Kinetics studies in laboratory lessons as a project-based learning approach in Chemical Engineering Education

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GOAL AND CONTENTS

The goal of this presentation is to show how project-based approach applied to experimental could improve the understanding of key chemical engineering concepts and strength theory

- Presentation of the subject and semester data
- Batch results
- Continuous results
- Comparison batch vs continuous

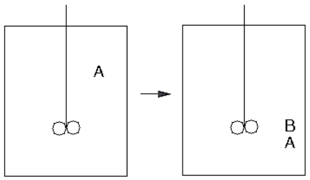
- Bachelor's degree in Chemical Engineering, ETSEIB , UPC
- Experimental subject "**Experimentation in Chemical Engineering II**" run the **6th semester** in parallel with key subjects as Unit operations, Kinetics and reactions and Fluid mechanics

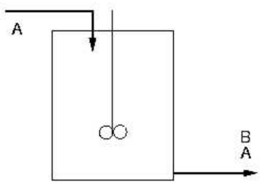
Sixth semester	Experimentation in Chemical Engineering II	4.5
	Fluid Mechanics	6
	Kinetics and Reactors	6
	Organisation and Management	4.5
	Project II	3
	Unit Operations	6

- Opportunity to strength experimental and theoretical concepts !

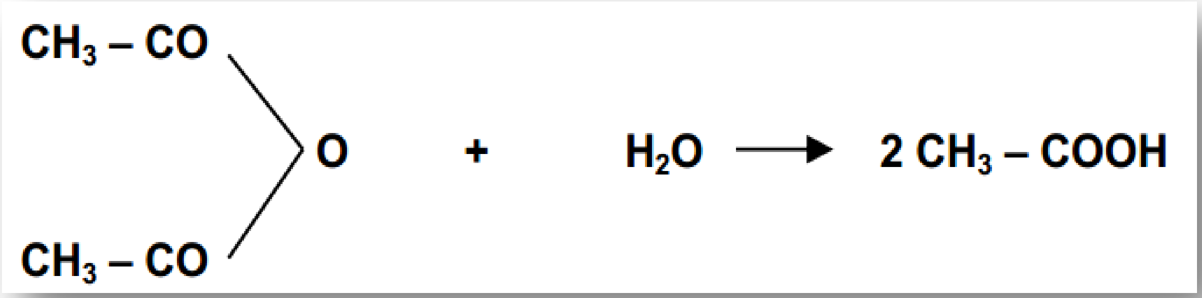
Three **laboratory lessons** considered

- **i) Batch Isothermal**
- ii) Batch Adiabatic
- **iii) Continuous Stirred Tank Reactor (CSTR)**





by using the same reaction: anhydride acetic hydrolysis.



The lessons i) and iii) (batch isot. vs continuous) will be compared in the present work

PROJECTS

Projects in this subject were performed with the following objectives:

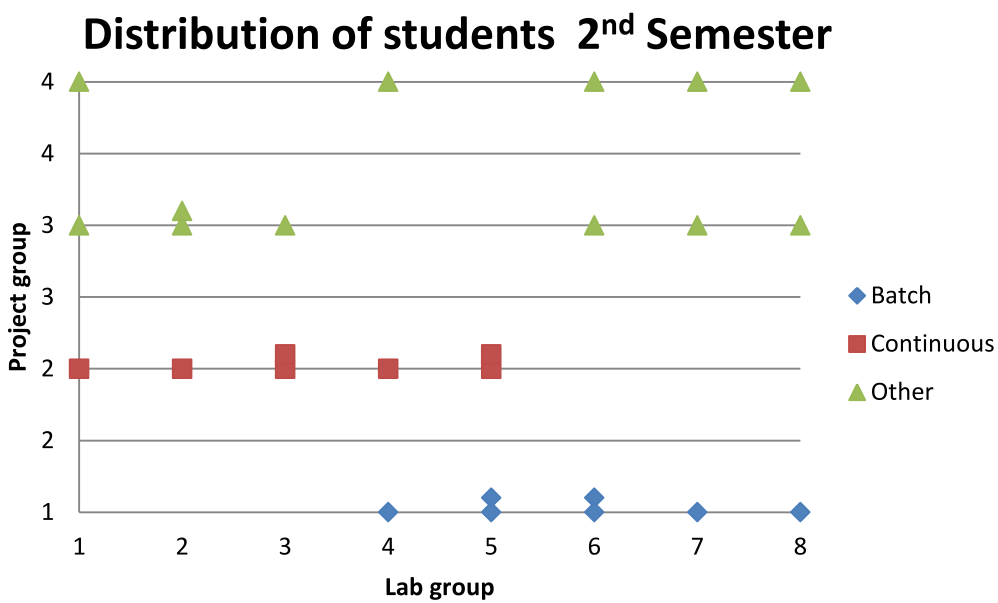
- Design the conditions to be performed in the lab lesson
- Study-modelize all the experimental data generated in the lab lessons

2 from 4 transversal projects were considered to focus on **isothermal batch and continuous reactions** mentioned before. The objectivesof these specific projects were:

- to explore the potential effect of several experimental factors over results
- to study the order of the reactions (order 1 or 2)
- to obtain kinetic constants (k)
- To obtain energy of activation (E_A) by using Arrhenius expression

Course 2014-2015:

1st semester: 18 students, 6 lab groups (3), 4 project groups
2nd semester: 25 students, 8 lab groups (3-4), 4 project groups



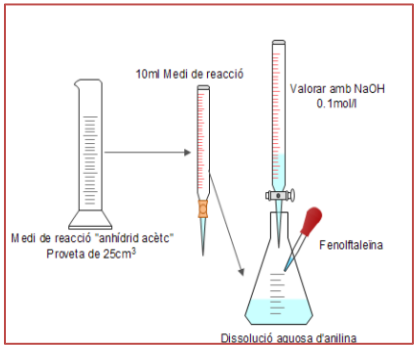
Half of the students Performed batch or continuous approach

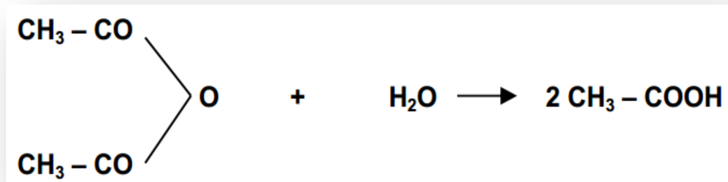
The students were grouped in lab-groups to perform lab lessons and in project-groups for the project-based approach.

GENERAL METHODOLOGY BOTH LAB LESSONS

Weak acid- strong base titration of **acetic acid** with NaOH 0,1 M and phenolphthalein formed from:

1) hydrolisis

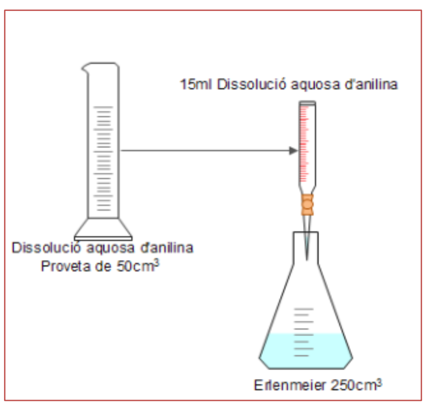


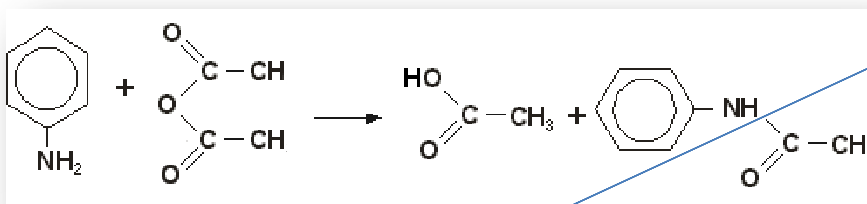


$$C_{A_0} = \frac{C_{NaOH} \cdot V_{(NB)}}{2 \cdot V_{A(NB)}}$$

Main experimental error in volum titration

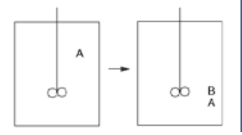
2) blocking reaction with aniline





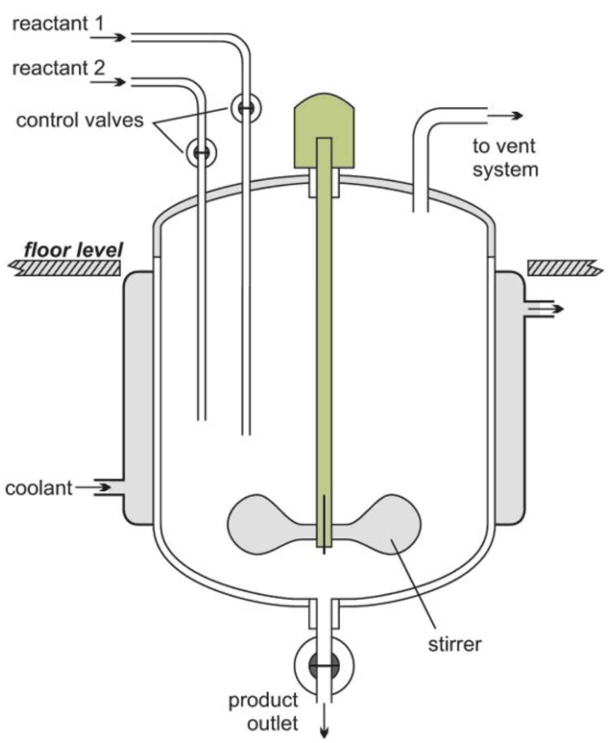
$$C_A = \frac{C_{NaOH} \cdot V_{(NB)}}{V_{A(NB)}} - \frac{C_{NaOH} \cdot V_{(B)}}{V_{A(B)}}$$

$$X_A = \frac{C_{A_0} - C_A}{C_{A_0}} = 1 - \frac{C_A}{C_{A_0}}$$



EXPERIMENTAL PROCESS

Batch Reactor



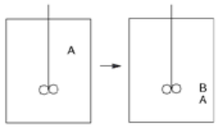
Preparation of solution of water saturated with aniline

Addition distilled water to the reactor isothermal and **temperature control.**

Addition volume of anhydride acetic reactor

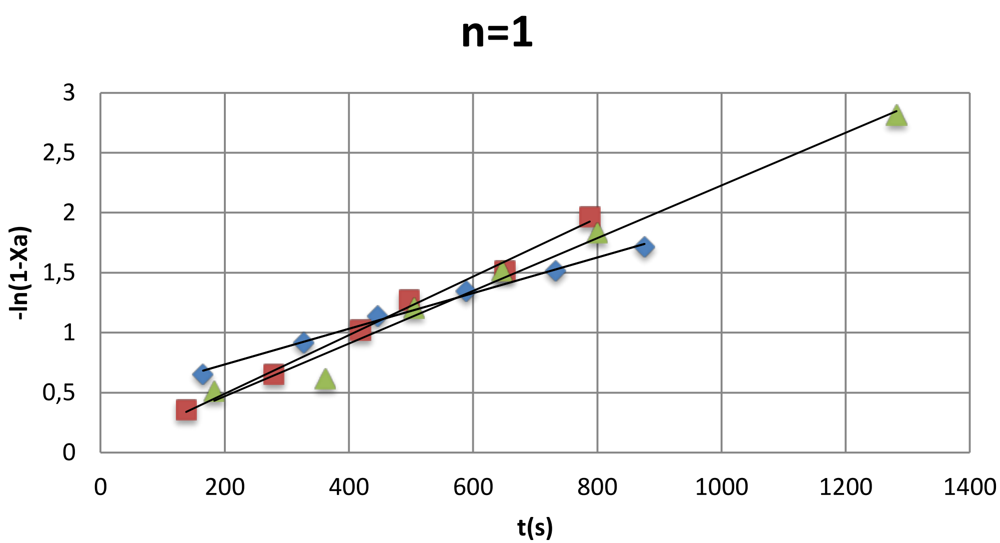
At certain times 6 samples extracted and add them to an Erlenmeyer with aniline.

Extraction a final sample without aniline to calculate CA_o



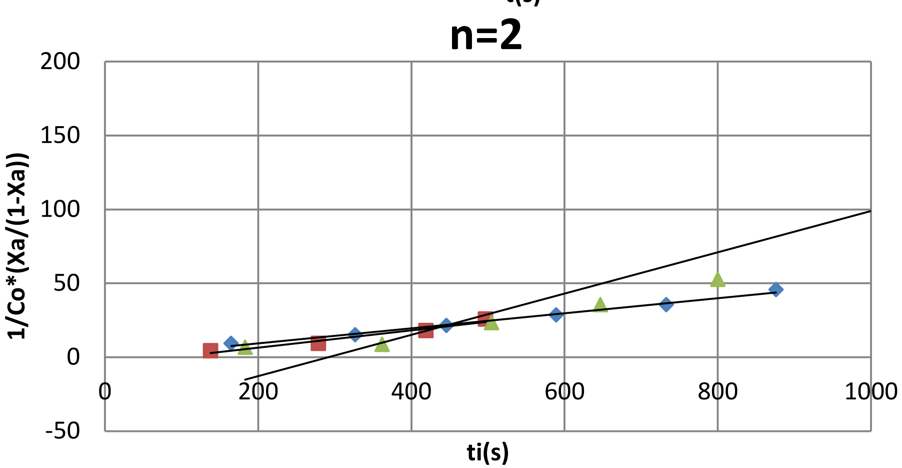
Comparative reaction order(n=1,2).

2nd semester



r^2(n=1): 0.9832,0.9929, 0.9942

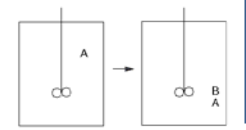
$$[A] = [A_0]e^{-a\cdot k\cdot t}$$



r^2(n=2): 0,8024, 0.8917,0.8925

$$\frac{1}{[A]} = \frac{1}{[A_0]} + a \cdot k \cdot t$$

Correlation data is very good for order 1 and better than order 2

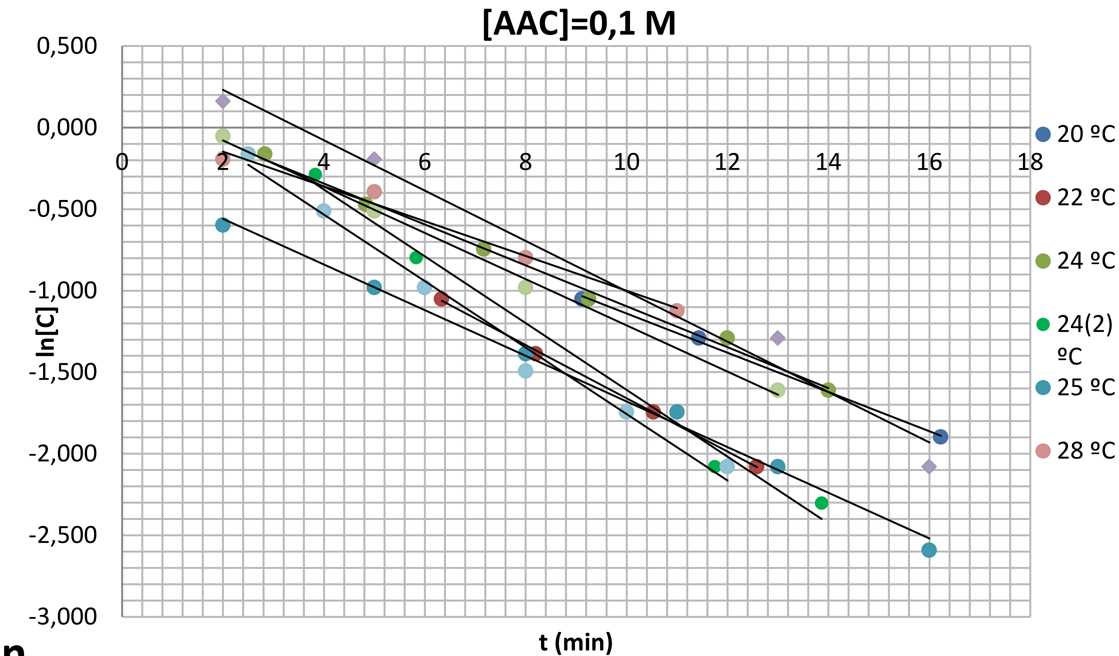


The processing of data gives us an order reaction n=1

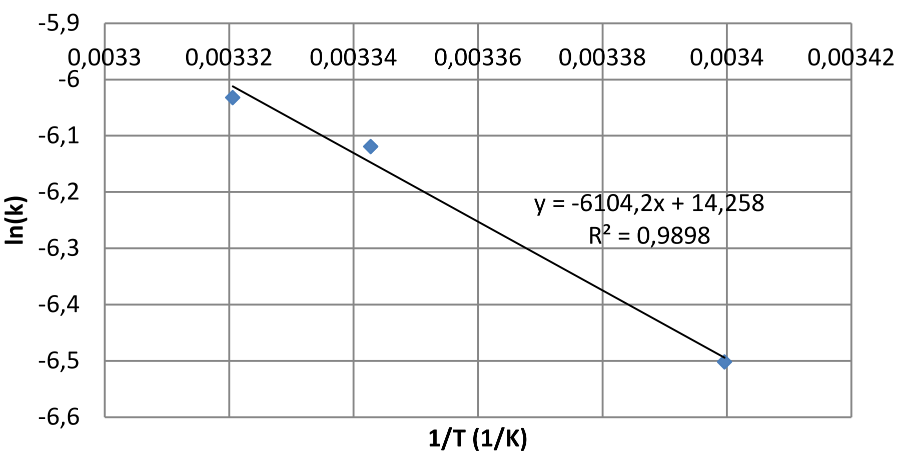
2nd semester

Temperatures(ºC) : 19 <T< 33
r^2 : 0.994919

$$[A] = [A_0]e^{-a \cdot k \cdot t}$$



Ea calculation

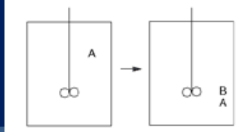


Group 6, 2nd semester

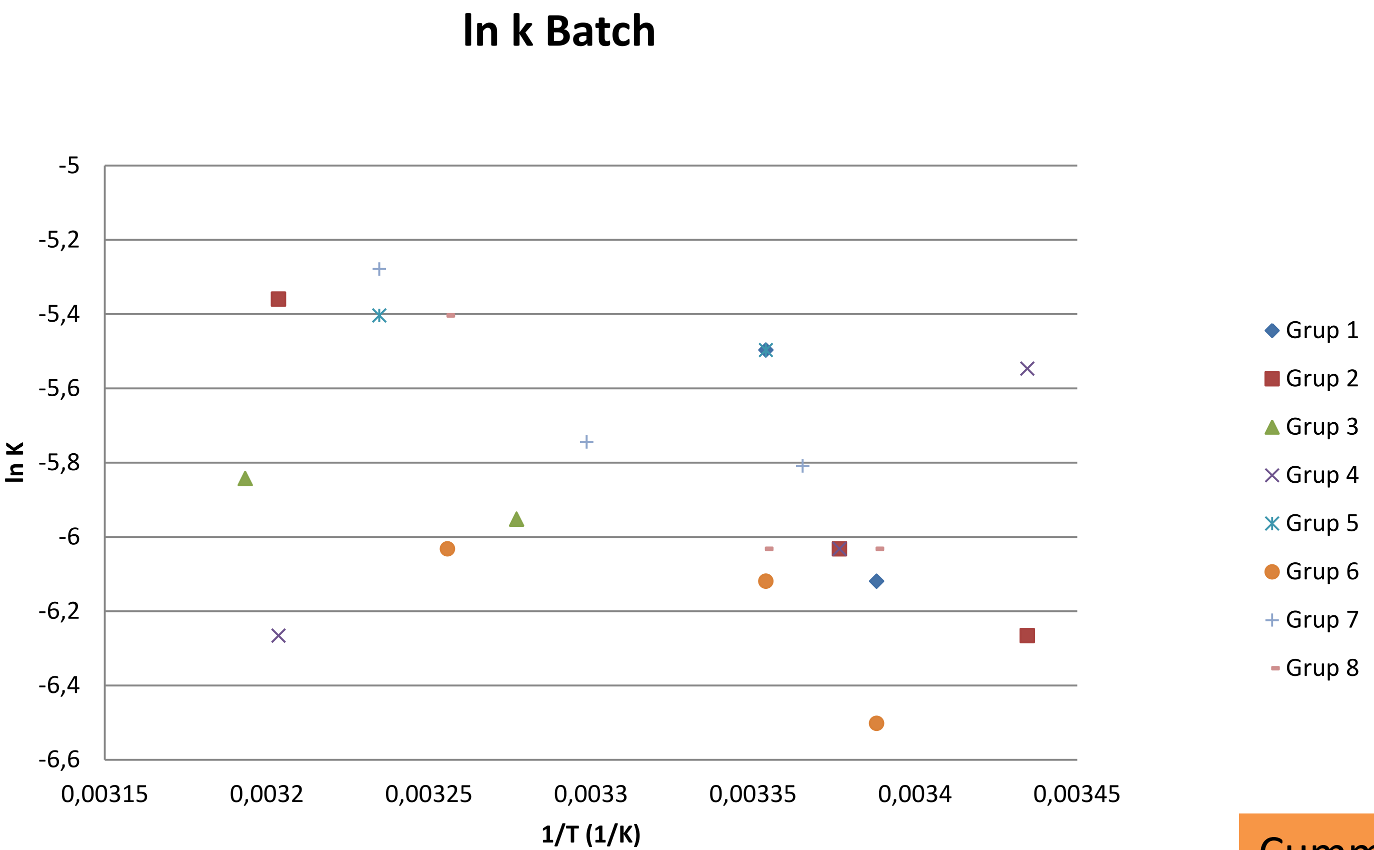
$$k = k_0 \cdot e^{\frac{-E_a}{R \cdot T}}$$

Fitting first-order k is good and the trend with T seems to fit well Arrhenius model

FITTING BATCH DATA TO ARRHENIUS (I)



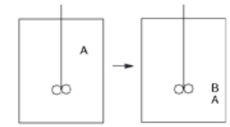
$$k = k_0 \cdot e^{\frac{-E_a}{R \cdot T}}$$

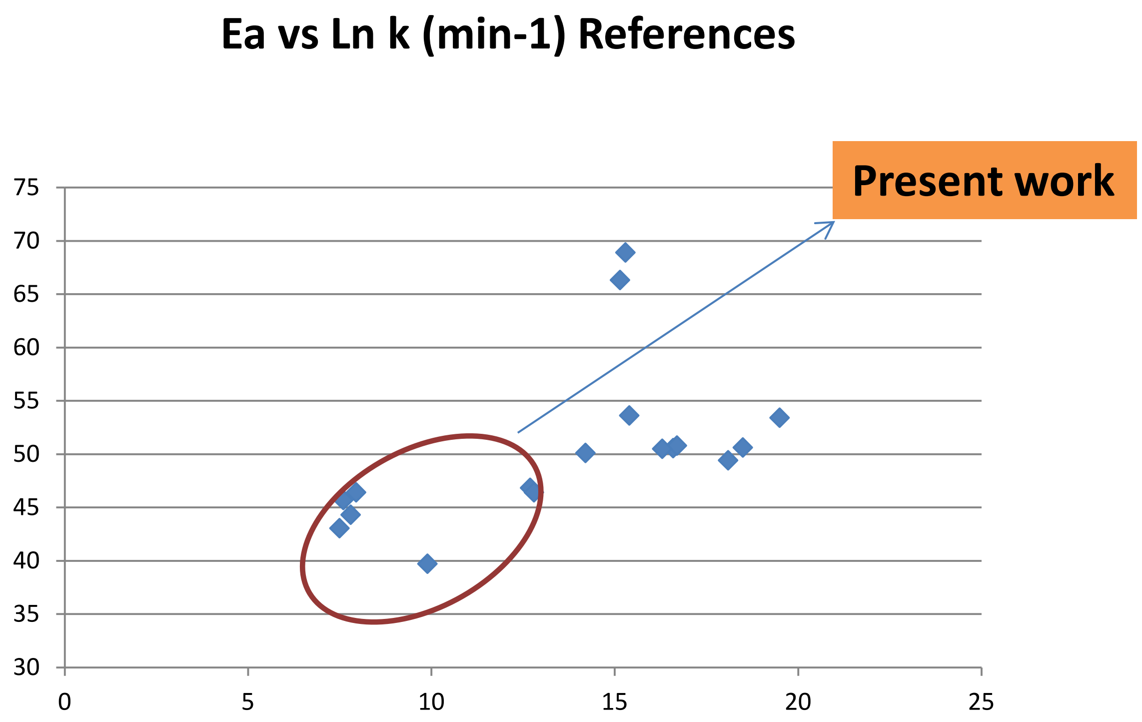


2nd semester

Cummulative effect of titration and T measuremet gives dispersion

FITTING BATCH DATA TO ARRHENIUS (II)

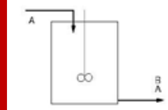


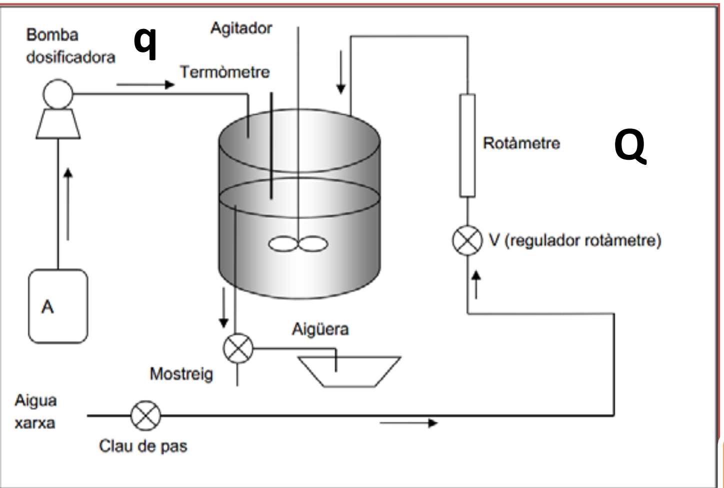


Ea (J/mol) References	Ea (J/mol) Present work	Ln k(min-1) References	Ln k (min-1) Present work
39.5<Ea<53.5	35< Ea<50	7.5<lnk<19.5	7<lnk<13

Experimental dispersion is similar to some ranges of reference data

METHODOLOGY CONTINOUS SYSTEM SETUP





$$\frac{d(C_A \cdot V)}{dt} = v_0(C_{A0} - C_A) - k.C_A.V$$

Check the steady state of water flow (Q) by measuring it

Dose pure acetic anhydride flow (q) by using a peristaltic pump. d and M density and mol. Weight acetic anhydride

Sample output dissolution each 10 minutes

let 10 min more to ensure complete hydrolysis and titrate to **determine CAo**

When CAo is constant steady state has been reached . Extract 3 samples and block with aniline

Titrate to obtain data to **calculate CA**, XA and K

$$vo = Q + q$$

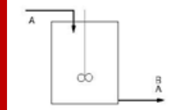
$$C_{Ao} = \frac{q \cdot d \cdot M}{vo}$$ Theoretical

Linear models

$$\frac{C_{A0}}{C_A} = 1 + k\tau$$

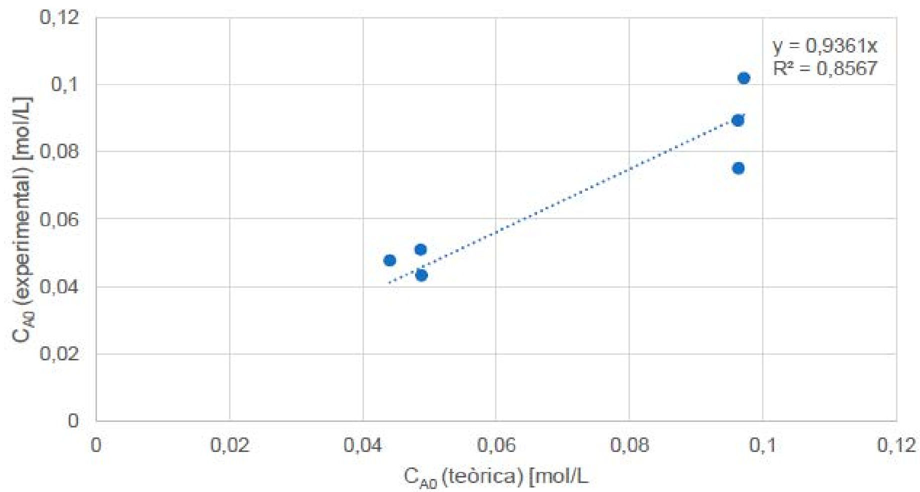
$$k \cdot \tau = \frac{X_A}{1 - X_A}$$

FITTING CONTINUOUS DATA-CONTROL QUALITY



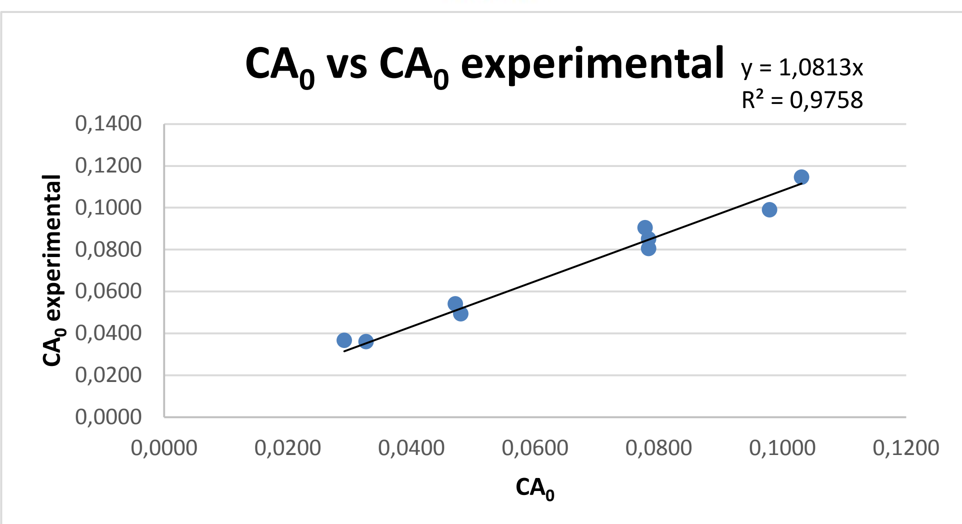
The comparison of theoretical and experimental initial concentration of anhydride acetic the reactor could be used as a “quality control” of the performance of the session

$$C_{Ao} = \frac{q \cdot d \cdot M}{vo}$$ Theoretical



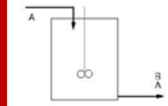
Gràfica 1

1st semester



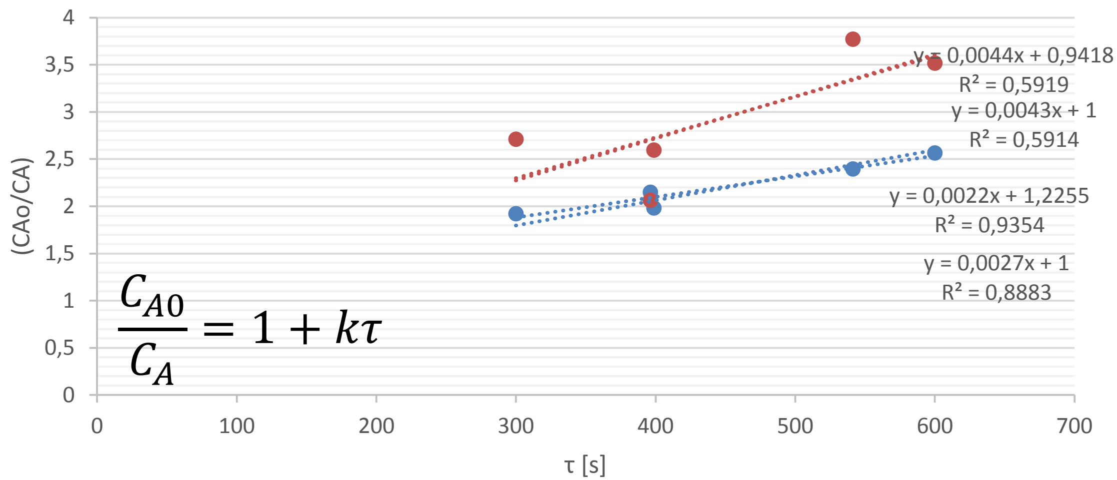
2nd semester

Control and measuremet of **vo** is a key parameter to get good results



FITTING CONTINUOUS DATA- K CALCULATION

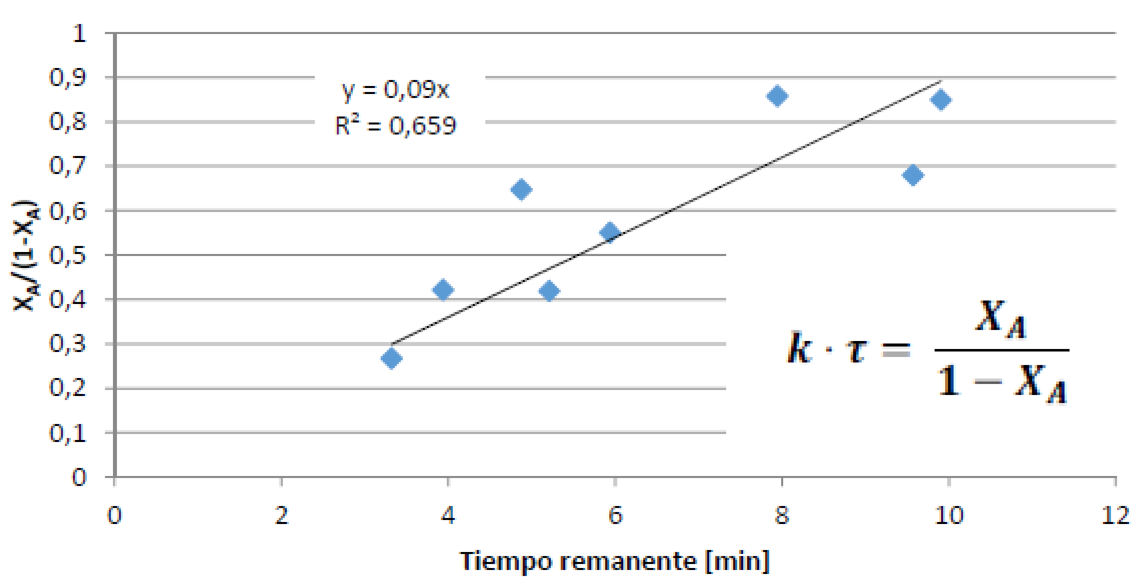
Fittings work quite well , but K are different between semesters



1st semester

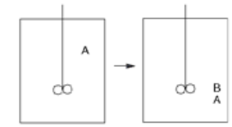
$K=0{,}0027\text{-}0{,}0044\ s^{-1}$

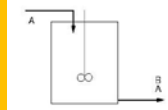
Cummulative effect of vo and titration gives dispersion



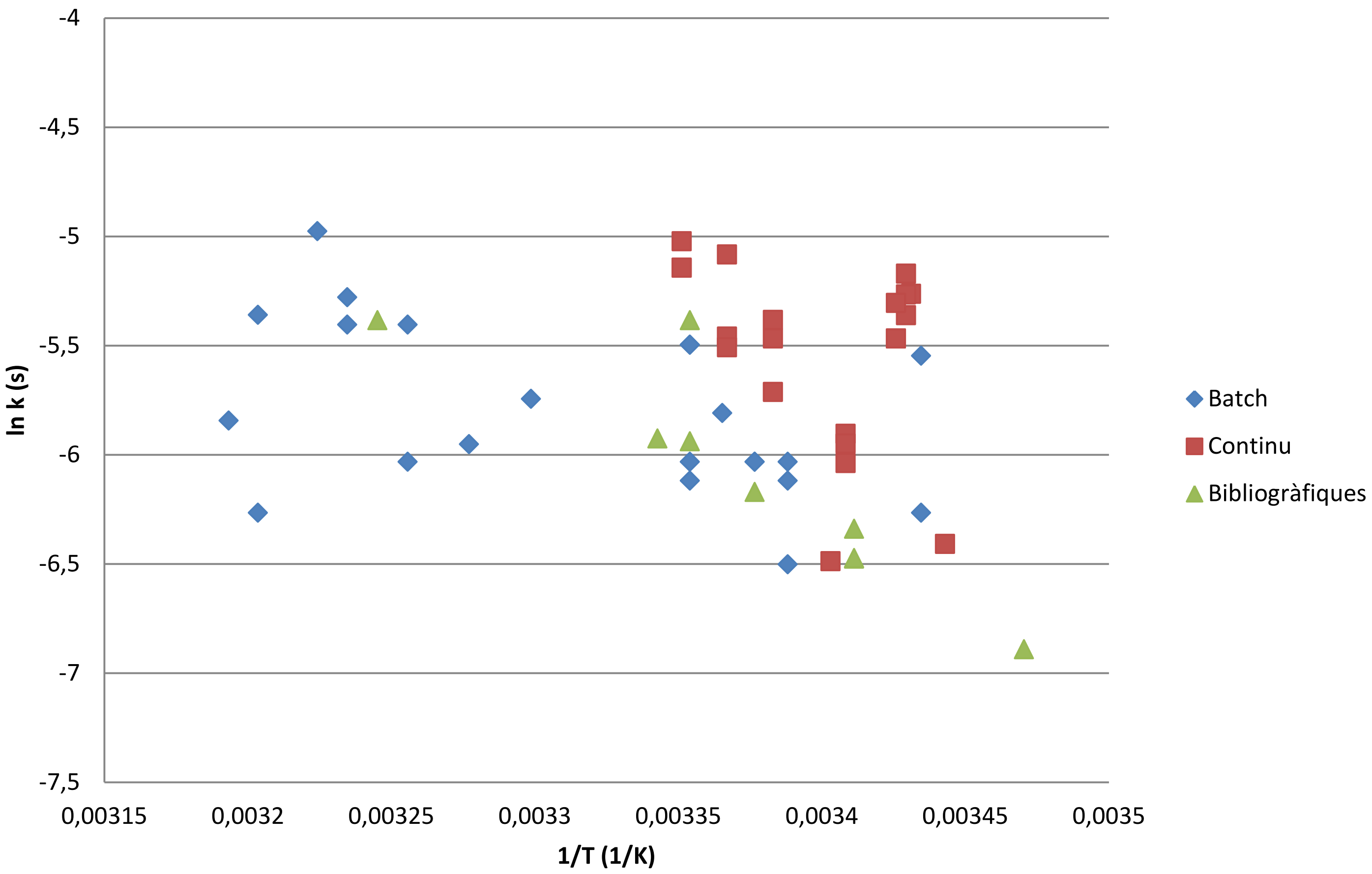
2nd semester

$K=0{,}09\ min^{-1}=0.0015\ s^{-1}$



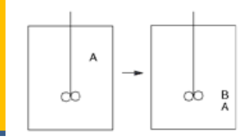


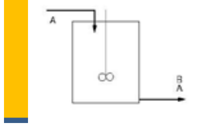
First-order k values- 2nd semester



Comparison batch-continuous give a broad range of k values due to dispersion but are of the same order of magnitude than literature

CONCLUSIONS





- Project-based learning **could be implemented easily** in experimental subjects
- For **batch**: Control of **titration and sampling time** needed to decrease dispersion. **Order and K values good**.
- **Very disperse fitting of Arrhenius**. Range of k values batch and continuous.
- For **continuous**: Control of **titration, sampling time and v_o** needed to decrease dispersion. CAo and K values good to obtain with disperse values.
- Using this experimental approach opens the possibility to learn a methodology based on theoretical and experimental correlation of different subjects and have a unique final vision of the same reaction.

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