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MATLAB: A Powerful Tool for Experimental Design in Chemical Engineering*

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Laboratory experiments in chemical engineering can be modelled by defining heat and material balances and considering transport phenomena in non-stationary conditions. Usually, these equations have no analytical solution and students cannot solve the problem easily to compare experimental results with theory. In this paper the use of MATLAB is presented as a powerful tool in order to solve chemical engineering problems numerically. A new laboratory experiment for third-year students in chemical engineering has been developed combining a laboratory rig with a computer-aided solution using MATLAB and Simulink. The experiment consists of three gas–solid fluidised baths, one of them prepared with two heaters and temperature transmitters to obtain non-stationary data. A fluidised bath is considered a globalise system owing to perfect mixing, so temperature gradients are negligible. The other two baths have different diameters and work at ambient temperature to give steady-state results for hydrodynamic conditions. This experiment is a partner-to-partner design between university teachers, a control engineer, a technical staff member and the students; contribution of each was crucial. A new laboratory plant for university students has been developed with a MATLAB-aided solution. The combination of theory, experimental results and simulation improves learning and safety in operation.

INTRODUCTION

AT THE END of the twentieth century some reports analysed future requirements in chemical engineering teaching practice. Thus, Felder *et al.* considered that the curriculum should concentrate on basic knowledge rather than specific topics [1]. In this way, the overall understanding of chemical processes could be improved by focusing on three aspects: 'multidisciplinary thinking', team-work and computer-aided simulation. In the same way, J. Gillet presented the conclusions of the working party 'Chemical Engineering Education' (EFCE) in his paper, *'Chemical Engineering Education in the Next Century'* [2].

There are two main points in this overall change, talking about teaching in chemical engineering. Firstly, the addition of new programmes, methods and educational materials aimed at improving the learning outcomes. These programs should include educational software development, engineering design during the first years and laboratory experiments. Laboratory work develops problem solving, teamwork [3], communication and creativity. And secondly, the university has realised the necessity of including these methods traditionally associated with school. Moreover, these reports suggest that the proposed projects should integrate both academic contents and real problems. Students must deal with such problems using issues from 'local' industries and the latest research. In this case, they will learn from people working with the latest in engineering knowledge and at the interfaces of engineering and science, academia and industry.

Therefore, an innovative curriculum should promote the development of technical expertise and non-technical skills in communication and management through a mix of team-based project work with traditional lecture-based courses, complemented by laboratory work. This should involved active learning and personal interaction between staff and students.

In order to improve academic training of chemical engineers and considering all trends previously mentioned a new laboratory pilot plant for the third-year students in Chemical Engineering has been developed. It summarises subjects such as fluid flow, studied in the second year and heat transfer, studied in the first semester of the third year. This experiment introduces process control and data acquisition, which are studied in the forth year and uses the MATLAB program as simulating software. The plant has been designed, built and tested by students [4], technical staff and lecturers in a partner-to-partner collaboration as an innovative project in our degree. Students, lecturers and technical staff spend a lot of time in the laboratory during the year. All their different

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points of view should be considered if the design is to be successful. As a trivial example, the selection of the position of the emergency button and the control panel changed drastically when one of the students confirmed that she was not tall enough to reach it.

LEARNING OUTCOMES

Time spent in the laboratory should make the link between theory and practice, connecting both of them with one aim: 'Make the basic concepts clear and put them into the real world'. The chemical engineering degree in Spain lasts 5 years. The first two years are dedicated to basic engineering (maths, physics, chemistry, etc.) and also to chemical engineering with fluid flow. The third year concentrates on heat transfer and kinetics. Work in laboratory begins with fluid flow and heat transfer. In the last two years students specialise in reaction, separation processes and process simulation.

We have developed a new practical experiment for the third year students. At the end of the practical work with this plant the student should be able to:

1. Describe the experimental aspects of gas-solid fluidisation.
2. Draw and understand the process flow diagram.
3. Start-up and operate a pilot plant with heating systems and blowers.
4. Use automatic controllers for temperature.
5. Measure data with automatic on-line acquisition systems and also with manual systems.
6. Derive equations to model the system in dynamic conditions.
7. Solve the model equations using MATLAB and Simulink.
8. Compare & Contrast experimental and simulated data to fit model parameters.
9. Predict the behaviour before doing the experiment.
10. Scale up the system.

These outcomes are well integrated with our teaching system because the students have two days for each experiment. On the first day they study the theoretical aspects and the start-up strategy. In this way, an unfinished Simulink program will be given to them in order to predict the start-up behaviour. Thus, they should see how the system should respond and can then design a proper start-up strategy under safe conditions. On the second day they should operate the pilot plant measuring all the variables. After that, they should check the agreement of the results and discuss them using a new model (improved by them).

EXPERIMENTAL SECTION

A process flow diagram of the pilot plant is presented in Fig. 2; a picture of the system is shown in Fig. 3.

The pilot plant consists of three sand baths, two of them made of methacrylate (200 mm and 250 mm diameter) to operate at room temperature and another one made of stainless steel (250 mm diameter) to study high temperatures (up to 200ºC). The baths are half-filled with alumina particles of 170–210 μm. When air is flowed at the bottom of the sand baths the bed experiences a volumetric expansion. Above a certain flow rate all the particles are suspended chaotically (perfectly mixed): this is called fluidisation [5, 6]. Under these conditions the solid has the same appearance as a boiling liquid, with breaking bubbles, as it is illustrated in Fig. 3.

Air is taken from outside and after filtration is pumped into the three baths with a low-pressure blower. Flow rates for each bath are controlled with a valve on each branch (one per bath). Flow rates are measured using air rotameters in the

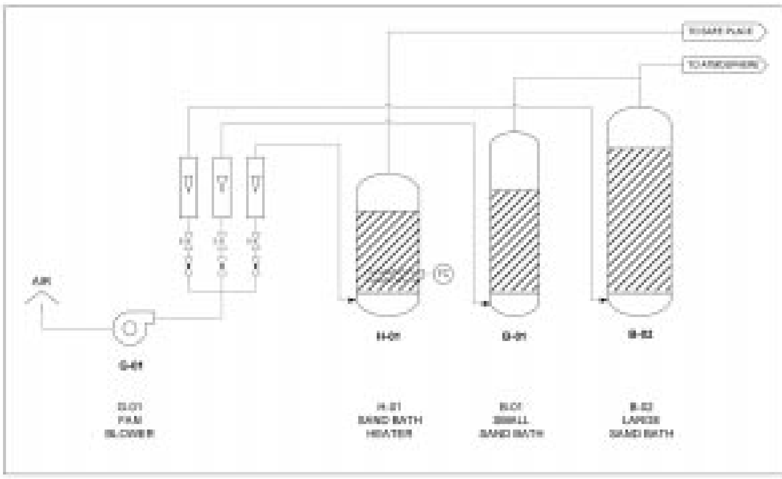

Fig. 1. Process flow diagram of the pilot plant.

Fig. 2. Laboratory plant general view.

Fig. 3. Fluidisation detail in the cold sand bath.

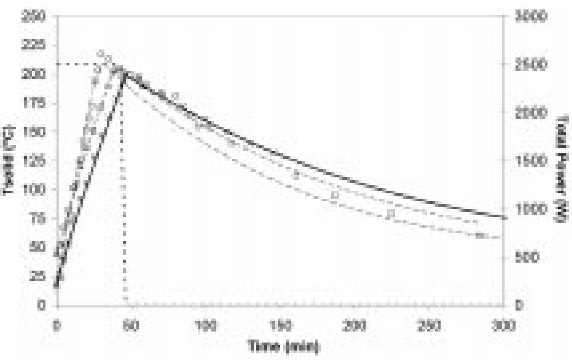

Fig. 4. Experimental (points) and predicted values (lines) for the Fluidized Sand Bath Heater at maximum power. (○ Continuous thick 25 kg; □ long dashed 30 kg; + dashed-dotted 35 kg).

range 1.8–18–m^3/h. Pressure drop is also measured using water manometers.

The metal bath has two cartridge heaters (1600 W each) controlled by manual potentiometers connected to an automatic controller (LS-3200, Design Instruments). The temperature is measured with two thermocouples inserted in the bath at a certain height.

FLUIDISATION AND HEAT TRANSFER: MATHEMATICAL MODEL

In order to test the system, twenty experiments were carried out in the metal sand bath. Fluidisation and heat transfer variables were studied for 25, 30 and 35 kg of alumina at three different heating powers. Results are shown in Fig. 4.

To model the system a globalised state is considered for the sand due to fluidisation conditions. Equation 1 is an ODE (ordinary differential equation) which describes the heat balance for the fluidised sand bath, where the change in temperature of alumina is proportional to power, enthalpy of the air and heat loss. This is a typical heat balance studied in third year, consequently students should be able to reproduce this model easily. Equation 2 is an experimental fit which describes the change in temperature of the air depending on sand temperature. Ideally in a perfectly mixed tank both temperatures should be equal [7]:

$$m_s Cp \frac{dT_s}{dt} = W - \dot{m} Cp_{air}(T_{air\_out} - T_{air\_in}) - q_p \quad (1)$$

$$T_{air\_out} = 0,962\, Ts - 2,822 \quad (2)$$

where: W = power (watt); m = air mass flow (kg/s); Cp_{aire} = specific heat capacity of air (J/kg K); T = temperature (ºC), q_p = conduction heat losses (W), m_s = mass of alumina (kg); Cp_s = specific heat capacity of alumina (J/kg K); t = time (min); T_s = temperature of particles (ºC); Ts_{air_in} = temperature of air at inlet conditions (ºC); Ts_{air_out} = temperature of air at outlet conditions (ºC).

An analytical solution for the model equations can be found under some assumptions. However, Equation 2 introduces non-ideal behaviour. Furthermore, mass flow rate of inlet air is controlled during the experiment because the increasing temperature decreases the density and

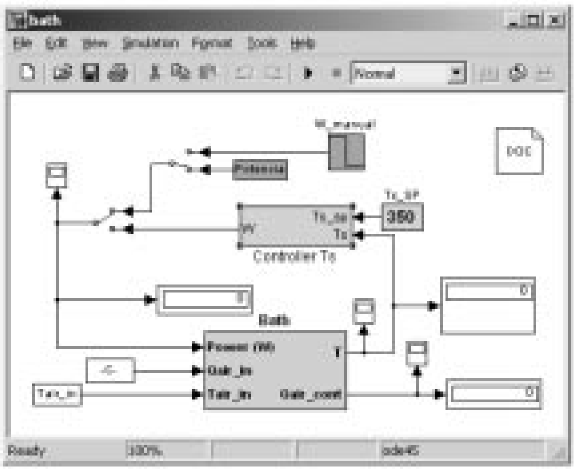

Fig. 5. Simulink main interface.

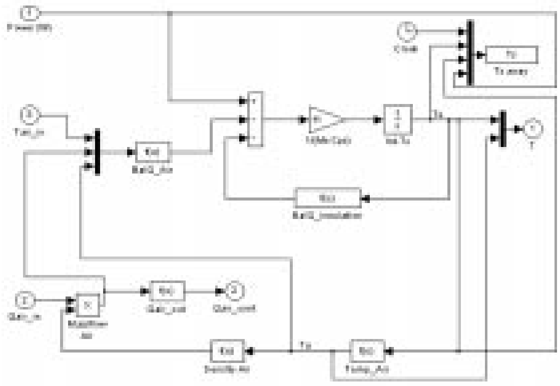

Fig. 6. Simulink model main balance.

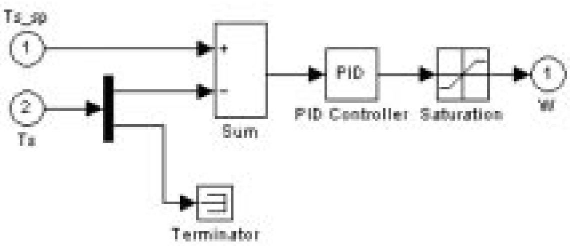

Fig. 7. Simulink model controller.

increases volumetric flow rate of air inside the bath. This can be implemented in the model by simply considering the ideal gas law to calculate instantaneous density (Equation 3).

$$m(t) = m_{air\_in} \cdot \frac{(T_{air\_in} + 273.15)}{(T_{air\_out} + 273.15)} \qquad (3)$$

All the values for the physical properties were extracted from the most common chemical engineer handbook, from the student library [8].

MATLAB: A POWERFUL TOOL

MATLAB 6.1 was the selected programming language for several reasons. Firstly, it is licensed in our university. Secondly, it is very easy to use and fully coupled to Excel having many engineering toolboxes. Thirdly, it is part of one of the subjects in the first year. And finally Simulink provides an educational conceptual approach to describe and solve dynamic systems. For these reasons we consider MATLAB a useful tool for educational purposes. More complex problems, such as transport phenomena equations, could require computer fluid dynamic modelling (CFD). This is also possible with MATLAB in conjunction with FEMLAB. Therefore, it is a good choice for the future. Moreover, to simplify the way to get the program files we have posted all the files to MATLAB Central File Exchange [10]. Thus, the program can be up-graded and the students should see the advantages of sharing the knowledge in this type of networks.

Direct ODE solving

The simplest model for our system is well described by Equation 1 where all the values apart from solid temperature and outlet air temperature (equal to solid temperature in ideal conditions) and time are constant. In this case, direct analytical solutions can be successfully attempted. However, most of the models cannot be solved analytically. We have detected that the students of the fourth and fifth year have great difficulty solving these models numerically even when they have studied them in lectures. Therefore, to address this lack of ability a numerical method is selected.

As recommended in MATLAB help, 'ode45' is the best function to apply as a 'first try' for most problems. This method is based on an explicit Runge-Kutta 4,5-formula, the Dormand-Prince pair [9]. The MATLAB commands are as follows where all variables can be easily identified comparing to Equation 1.

```
[t,Ts] = ode45(@fbath,[t0
  tf],[Ts0],[],p,Qr);
fbath.m
function dTsdt = fbath(t,Ts,p,Qr)
dTsdt = (60/(Ms*Cps))*(Qr-m_aire*
  Cpa*(Ta-Ta0));
```

SIMULINK model and user interface

Modular programming gives the possibility of dividing the problem into pieces for better understanding. Our system has been divided into two main blocks. The first block is the heat balance; the second block is an additional control box for the power. Figure 5 shows the graphical user-interface; manual or automatic control can be selected by manual switching. Figure 6 shows the heat balance; all the heat contributions are separated in functions. The insides of the controller are revealed in Fig. 7; power is the manipulated variable while solid temperature is the setpoint.

During the practice preparation students should understand and use this model to predict the

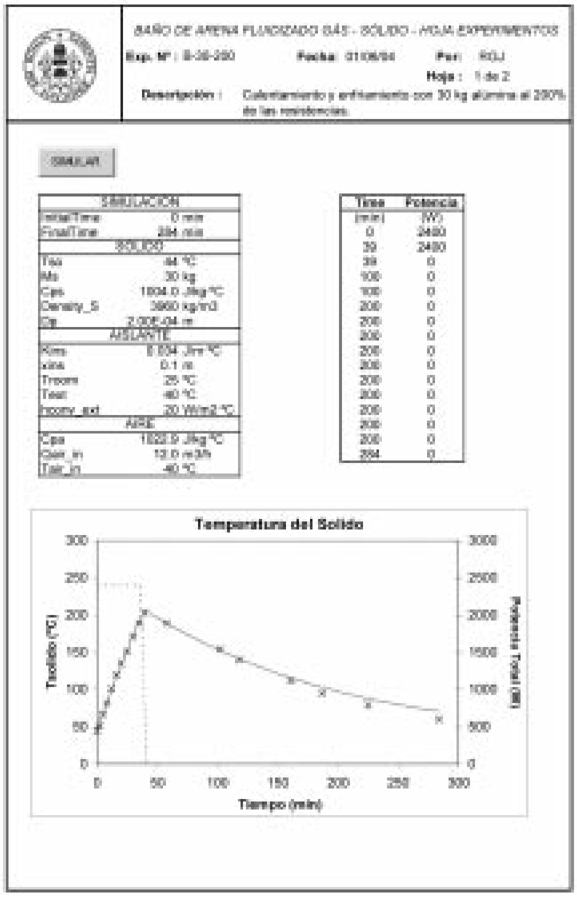

Fig. 8. Excel interface for bath.mdl.

behaviour of the system. The model will be given unfinished to force them to find the errors or improve actual simulation.

Excel interface: preparing data sheets

The use of datasheets to present lots of data is widespread nowadays, specially in laboratory data. So, an Excel friendly-interface (see Fig. 8) was developed in order to simplify data collecting and results presentation; the current Spanish version is presented. This was achieved using an add-in, the MATLAB Excel link. The simulating data sheet is divided into: simulation parameters, physical properties, experimental data, instant power and results.

TEAMWORK, COMBINING SKILLS

The project began in February 2003 from a heating solution given in our research group (High Pressure Processes Group, University of Valladolid). The lack of fluidisation experiments in our laboratory and experience of working with solids had to be addressed. Therefore, the topic was proposed as a basic design to 8–10 students working in pairs during laboratory practices. They made a report with all the gathered information, calculations, flow diagrams and technical specifications. The interest and enthusiasm of some students for the system caught our attention, which lead to the proposal that students could themselves design, construct and operate a pilot scale plant.

From the outset, responsibilities were delegated amongst the project group. The project group was formed by a manager (professor), process leader (assistant lecturer and chemical engineer), technician, two students and a control consultant (chemical engineer, actual job control engineer). We have taught each other a great deal during these months. Some solutions to the real problems are compiled below; they show how extremely important the relation between staff and students is to improve Academia.

- *Problem 1:* Lack of knowledge of fluidisation in gas-solid systems, no equations at all to calculate air requirements. There is nothing an engineer can do if he/she does not have the proper previously-measured equations. Our technician built in only one hour two mini-scale baths with a PET bottle, cotton wool as filter and an old fan. The scale-up calculations were then trivial.
- *Problem 2:* temperature is not controlled properly by the automatic controller and the PID tuning was not successful. The control engineer suggested that our system should have a very different dynamic response for heating up and cooling down. It is a special case and a typical PID real controller cannot overcome this problem. At that point we tried to model the system in order to change the power manually during the experiment to equilibrate the dynamic properties. Now the system works!
- *Improvement:* how often is required to measure the temperature? Each heat experiment takes about four hours, therefore measuring each five minutes we will have eighty data points per experiment manually written down by the students. Should the students focus their attention in reading temperatures or should they have time to think about what is going on? In this way, the next attempt is to install an automatic data acquisition system into Excel.

The students used all their engineering knowledge and made all the calculations, placed orders and even built the apparatus with the technician. The working group is presented in Fig. 9 in one of the meetings during the project.

CONCLUSION

A new laboratory pilot plant for third-year students in chemical engineering has been developed. The lack of fluidisation experiments in our laboratory and experience of working with solids has been addressed. The experiment combines some of the main subjects in chemical engineering, i.e. fluid flow, heat transfer and process control.

Fig. 9. The working group in Maria Jose's office. From the left, Eduardo, Rebeca, Juan and Alvaro.

Practical knowledge links teaching and learning in an easy way. Thus, in this experiment, process control is introduced to the students without been studied previously, but they did not have any problem. A dynamic model for a fluidised sand bath heater has been validated and tested. The model equations have been solved numerically using MATLAB and Simulink. Therefore, at the end of the experiment the students should be able to solve model equations numerically.

The combination of the interest and enthusiasm of the team and the partner-to-partner collaboration made the project real. Sometimes it was the only reward for lecturers, technicians and students who suffer the lack of means, support and institutional greetings.

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