

Process Experimentation Laboratory: Use of Open Source Software in the Chemical Engineering Degree: Case study.

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Abstract: Lab courses are considered of paramount importance in the education of future engineers, as it is the case of chemical engineers. The exponential growth of simulation software in the field of chemical engineering has opened the door to a powerful tool in teaching duties. Hence, use of specific software constitutes a valuable instrument aiding students to develop their creativity. Additionally, simulations can check the performance of distinct scenarios in short times, save in reagents and apparatus lifetime, and visualize expected results in real experiments. Access to adequate software is sometimes prohibitive from an economic point of view. Accordingly, availability of freeware to students and institutions is of paramount importance if computer simulations are to be introduced in the teaching procedure. In this work, the introduction of several open PC programs is presented and applied to a specific experimental work completed in the last course of the undergraduate ChE curricula at the University of Extremadura (Spain). The case belongs to the subject "Experimentation in processes" and conjugate different disciplines that students should theoretically know. Hence, knowledge in electrical and electronic assemblies (software used: CadeSimu and PCSimu), sequential control (software used: Logo Soft Comfort) and interface programming (software used: Logo Web Editor) are explained and combined in an unique experiment.

Key-words: Freeware; Scada; process lab; simulation

1. Introduction

The degree in chemical engineering is characterized by taking into consideration several branches in the field of engineering. Hence, the grade in Chemical Engineering contemplates knowledge in subjects such as chemistry, process control, material engineering, instrumentation, electronic engineering, electrical engineering, etc. Acquisition of skills during the degree rely not only on theoretical background comprehension, but also on the adequate planification of experimental lab courses [1]. Lab experimentation is of paramount importance to acquire professional skills [2]. With the fast development of computer science and capabilities [3], scientific software has become a valuable tool in lab courses. Use of specific software should not be used as a substitutive tool of actual experimentation, but as an aiding instrument to complement the course. Computer aided lab offers several advantages in teaching duties. For instance, software is an economical methodology to test several alternatives of conducting any specific task. Savings in reagents, electricity, apparatus useful lifetime, etc. can be obtained. Additionally, previous software simulations can increase the safety in the lab, preventing potential procedure mistakes when handling chemicals, electricity, hot surfaces, high pressure systems, etc. also extending the lifetime of equipment if misused.

Data obtained in simulations offer an important tool to detect errors in actual experiments. The power of simulation software induces the students to stimulate their critical scientific reasoning.

Taken into consideration the aforementioned advantages, open source software facilitates the access of students and institutions encouraging the cooperative work and becoming a strategic factor for scientific development [4, 5].

In this line, in this work use of free software is proposed as a valuable tool to complete an experiment compiling knowledge in reaction kinetics, process control and instrumentation, electronic and electric engineering, programming, etc. The experiment is included in the subject "laboratory of processes" which is offered in the fourth course of the chemical engineering degree at the University of Extremadura (Spain)

2. Experimental set-up

The installation shown in Fig. 1 was implemented. The objective of the experiment was to carry out a reaction in batch mode by sequentially controlling the feed of reagents and reaction temperature.

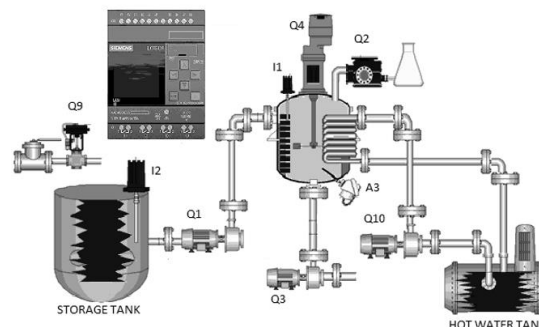


Fig. 1. Pilot plant used in experiments

In Fig. 1 the electro valve (SMC Solenoid Valve VXS245GLA) Q9 feeds a solution of compound A to the storage tank. The electro valve actuates controlled by the I2 level sensor (Toscano Vigilec® TH1). The centrifugal pump Q1 (CALPEDA NM2m/A/A 0,75kW) feeds the previous solution to the reactor until level sensor I1 indicates maximum volume achieved, at this time the agitator Q4 is switched on. Once reactor temperature is reached, the peristaltic pump introduces a solution of compound B to the reactor during a pre-specified time (depending on flowrate and desired concentration in the reactor). After the reaction between A and B is completed, the agitation stops and pump Q3 drains the reactor initiating a new cycle.

Reactor temperature measured by the thermocouple A3 is controlled by circulating (pump Q10) hot water through an internal coil. Kinetics of the reaction at the conditions used in the experiments are deduced from virtual experiments completed with a programmed Matlab function which has three entries (initial concentrations of two reactants and reaction time) and one output in graphical form. Data allow students to apply the differential and integral methods to obtain reaction order and rate constant.

3. Sequential control of the process. Programming Logo Soft Comfort V8.3

The aforementioned sequential process is controlled by a Siemens LOGO! 24 CE - 6ED1052-1CC08-0BA1 apparatus. This PLC is a cheap and reliable controller suitable for basic control tasks. Up to 8 digital inputs (I) are available (4 of them can be used as analog inputs) with 4 relay type digital outputs (Q).

The PLC can be programmed by the SIEMENS freeware Logo Soft Comfort V8.3 [6]. The software allows for the codification of the sequential control required by means of different instructions including analog and digital signals, relays, timers, etc. The program is depicted in Fig. 2.

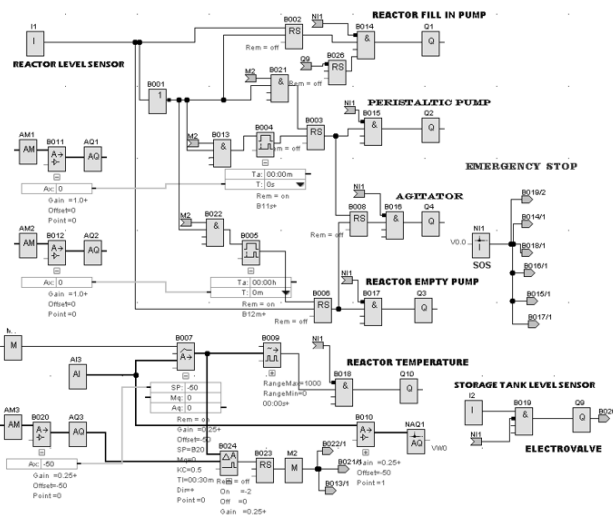


Fig. 2. Function diagram applied to pilot plant control

In Fig. 2 the following instructions are implemented:

- An emergency stop button controlled from the web based interface explained in section 5 (variable V0.0 corresponding to block NI1) would eventually disconnect all output variables.
- Level sensor I2 determines the action of electrovalve Q9, provided that the emergency input (V0.0) is low.
- Reactor level sensor I1 activates the latching relay B002 which switches on the reactor filling pump Q1. This action is contingent upon storage tank is not initially empty by means of an “AND” instruction (B014).
- Latching relays B003 and B008 govern the peristaltic pump and the agitator while B006 relay operates on the empty pump Q3. B003, B008 and B006 are not activated unless reactor temperature is sufficiently close to set point. Analog comparator B024 determines the difference between setpoint and actual temperature allowing the normal function of latching relays.
- Peristaltic pump is switched off after a pre-specified time introduced in the connection time delay B004.
- Agitator is stopped after the reaction time considered in the time delay function B005 is completed.
- The previous signal initiates the reactor drainage (Q3).
- Several parameters are introduced through a web based interface by means of analog or digital marks.

4. Wiring checking. Use of CadeSimu and PCSimu.

CadeSimu is an open software intended to easily simulate electric schemes in low voltage [7]. The following elements were connected to simulate the experimental setup (see Fig. 3):

- From the electricity sources tab, the alternate current was directed to the corresponding electrical circuit breaker.
 - The continuous 24V current generator was taken from the I/O tab. This generator fed the PLC, extensions and sensors (if required).
 - Siemens LOGO! 24 CE - 6ED1052-1CC08-0BA1 apparatus and extensions were also selected and withdrawn from the I/O tab of the program.
 - Switches S1 and S2 can be used as level sensor signals, however, in this work, level sensors will be added to the program from sensors tab and simulated from PCSimu software [8].
 - Outputs from Siemens PLC are wired to relay devices.
 - Actuators are assigned to motors, although in the actual experimental setup final actuators are pumps and valves. The latter will be simulated in PCSimu.
- If wiring is correct, when running the program, the PLC screen will be switched on and will show the active signals, both inlet and outlet. Actuators will also depict their ON or OFF state.

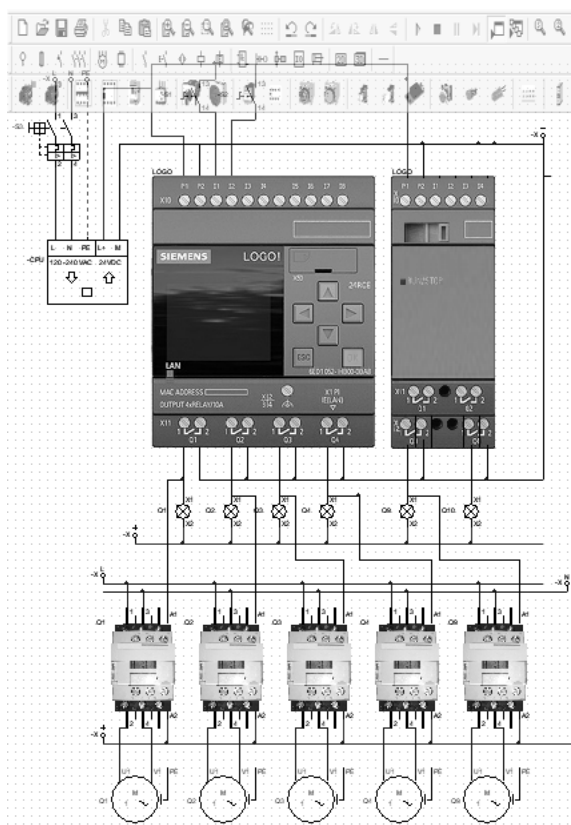


Fig. 3. Wiring simulation of PLC, inlet and outlet signals in CadeSimu.

The scheme implemented in LOGO Soft Comfort, with some differences, must be programmed in Cade Simu to check the correct sequential control actions. Figure 4 depicts the program inserted in Cade Simu through the Ladder tab.

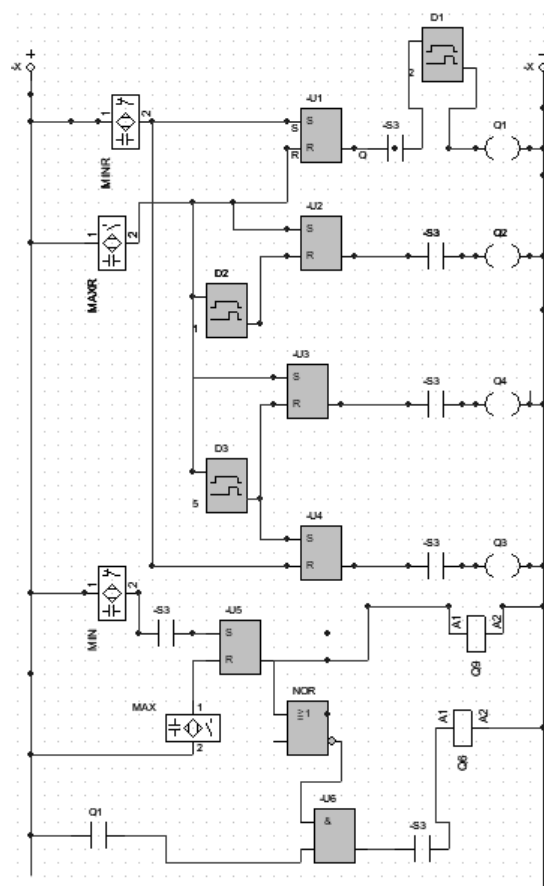


Fig. 4. Ladder program in CadeSimu.

In Fig. 4, MINR and MAXR represent the minimum and maximum liquid level transmitted by the sensor in the reactor, activation of signals is simulated in PCSimu. S3 is the electricity breaker.

MIN and MAX are level signals corresponding to the storage tank. These signals are connected to a latching relay which govern the electrovalve Q9.

When MINR is active, latching relay U1 is activated and reactor filling pump Q1 switched on. Certain delay (D1) is allowed to avoid pumping the liquid if storage tank is empty. After maximum level is reached, U1 reset activates the peristaltic pump Q2 through latching relay U2. Time of peristaltic pump operation is controlled by delay D2. Additionally, reactor agitation (Q4) also begins once the reactor is at maximum level. Reaction time and agitation are controlled by delay D3 which reset agitation and set empty pump Q3 by means of latching relay U4.

Electrovalve Q6 allows pass of the liquid from storage tank only when the reactor is being filled up and the storage tank is not at minimum level.

Temperature control is not simulated in CadeSimu because analog signals are not handled in this software.

Interaction between CadeSimu and PCSimu is achieved after defining inlet and outlet variables (Fig. 5)

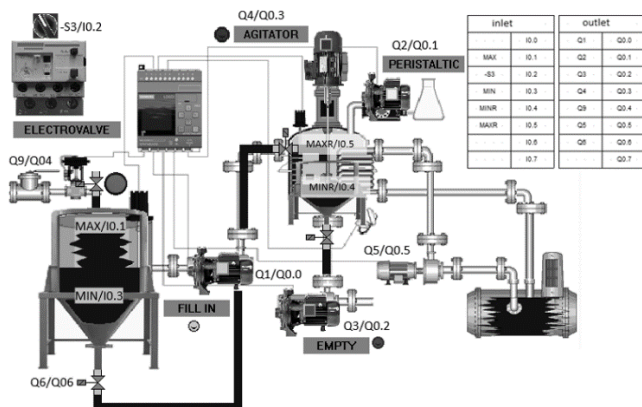


Fig. 5. Correspondence in variables between CadeSimu and PCSimu. Interface in PCSimu

Variables shown in Fig. 5 are shared by CadeSimu and PCSimu. Interface is programmed in PCSimu. The latter software not only can be virtually connected to CadeSimu but also can interchange variables with LOGO OBA7/OBA8, Siemens S7-200/1200/1500 and Arduino by means of IP or serial port.

5. Logo Web Editor

Logo Web Editor (LWE) is an open source web editor capable of acting as interface connecting the experimental hardware (pumps, electrovalves, thermocouples, etc) – Logo Soft Comfort – Logo Web Editor. LWE is capable not only of visualizing output signals, but also can introduce inlet parameters to Logo Soft Comfort [9].

Fig.6 shows a screen shot of the program. In this scheme the following associations can be mentioned.

- The emergency button is linked to the local memory variable V0.0 in net inlet block NI1(see Fig. 2). This writable button allows to stop the experiment at any time by just clicking on it.
- Pause indicator reflects the state of the electrovalve Q9 which controls the storage tank level.
- Hourglass indicator Q1 depicts the state of reactor filling pump. Similarly, Q2 and Q3 indicate the state of the peristaltic and empty pumps, respectively.
- The enable hand, near the peristaltic pump, is a non-writable mark (M2) that prevents the peristaltic pump to be switched on unless reactor temperature is sufficiently close to the desired set point. Reactor temperature setpoint is manually introduced through analog mark AM3 which is compared to actual temperature (analog comparator B024 in Fig. 2) activating M2 when temperature difference is less than 2 °C. Proportional integral (B007) control of temperature is enabled by means of mark M1 in the interface. Temperature is visualized by means of variable VW0 from net analog output NAQ1
- Time of peristaltic pump and agitator operation are introduced through analog marks AM1 and AM2, respectively.

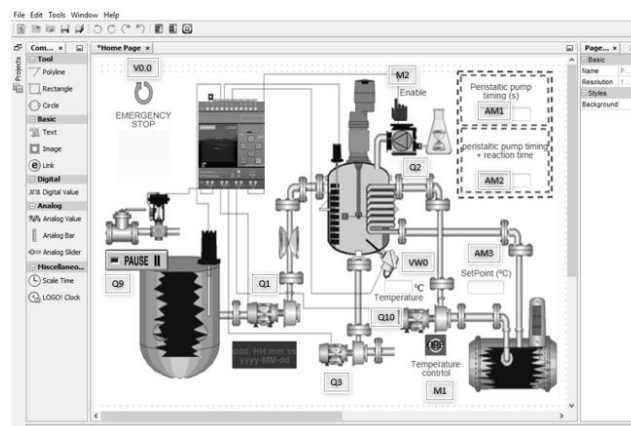


Fig. 6. Logo Web Editor interface.

6. Students tasks

Accomplishment of the lab experiment involves the following tasks to be completed by students:

*Determination of reaction kinetics (reaction rate and reaction order). Kinetic parameters will be obtained by designing the adequate experiments using a programmed function in Matlab. Students must propose the conditions to be used (initial concentrations, reaction time, etc) to apply the differential and integral methodologies of reaction kinetics. The reaction occurring in the reactor is the oxidation of methylene blue (MB) by potassium monopersulfate. A first idea of the kinetics can be extracted from bibliography [10]. Figure 7 shows the Matlab program used for the second order reaction with $k = 6 \text{ M}^{-1}\text{s}^{-1}$. Since MB is measured by UV absorption, concentration to be virtually analyzed must be sufficiently low to follow Lambert Beer equation (if dilution of samples is to be avoided). A “while” instruction prevents absorbance to be above 2.

```
function [] = cinetica(CBo,CAo, tf)
while 35000*CBo > 2
fprintf('Initial Methylene Blue concentration too high.
Range outside Lambert Beer law')
CBo=input('\n\n Please, introduce new initial Methylene
Blue concentration (M)');
fprintf('_____
\n\n')
end
time=linspace(0,tf,25);
k=6;
syms CB
for n=1:1:25
solve(log((CAo-(CBo-CB))*CBo/CB/CAo)-(CAo-
CBo)*k*time(n)==0,CB);
CB_t(n)=double(ans);
end
figure
plot(time,CB_t,'o')
grid on
xlabel('time, min')
```

```
ylabel('Concentration MB, M')
pause
clc
end
```

Fig. 7. Matlab function to determine second order reaction kinetics

*Once the objective of the experiment is clear, students must build the block diagram in Logo Soft Comfort by considering the time the peristaltic pump must be ON and the time of reaction to achieve a pre-specified conversion. Undergraduates must be familiar with the performance of latching relays, connection delays, proportional integral control and the concept of Pulse Width Modulation, needed to combine analog and digital signals in temperature control.

*Adequate electrical connection must be checked before carrying out the reaction. Cade Simu allows for the simulation of the electrical wiring. Continuous and alternate current devices are connected with the use of relays, electrical breakers, continuous current sources, temperature transducers, etc. CadeSimu in conjunction with PCSimu let students to check the correct performance of the sequential program applied. Additionally, PCSimu can be directly connected to the PLC Logo, although in this case, the Logo Web Editor is preferred as interface. Besides the adequate wiring, the sequential program implemented in Logo Soft Comfort (or similar) must also be checked in Cade Simu.

*Finally, students must identify actual inlet and outlet signals from LOGO and introduce the information into the Logo Web Editor interface. Analog, digital, and net signals have to be considered in the process. Additionally, students must differentiate between writable and non-writable variables (indicators). The final result should be an interface easy to understand and manage. Experimental data can be downloaded as SCV file for further analysis.

7. Results

Previous simulation by the adequate software has resulted in a deeper comprehension of each of the parts configuring the whole experiments. Hence, potential wrong connection of devices has been avoided, as for example feeding the LOGO PLC with alternate current, or directly connecting power apparatus such as pumps to the LOGO outlets. Students have also understood differences between two or three wire thermocouples and the connection scheme. Use of the kinetics has allowed them to calculate reaction times, pumping periods, etc. These calculations have consolidated their knowledge in reactor design and applications. In case of wrong calculations, no wastage of reagents or time has been achieved.

Additionally, undergraduates have applied concepts of sequential control and PI control checking the correct performance by LOGO Soft Comfort with no risk for the actual setup.

Approaching to SCADA concept has been accomplished by means of Logo Web Editor. Students have been able to differentiate between analog and digital signals and how to interact with the experiment through the PC. They are free to register/visualize any variable, so a deep knowledge of the experiment, objectives and goals has to be considered.

Broadly speaking, undergraduates gain a higher understanding of the experiment before conducting it.

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