the differential method may be used.

However, by utilizing the method of excess, it is also possible to determine the relationship between $-r_A$ and the concentration of other reactants. That is, for the irreversible reaction



where α , β are both unknown, the reaction could first be run in an excess of B so that C_B remains essentially unchanged during the course of the reaction and

$$\begin{aligned} C_B &=C_{B0} \\ k' &=kC_{B0}^\beta \\ -r_A &=k'C_A^\alpha \end{aligned} \quad (26)$$

Both α and β can be determined by using the method of excess when coupled with differential method of analysis.⁴

2.5.1.1 Differential Method of Analysis

To outline the procedure used in the differential method of analysis, we consider a reaction carried out isothermally in a constant-volume batch reactor and the concentration recorded as a function of time. By combining the mole balance with the rate law given by Equation (26), we obtain

$$-\frac{dC_A}{dt}=k'C_A^\alpha \quad (27)$$

After taking the natural logarithm of both sides of Equation (27)

$$\ln\left[-\frac{dC_A}{dt}\right]=\ln k'+\alpha\ln C_A \quad (28)$$

observe that the slope of a plot of $\ln(-dC_A/dt)$ as a function of $(\ln C_A)$ is the reaction order, α .

To obtain the derivative $-dC_A/dt$ used in this plot, we must differentiate the concentration-time data either numerically or graphically. There are different methods to determine the derivative from the data giving concentration as a function of time. One of these methods is *Numerical Method*.⁴

Numerical Method

Numerical differentiation formulas can be used when the data points in the independent variable are equally spaced, such as $t_1 - t_0 = t_2 - t_1 = \Delta t$.

The three-point differentiation formulas

$$\left(\frac{dC_A}{dt}\right)_{t=0} = \frac{-3C_{A0} + 4C_{A1} - C_{A2}}{2\Delta t} \quad (29)$$

$$\left(\frac{dC_A}{dt}\right)_1 = \frac{C_{A,1} - C_{A,0}}{2\Delta t} \quad (30)$$

.....

$$\left(\frac{dC_A}{dt}\right)_n = \frac{C_{A,n-2} - 4C_{A,n-1} + 3C_{A,n}}{2\Delta t} \quad (31)$$

can be used to calculate dC_A/dt . Equations (29) and (31) are used for the first and last data points, respectively, while Equation (30) is used for all intermediate data points.⁴

2.5.2 The Effects of A Change in the Temperature

The heat absorption or irradiation in the reaction always causes a chemical change in the process. It does not only influence the velocity of the reaction but also the balance and the composition of the products. In 1889, *Arrhenius* could demonstrate that the constant $k(T)$ of many reactions could be described by the next expression:⁴

$$k = Ae^{\frac{-E_a}{RT}} \quad (32)$$

where A and E_a are characteristic constants of the reaction and R is the constant of the gases. E_a is the *activation energy of the gases* and A is the *pre-exponential factor* or *factor A of Arrhenius*. A and k have the same units; E_a and RT also have the same units (*energy/mol* => *Kcal/mol*, *kJ/mol*).

Arrhenius got the previous equation considering that the influence of the temperature over the kinetic constant would probably be similar with the influence of the temperature in balance constants.

$$\ln k = \ln A - \frac{E_a}{RT} = \log A - \frac{E_a}{2.303RT} \quad (33)$$

If the Arrhenius equation is true, a graphic representation of **logk** versus **1/T** is a straight line. The slope is $-E_a/2.303R$ and the origin ordinate is **logA**. It will be able, then, to obtain E_a and **A**. A typical experimental error of E_a is about 1 Kcal/mol and the error of **A** is a factor equal to 3.

Notice that starting from the Equation (32), small activation energy bears fast reactions and big activation energy bears slow reactions.

3. EXPERIMENTAL SECTION

3.1. Equipment Description

The **liquid phase chemical reactor** is specially used for the kinetic study of liquid-liquid homogeneous reactions and gas-liquid heterogeneous reactions.

The equipment is constituted by the following elements:

3.1.1 Base module and interface

They provide the necessary elements for the use of the diverse reactor modules. These elements are constituted by:

- Feeding circuits of reagents
- Flow control system
- Temperature control system
- Data acquisition and process control system
- Collecting circuit of products

The feeding circuit of reagents consists of two tanks made of glass, two pumps and the necessary joints.

The **flow control system** consists of two dosing pumps, two flowmeters of direct measure for the feeding pumps of reagents. It also has another rotation meter to measure the flow of the gas.

The **temperature control system** is constituted by a thermostatic bath (we can control the temperature in function of the temperature of the reactor) and an impulse valve of water coming from thermostatisation.

The **data acquisition and process control system** is centralized in the electronic interface connected to the elements that constitute the base module and the reactor module.

The **collecting circuit of products** makes easier the collection and conduction of the products obtained in the reactions. The products go directly to their corresponding deposit.

3.1.2 Chemical reactor module in liquid phase

The following sections constitute it:

- Reactor at constant temperature
- Stirring system

The **Pyrex-glass reactor**, insulated and with a maximum capacity of 2 liters, allows us to work in discontinuous and in continuous. The temperature regulation is carried out in an external thermostat.

The **agitation system** with speed control and indication allows the study of the influence of the agitation, continuously and also discontinuously, in the reaction kinetics.

The **control of the reaction** is carried out using a conductivity cell with conductimeter, which allows measuring the evolution of the reaction in real time.

3.1.3. Specifications

In this section, we can separate in two parts: Base module and reactor module.

3.1.3.1 Base module and interface

- Interface
- Two dosing pumps of with a maximum flow of 14 l/h.
- Three deposits of 10 liters made of Pyrex-glass: two of them for the reagents and the other one for the products.
- Two rotameters to measure the flow of liquids. Flow range: 0.7-7 and 0.54-5.4 l/h
- A thermostatic bath of 9 liters, that regulates the temperature between + 5 and 200 °C
A magnetic-creep pump to impel the water that comes from the thermostatic bath and goes to the reactor module.
- A J type thermocouple to get the temperature of the reactor in a continuous way
- Connection systems for the laboratory substances
- All elements of this equipment are chemically resistant
- Control system of the reaction. In this reactor, the control of the reaction is carried out by means of a conductivity cell and conductimeter, connected to the electronic interface.

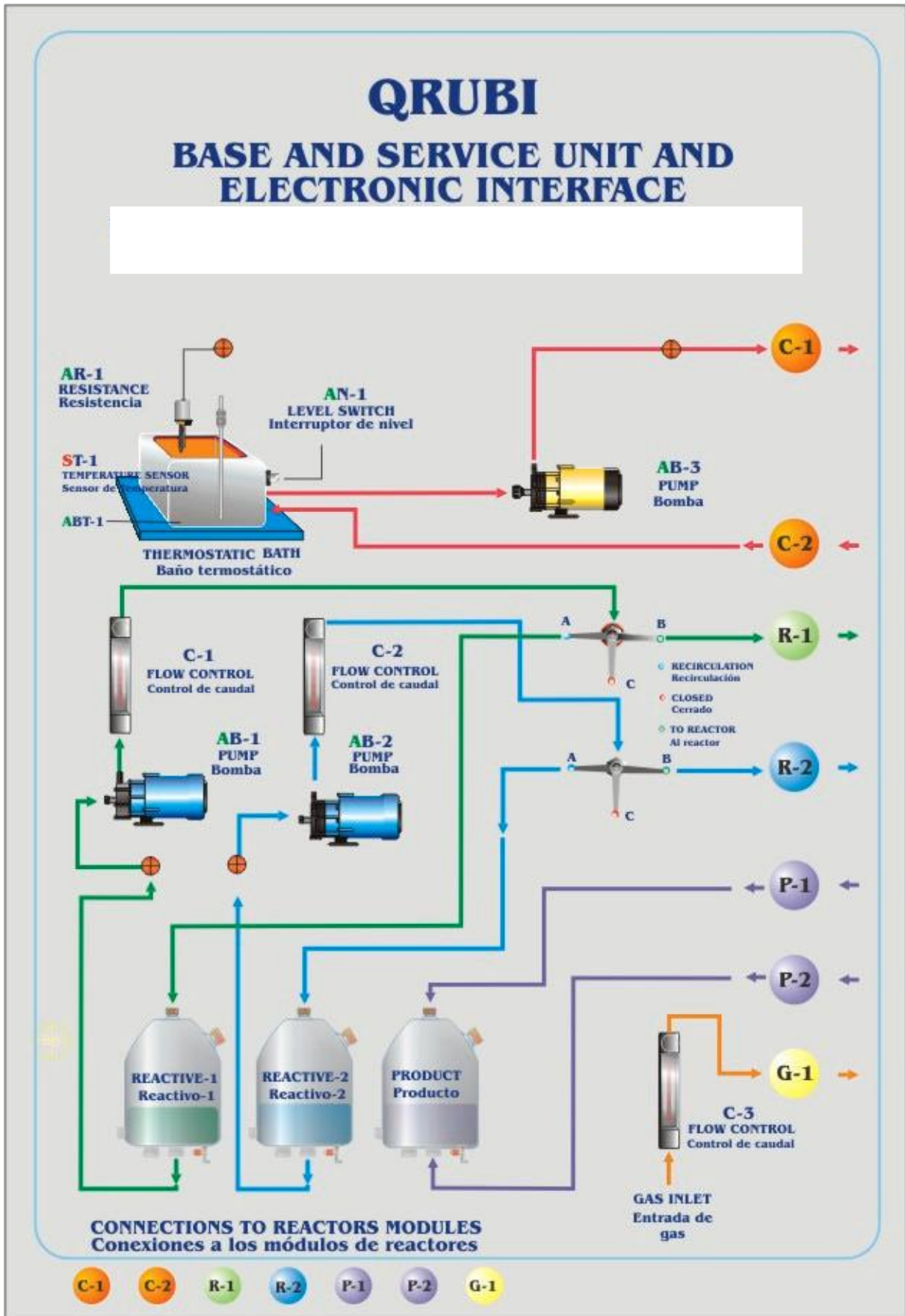


Fig. 4 Base and service unit and electronic interface

3.1.3.2 Reactor module

The module of the chemical reactor in liquid phase has the following elements:

- Reactor insulated made of Pyrex-glass, with a maximum volume of 2 liters.
- Agitation system with agitation speed control and indication from 0 to 2000 rpm.
- Safety, easy and quick connections
- All elements of this equipment are chemically resistant.

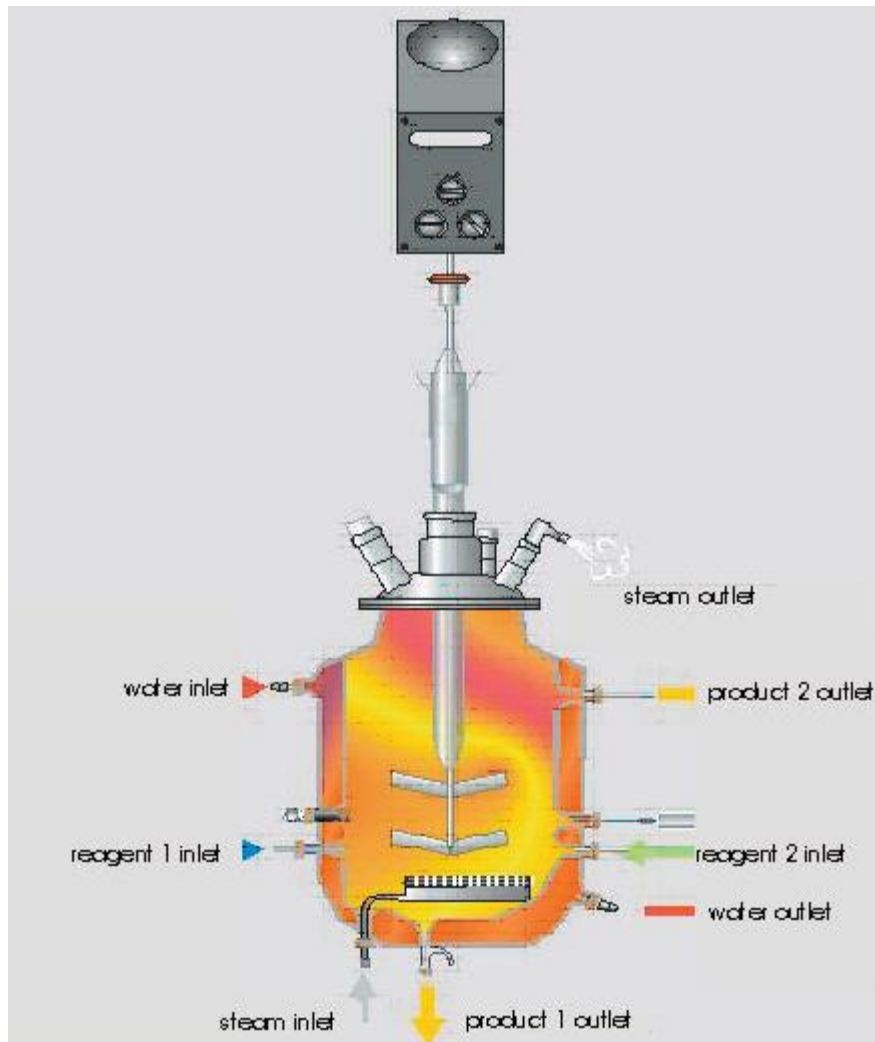


Fig. 5 Outline of the chemical reactor module in liquid phase

3.1.4. Accessories

Chemical reagents:

- Ethyl acetate and Sodium hydroxide

Laboratory materials:

- 5-liter plastic cans, draining containers

3.1.5. Required services

- Electric supply: 210 V / 50 Hz.
- Water supply.

3.2. Laboratory Practice

3.2.1 Experimental installation

The Figure 3.1. shows an outline of the experimental installation without the electronic interface.

Before the starting up of the equipment the following things should be checked.

- **Base module connections**

It is very important to check that the inlets of the pumps are connected horizontally, that the inlet of the flowmeters are connected to the downwardly.

In the thermostatisation circuit, it should be checked that the resistance is fastened and that the filling and drainage tubes do not reach it. Also, the level switch should be checked that it is not obstructed and that the inlet and outlet of the pump has a correct position.

- **Connections between the base module and the reactor**

Check each one of the joints. Close the diverse couplings to prevent leaks and fuses.

- **Connections of the reactor**

Using the Figure 3.3. as a guide, check that the connections of the rear part of the module of the reactor correspond to the diverse inlets and outlets of the reactor.

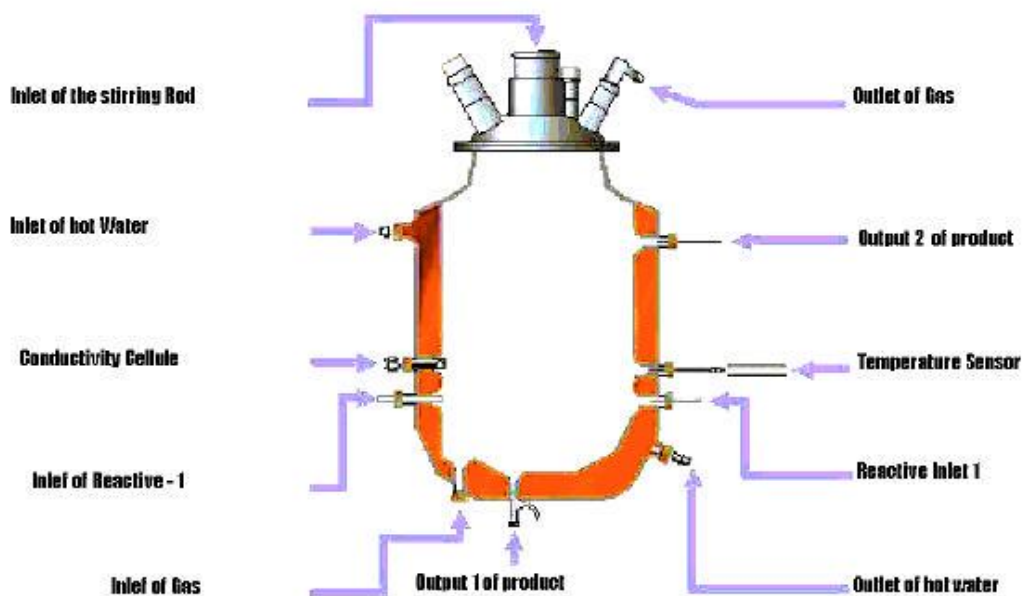


Fig. 6 Connection diagram of the reactor

➤ *Assembly of the stirring system*

Due to the high power of the stirrer and the need of avoiding breakings in the glass elements, before starting up the equipment, check manually that the stirrer do not touch any of the elements of the reactor.

➤ *Connections of the base module and the module of the reactor to the electronic interface*

In this part of the interface there are three places to connect the level switch, the temperature sensor and the conductivity meter. Be very careful with the connection wires for not being an impediment for the equipment working. In the rear part of the equipment we should connect the three pumps, and following the instructions of the diagram, we should connect the conductivity meter and the supply of the resistance.

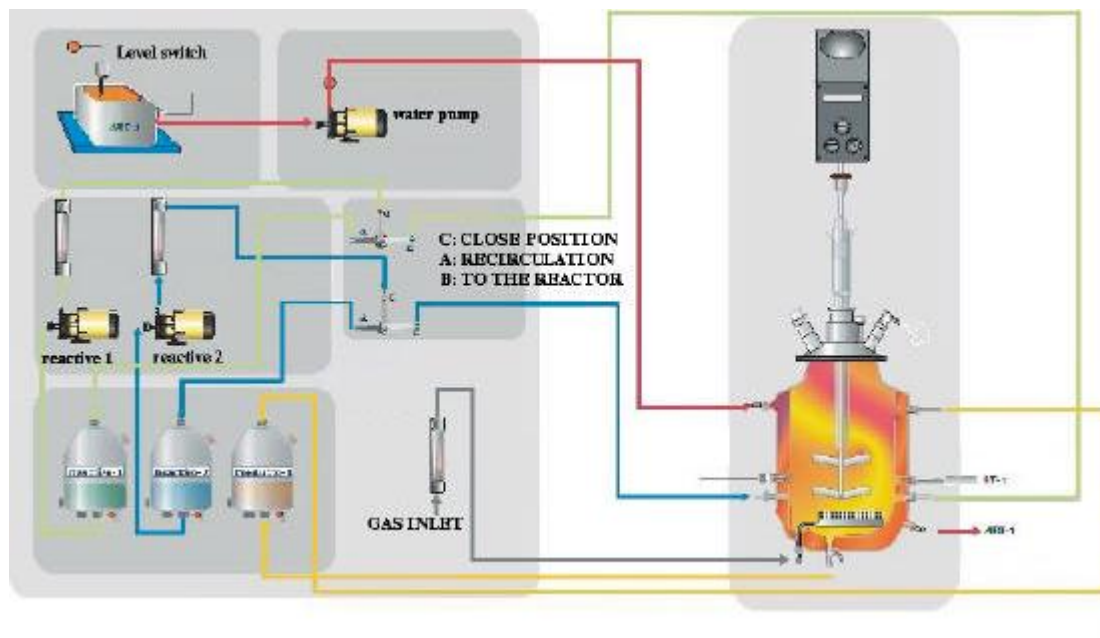
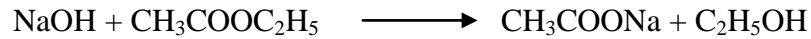


Fig. 7 Complete diagram of the liquid phase reactor

3.3. Experiments

3.3.1. Saponification of EthylAcetate

A process in which esters in fats are hydrolyzed with sodium or potassium hydroxide to produce a carboxylate anion which can act as a surfactant.



The irreversible reaction below will be carried out isothermally both in discontinuous and continuous reactors.

3.3.2. Discontinuous Isothermal Operation (Batch System)

3.3.2.a. Obtaining the reaction rate constant (k) and the reaction order (α) with respect to ethyl-acetate.

Objective: Demonstrate that the saponification of the ethyl-acetate with sodium hydroxide is a reaction of first order respect to ethyl-acetate. And find the reaction rate constant and make an assessment between the experimental and theoretical values of k.

Required elements

- ✓ 0,02 M , 5 liter Ethyl-Acetate (EtOAc) solution.
- ✓ 1 M , 5 liter Sodium hydroxide(NaOH) solution
- ✓ QRIA system
- ✓ Software SACED-QRIA
- ✓ QRIA practice manual

Practice development

The procedure to carry out this practice is:

1. Start the SACED-QRIA software
2. Press START and input the data filename as (Batch,25^oC,Group No).
3. Put the corresponding reactants in the deposits.
4. Start the QRUBIA and QRIA.
5. Recirculate water until a constant flow is obtained.
6. Start the thermal system and set the desired working temperature to 25°C

7. Open the sodium hydroxide valve to the “To Reactor” position and allow 1 liter of solution to the reactor. Once the desired amount of reactant is in the reactor, turn the valve to the “Recirculation” position.
8. Start the stirrer to help the thermal homogenization. Wait to the temperature to be stable around 25°C.
9. Measure the conductivity of the ethyl acetate solution.
10. Open the ethyl-acetate valve to the “To Reactor” position and allow 1 liter of solution into the reactor. Return the valve to the “Recirculation” position.
11. Once the conductivity is stable the reaction is finished.
12. Stop the stirrer.
13. Empty the reactor through the “Product Output 1” valve.
14. Fill the table with the obtained data.
15. Add 1 lt of water to the ethyl-acetate reactant deposit.
16. Repeat points 1 through 16 for four different concentrations.
17. Stop the feed system.
18. Turn the three-way valves to the “Close” position.
19. Turn off the stirrer.
20. Turn off the thermal bath heating element.
21. Empty the product deposit.

Results and tables

Time (min)	K	Csodium hydroxide	Cethyl acetate
1			
2			
3			
4			
5			
6			
7			
8			
9			
10			
11			
12			
13			
14			
15			
.			
.			

When the obtained data has been noted, carry out the necessary calculations and find **k** and **α** .

T	K	A
25 °C		

3.3.2.b. Variation of the kinetic constant with temperature, Arrhenius Equation.

Objective: Demonstrate the dependency of the velocity constant with temperature obeying the law of Arrhenius:

$$k = Ae^{\frac{-E_a}{RT}}$$

where A and E_a are constants characteristics of the reaction and R is the gas constant. E_a is known as the Arrhenius activation energy and A is the Arrhenius factor A.

Practice Development

Set the reaction temperature 35°C and apply the same procedure as described in section 3.3.1.a.

Results and tables

Time (min)	K	Sodium hydroxide	Ethyl acetate
1			
2			
3			
4			
5			
6			
7			
8			
9			
10			
11			
12			
13			
14			
15			
.			
.			

When the obtained data has been noted, carry out the necessary calculations and find reaction rate constant, k.

T	k
35 °C	

3.3.3. Continuous Operation, CSTR System.

Objective: Study the difference between discontinuous and continuous operation.

Required elements

- ✓ 0,02 M , 5 liter Ethyl-Acetate (EtOAc) solution.
- ✓ 0,02 M , 5 liter Sodium hydroxide(NaOH) solution
- ✓ QRIA practice manual
- ✓ QRIA equipment
- ✓ SACED-QRIA software

Practice development

1. Start SACED-QRIA
2. Press the START button and enter the data filename as (Cstr,25^oC,Group No).
3. Set 25°C as working temperature.
4. Set an equal flow for both reactants keeping the system in “recirculation”.
5. When a steady flow is achieved turn the valve to the “to reactor” position.
6. When the reactant level reaches the stirrer’s blades, start the stirring system.
7. Keep the system working for 1 hour.
8. Turn the reactant valves to the “recirculation” position.
9. Stop the system.

Results and tables

Time (min)	K	Csodium hydroxide	Cethyl acetate
1			
2			
3			
4			
5			
6			
7			
8			
9			
10			
11			
12			
13			
14			
15			
.			
.			

When the obtained data has been noted, carry out the necessary calculations and find conversion, x .

T(min)	K	Csodium hydroxide	Cethyl acetate	x

4. SAFETY

In case of emergency, necessary precautions should be taken according to the following MSDS of chemicals that are used in the experiment.

Chemical Safety Data: Ethyl acetate



Common synonyms	Ethyl ethanoate, acetic acid ethyl ester, ethanoic acid ethyl ester
Formula	$\text{CH}_3\text{COOC}_2\text{H}_5$
Physical properties	Form: Colourless liquid with a sweet, fruity smell Stability: Stable, but highly flammable Melting point: -84 C Boiling point: 77 C Water solubility: soluble Specific gravity: 0.9 Flash point: -4 C
Principal hazards	*** Ethyl acetate is very flammable
Safe handling	Wear safety glasses. Make sure that there is no source of ignition near where you work. The vapour may be ignited by contact with a hot plate or hot water pipe - no naked flame is needed.
Emergency	Eye contact: Immediately flush the eye with plenty of water. If irritation persists call for medical help. Skin contact: Wash off with water. If swallowed: Flush the mouth out with water if the person is conscious. If the amount swallowed is substantial call for medical help.
Disposal	Small amounts of ethyl acetate can be flushed down a sink with a large quantity of water, unless local rules prohibit this. This material is very flammable, so care must be taken to avoid any build-up of vapour in sink or sewers.
Protective equipment	Safety glasses. If gloves are required, use polyvinyl alcohol (PVA).

Chemical Safety Data: Sodium Hydroxide

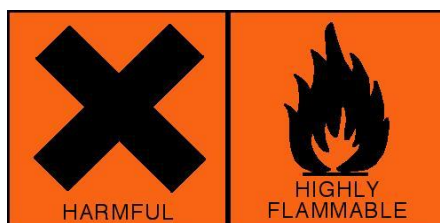


Common synonyms	Caustic soda, soda lye
Formula	NaOH
Physical properties	Form: White semi-transparent solid, often supplied as pellets weighing about 0.1 g Stability: Stable, but hygroscopic . Absorbs carbon dioxide from the air. Melting point: 318 C Water solubility: high (dissolution is very exothermic) Specific gravity: 2.12
Principal hazards	*** Contact with the eyes can cause serious long-term damage *** The solid and its solutions are corrosive *** Significant heat is released when sodium hydroxide dissolves in water
Safe handling	Always wear safety glasses. Do not allow solid or solution to come into contact with your skin. When preparing solutions swirl the liquid constantly to prevent "hot spots" developing.
Emergency	Eye contact: Immediately flush the eye with plenty of water. Continue for at least ten minutes and call for immediate medical help. Skin contact: Wash off with plenty of water. Remove any contaminated clothing. If the skin reddens or appears damaged, call for medical aid. If swallowed: If the patient is conscious, wash out the mouth well with water. Do not try to induce vomiting. Call for immediate medical help
Disposal	Small amounts of dilute sodium hydroxide can be flushed down a sink with a large quantity of water, unless local rules prohibit this. Larger amounts should be neutralised before disposal.
Protective equipment	ALWAYS wear safety glasses when handling sodium hydroxide or its solutions. If you need gloves, neoprene, nitrile or natural rubber are suitable for handling solutions at concentrations of up to 70%

Chemical Safety Data: Sodium acetate

Common synonyms	Sodium ethanoate, ethanoic acid sodium salt
Formula	CH ₃ COONa
Physical properties	Form: white crystalline powder Stability: Stable Melting point: 58 C Boiling point: decomposes at temperatures above about 120 C Specific gravity: 1.52 Water solubility: high
Principal hazards	Sodium acetate may be harmful if a large amount is swallowed..
Safe handling	Wear safety glasses if required by local rules.
Emergency	Eye contact: Immediately flush the eye with water. If irritation persists, call for medical help. Skin contact: Wash off with water. If swallowed: Call for medical help if the amount swallowed is large.
Disposal	Small amounts can be washed down the sink unless local rules prohibit this.
Protective equipment	Safety glasses if required by local rules.

Chemical Safety Data: Ethyl alcohol



Common synonyms	Ethanol, alcohol, grain alcohol, fermentation alcohol, fermentation ethanol
Formula	C ₂ H ₅ OH
Physical properties	<p>Form: colourless fragrant liquid</p> <p>Stability: Stable, but highly flammable</p> <p>Melting point: -144 C</p> <p>Boiling point: 78 C</p> <p>Water solubility: miscible in all proportions</p> <p>Specific gravity: 2.12</p> <p><u>Explosion limits</u>: 3.3 - 24.5%</p>
Principal hazards	<p>Contact with the eyes can cause considerable irritation.</p> <p>"One-off" consumption of small amounts of ethanol is not likely to be harmful, but consumption of large amounts can be (and has been) fatal. Chronic (long-term) ingestion of ethanol may lead to damage to a variety of organs, such as the liver, and may increase the risk of cancer.</p> <p>Ethanol is very flammable, so constitutes a fire risk.</p>
Safe handling	Wear safety glasses. Ensure that no sources of ignition, such as a gas flame, hot plate or hot air gun, are present in the working area. Check that ventilation is good; use a fume cupboard if possible.
Emergency	<p>Eye contact: Flush the eye with plenty of water. If irritation persists call for medical help.</p> <p>Skin contact: Wash off with water.</p> <p>If swallowed: If the quantity swallowed is large, call for medical help</p>
Disposal	Small amounts of ethanol can be flushed down a sink with a large quantity of water, unless local rules prohibit this. Do not forget that this material is very flammable, so precautions must be taken to ensure that flammable vapour does not build up in the sink or drains.
Protective equipment	Safety glasses

4. REFERENCES

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2. Practical manual, Unit ref: QRAD/ Elias Bonilla, Nov 2009, Pg: 16/104
3. Practical manual, Unit ref: QRFT/ Elias Bonilla, Sept 2008, Pg: 23/59
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NOMENCLATURE

A ; pre-exponential factor or factor A of Arrhenius

C_{A0} ; concentration of the reagent A at the beginning, mol/l

C_i ; concentration of i component, mol/l

C_{i0} ; initial concentration of i , mol/l

E_a ; activation energy of the gases, J/mol

F_{A0} ; molar flow of the reagent A that is fed to the reactor, mol/s

k ; reaction rate constant

N_{A0} ; moles of the reagent A at the beginning of the process, mole

Q ; volumetric flow rate of the reagent, l/s

$(-r_A)$; disappearance velocity of the reagent A (reaction rate of A)

r_i ; reaction rate of i component

R ; constant of the gases, J/mol.K

t ; time, s

T ; temperature, K

V ; volume occupied by the reaction mixture, l

x_A ; conversion factor

τ ; spatial time, s

ΔV ; differential element of volume, l

θ ; resident time, s

α, β ; reaction order