World Transactions on Engineering and Technology Education
Vol.4, No.2, 2005

Experiential engineering e-learning: the concept of *soft reaction*

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ABSTRACT: Advances in computers and information technology have meant ever-increasing ease of computation and data transfer. Engineering education is set to reap large benefits from the integration of these technological advances. Many academic institutions have already capitalised on the use of the Internet to deliver courses to students in remote locations, thus redefining the boundaries of education instruction. Because engineering is a practical subject, the big challenge facing engineering educators is how to deliver distance engineering education without compromising the practical components. In this article, a solution to this problem is described with the presentation of a *Web plant*, consisting of a hybrid between a real plant and a simulated one. The real plant is a flexible multi-purpose facility that is interfaced to advanced modelling software simulating many types of reactions. The real and simulated parts of the Web facility interact and exchange data seamlessly, and this data is, in turn, available to students locally in the laboratory via the control system or remotely via the Internet. The concept of *soft reaction* is defined where reaction process models and kinetic data are used allowing students to investigate various reaction systems, including chemical and biological ones.

INTRODUCTION

The face of tertiary education is a constantly changing environment where learning outcomes are being regularly assessed with a view to meeting current demands. Advances in information technology have seen the ever-increasing electronic delivery of course materials through Web-based systems (eg *WebCT*, *Blackboard*) and CD-ROM programs. For instance, Process system engineering courses can profit most from these technologies because of their unique features inherent in their theoretical discussion and practical investigations [1]. The Internet or World Wide Web (WWW) has played a major role in the development of these tools and has opened education to distant areas and to people who did not have access to these resources in the past. With today's accelerated improvement of the WWW and visualisation technologies, many different educational courses can benefit and decrease their deficiencies in the delivery of conventional lecture and laboratory courses [2]. However, the challenge is to be able to deliver programmes that meet strict learning outcomes and which can be readily assessed. This challenge is even more defying when considering online experiential learning for outcomes associated with laboratory engineering education. It is not a trivial task to provide online tuition to educate engineers about process behaviours. The virtual laboratory is emerging as a new concept where students can perform virtual online experiments or operate virtual online plants as part of their degree programme [3-5].

One of the salient features of engineering education is the combination of theoretical knowledge with practical experience. In conventional education, theoretical knowledge consists of lectures, exercises, lectures notes and textbooks. Practical experience utilises highly resource-demanding laboratory courses. Within this context, the availability of funding and, consequently, the availability of laboratory facilities and staff present restrictions to student enrolments. Experiential active problem solving and visual feedback on the part of students can provide valuable insights into engineering systems dynamics. For this reason, students need to be in the laboratory to gain invaluable hands-on-experience. Developments in information technology have opened new opportunities for students to take advantage of a remote laboratory, where a multimedia interface together with a collaboration tool, gives them the feeling of being in the laboratory.

Process simulation is a core component in any engineering degree. The advent and rapid growth of digital computers has revolutionised and broadened the use of dynamic simulation. It is now possible to develop and validate mathematical models for very complex industrial processes using the latest commercial software. These simulations can then be used to develop and test advanced operational strategies, which can then be implemented into real plants. Moreover, a simulated experiment offers an edge of moving beyond the realms of real hardware with the following benefits:

- *Providing more laboratory facilities to be experienced by students*: By increasing the number of experiments in order to enhance the understanding of chemical process unit operations, students can investigate experimental conditions that cannot be investigated in real plants due to safety and cost concerns.
- *Eliminating all types of hazards by modelling dangerous experiments*: By modelling dangerous experiments, students can conduct dangerous operations previously not possible or only possible after strict training.
- *Decreasing cost by modelling of expensive equipment*: Chemical engineering laboratories are very expensive to set-up and have high running costs. By modelling these kinds of facilities, students can perform numerous experimental runs without worrying about the associated costs.

- *Increasing number of simultaneous users*: When coupled to the Internet, there is no limit with respect to the number of users of the virtual laboratory [6].

The WWW provides significant new functionality in transmitting information to students and provides an effective mechanism for integrating tools into a single user interface. The integration of multimedia elements has significantly enhanced the ability to train and educate electronically. Virtual education explores a new way of teaching and learning that, instead of restricting itself only to enrolled students, addresses a larger audience. Therefore, it can be used for advanced training.

Consequently, an alternative less resource-demanding approach to engineering education is to combine the real laboratory with a simulated one. This may be realised by simulating real-world systems and animating experiments in a highly interactive environment. Such a virtual laboratory, with additional distance education in the form of courses offered across the Web, can fully engage students in the learning process through an interactive and dynamic environment.

THE WEB PLANT

The development of an experimental system to provide a flexible environment that can deliver both practical experience and Web-based learning modules to students was undertaken in the Department of Chemical Engineering at the University of Sydney, Sydney, Australia. This Web plant (WP) system was designed to exploit advances in information technology and seamless connectivity between plant equipment and process modelling software. A schematic of the main components in this Web-based laboratory facility is shown in Figure 1. The WP system was commissioned as a flexible experimental pilot scale plant to support education and research, and to provide a platform from which technological advancements in data management and communication may be exploited. In this role, the WP can directly support learning outcomes in the practical modules in all years of the undergraduate degree, as well as in postgraduate research and training. Further, it will provide the tools for developing Web accessible experiment-based courses for long distance learning and vocational training.

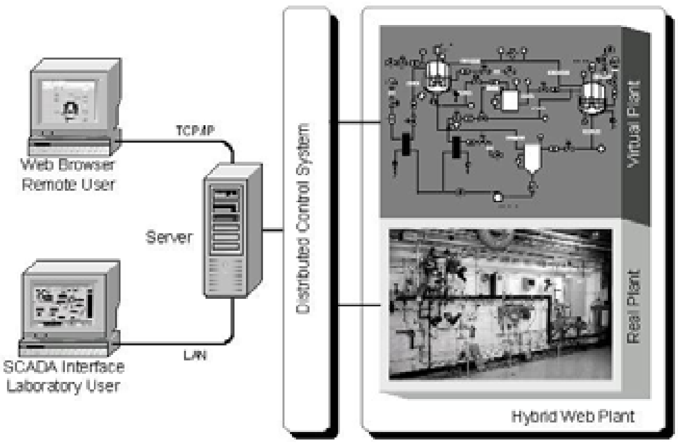

Figure 1: Components of the hybrid Web-based facility.

The WP hardware consists of two stirred reactors in series with an inline mixer, feed heat exchangers and a feed tank. Central utilities provide both cooling water and steam to the plant. The systems flexibility means that the experiment may be configured to operate in a number of modes including: as two stirred reactors in series; as two stirred reactors in series with second feed to reactor 2; and as two independent single reactor systems. Figure 2 shows the plant layout in the laboratory, while Figure 3 shows the process and instrumentation diagram (P&ID). The process involves the pumping of water in a closed circuit. Steam and cooling water are used to provide, respectively, heating and cooling to both reactor feed lines and reactor jackets. Plant information is collected from a range of sensors, including liquid levels, process flows, temperatures, agitation speed and the status of other digital devices. Water is the only chemical ever used in the plant, mainly for safety considerations. Other chemical components are introduced by a simulation described below.

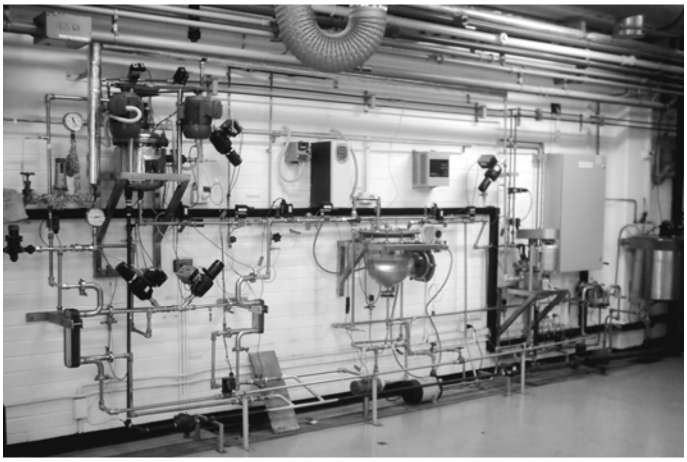

Figure 2: The Web plant.

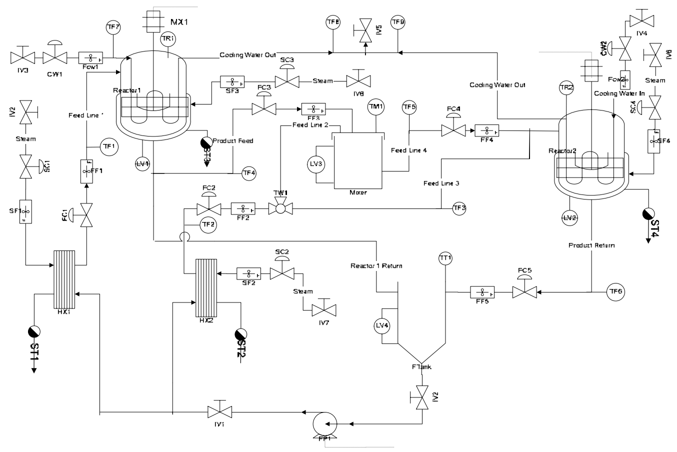

Figure 3: P&ID of the WP.

This unique facility combines both industrial plant equipment and advanced simulation to deliver a set of experimental-based learning modules that may be completed by students from local control stations or over the Internet using a standard Web browser. The simulation component is designed to model a process or reaction and interact with the real plant data, such as liquid flows, temperatures and vessel levels. There is a library of pre-built virtual reactions from which a student can select to investigate.

The concept of *soft reaction* is introduced here to describe these virtual reactions that could include chemical and biological reactions, among others. Models and kinetic data for these soft reactions have been built using advanced modelling packages, including *Matlab* (Mathworks), *gPROMS* (Process Systems Enterprise) and *Concept* (Schneider). Each soft reaction generates additional simulated plant information that is synchronised with, and calculated based on, actual real-time plant data. After choosing the reaction system to be investigated, students are able perturb the process into a range of scenarios.

Human machine interfaces (HMI) have been developed as part of this program to provide students access to the WP – both locally in the laboratory or control room using an interface the same as can be found in commercial systems used by industry, and remotely over the Internet. The local interface is a commercial and widely used product that has the added advantage of exposing students to current industrial technology. Students can interact with the process through the SCADA interface (Figure 4) if they are working in the laboratory or are connected to the local area network (LAN). If they are at a remote location, students can log on using a standard Web browser (Figure 5) to invoke plant changes. It is also possible to access real-time data and monitor this using trend displays via the LAN (Figures 6) and via the Web (Figure 7), or extract data out to other applications for further visualisation and analysis. The network interface was developed in-house, using java applets as the communication engine. This interface opens the way for delivering learning modules over the Internet. In addition to the real measurements, the simulation component can also extend beyond the limits of real instrumentations, providing inferred information like reactant conversion, viscosity, density, product concentration and heat of reaction.

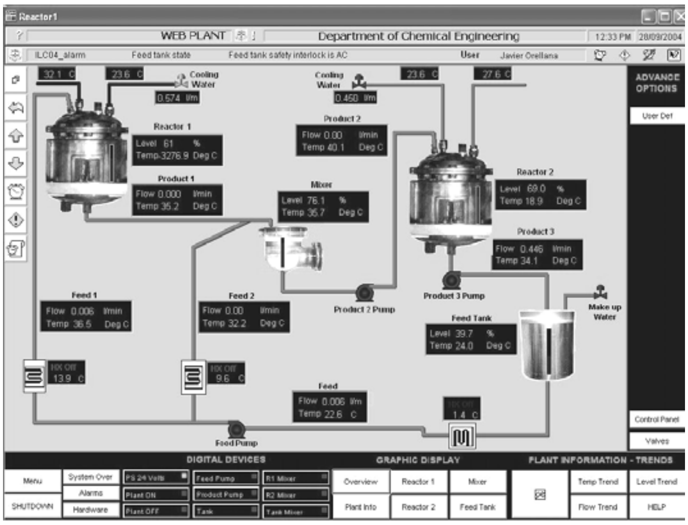

Figure 4: LAN SCADA interface showing the overall plant.

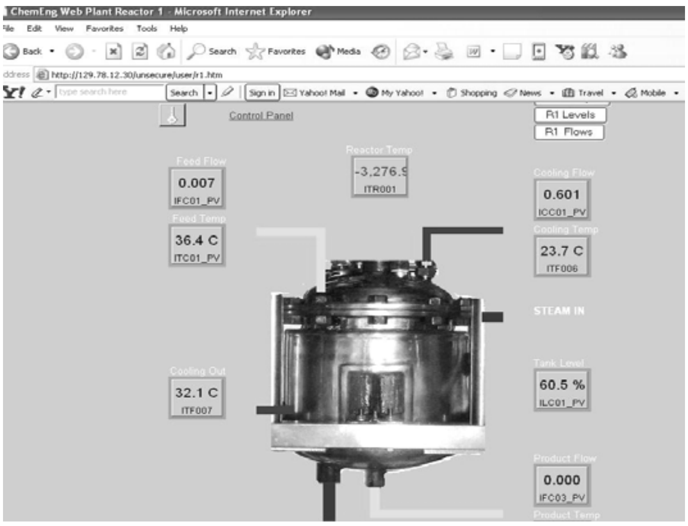

Figure 5: Remote Web browser view of the CSTR.

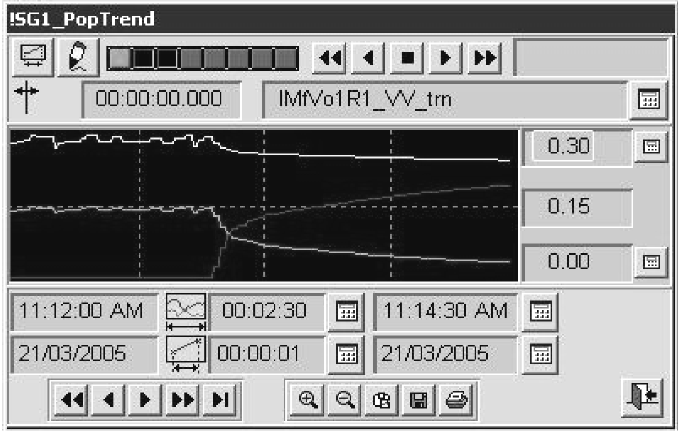

Figure 6: Trend display via the LAN.

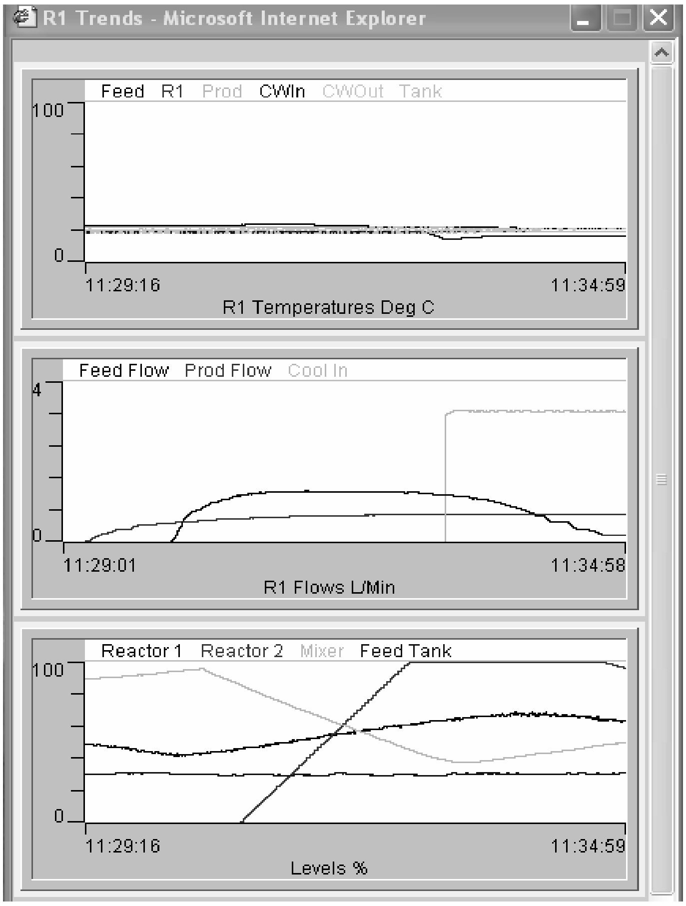

Figure 7: Trend displays via the Web.

SOFT REACTION CASE STUDY

Process modelling is used to provide a set of reactions that interact with real plant data, giving the impression that the reaction is occurring in the experimental rig. Since water is the only substance used in the WP, a series of mechanisms had to be devised to provide information to the control system of the *virtual* process phenomena occurring in the process system according to the concept of *soft reactions*. In this context, the WP has been set up as a true hybrid experimental laboratory facility, where real-time hardware-related process data from the control system is merged seamlessly with extended software-based data emerging from the soft-reaction simulation.

The general approach is now explored by means of the case-study of a saponification reaction already implemented in the WP and incorporated into a 1st year engineering subject. In this course, students are expected to familiarise themselves with the fundamentals of chemical engineering science by tackling the optimisation of a soap-making production facility from a holistic approach. First, students explore the behaviour of the reactions of saponification occurring within a CSTR in a simulation enviro-nment implemented in *Simulink*. Figure 8 is a screenshot of the simulation interface showing the main window (left) where manipulations can be made and trends (right) to monitor reagent consumption, reaction conversion rate and product concentration.

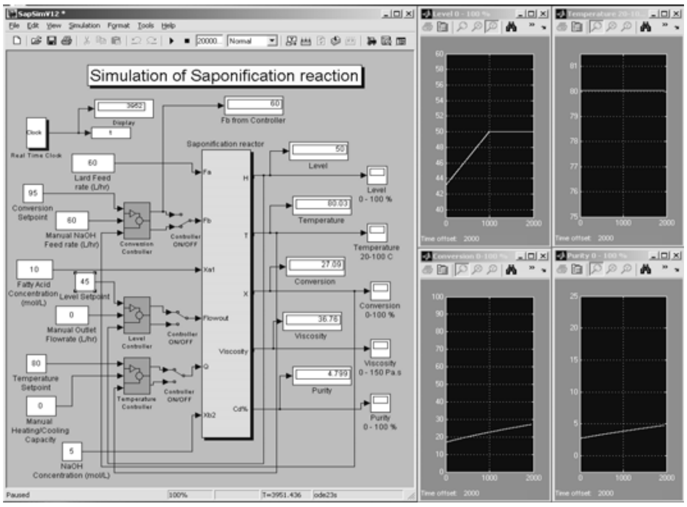

Figure 8: The simulation interface.

Once students have increased their understanding of the phenomenological behaviour of this reaction system and realised the potential for improving the operating conditions, they are introduced to the WP. Not only do they become acquainted with hardware and software systems supporting modern manufacturing processes, experience the sounds and visualise the physical and chemical changes associated to industrial manufacturing plants, but they are also prevented from the hazards associated with reagents according to the benefits intrinsic to the concept of *soft reactions*. Since an Internet camera is available for students to visually monitor the process, the WP can also support the remote or long distance education of experimental courses and modules via the Internet.

The concept of soft reaction is illustrated in concordance to the aforementioned case study. Consider a general mass balance (Equation 1) and associated constitutive/fundamental relations (Equation 2) in one of the two CSTRs:

$$\frac{1}{\breve{V}} A \frac{dh}{dt} - \frac{V}{\breve{V}^2} \frac{d\breve{V}}{dt} = \frac{1}{\breve{V}^0} \cdot \dot{V}^0 - \frac{1}{\breve{V}} \cdot \dot{V} \qquad (1)$$

$$\breve{V} = f(T, P, x) \approx \sum x_i \cdot \breve{V}_{0,i}(T) \qquad (2)$$

In the equations above, h denotes the height of liquid in the CSTR (state variable), $\breve{V}$ indicates the specific volume of the process fluid, and $\dot{V}$ denotes the volumetric flow-rates. The individual mass-fraction compositions are given by x_i (state variables), $\breve{V}_0$ denotes the specific volume of the pure components, and T is the mixture temperature (state variable); the superscript *0* is used to denote inlet conditions. Nothing is lost nothing and simplicity of analysis gained if the second differential term on the LHS of Equation (1) is ignored. Naturally, the plausibility of this simplification depends on the system under study.

With the availability of abundant process instrumentation as is the case of the WP, the magnitude of the process variables h, $\dot{V}^0$ and $\dot{V}$ and T would be available from the control system. On the contrary, information on $\breve{V}^0$ and $\breve{V}$ would not be readily available, not only due to the lack of appropriate instrumentation, but also because the value of these process variables does not correspond to any physical phenomena occurring in the process system. Despite this, by combining Equation 2 and real-time plant data, it is possible to calculate the unknown and *virtual* specific volume of the reaction mixture at the inlet $\breve{V}^0$ and outlet conditions $\breve{V}$.

Extending this approach, for example, to the calculation of the viscosity of the reaction mixture (a constitutive relationship used very frequently as an experimental measure of the degree of saponification), increased knowledge of the status of the soft-reaction process system can be obtained. Consider a particular mass balance in one CSTR:

$$x_i \frac{1}{\breve{V}} A \frac{dh}{dt} - \frac{V}{\breve{V}} \frac{dx_i}{dt} = \frac{1}{\breve{V}^0} \cdot \dot{V}^0 \cdot x_i^0 - \frac{1}{\breve{V}} \cdot \dot{V} \cdot x_i + R_i \qquad (3)$$

Combining Equations 1 to 3 and assuming x_i^0 or, more conveniently, obtaining x_0 from calculations of other process equipment within the process system, it is possible to calculate the vector of compositions x_i in the reaction mixture. From this information, the conversion of the saponification reactions, for instance, can easily be obtained.

Interestingly, an appropriate combination of Equations (1) and (2) and plant data also clarifies some advanced process-engineering concepts. Indeed, by determining unmeasured process variables or calculating redundant process information (eg the magnitude of the state variable h) from additional mechanistic relationships, it is possible to illustrate to students the ideas behind soft-sensing and inferential control, or explore the theory and practice of data reconciliation in advanced senior courses. However, in junior courses, one would be more interested in supporting the learning process by exploring experimentally diverse process phenomena, particularly concepts related to mass and heat transfer and reaction engineering, as explained above.

From the perspective of the implementation of the proposed approach into the WP, the three following main considerations were kept in mind:

- Robustness of the application;
- Robustness of data communication;
- Seamless interconnectivity among software components.

Needless to say, all inherent complications to these three matters can be lessened or avoided by a suitable choice of the modelling environment. Although other alternatives are currently being explored, *Concept* has been chosen for implementation purposes. *Concept* is an environment for high-level block-oriented PLC-language programming. The resulting instructions are embedded into, and processed within, the controller CPU. An immediate consequence of this is that there are no issues associated with the robustness of the numerical solution since, in the worse-case scenario, the simulation would drift from physically meaningful values, but would not fail numerically. A simple re-initialisation of the hybrid simulation would be sufficient to tackle this inconvenience. Additionally, process data is readily available at the controller CPU level and, hence, there are no communication issues related to making process data available to a software application external to the PLC control system.

Each process modelling component (unit operations, chemical reactions, physical properties, etc) is distributed in different re-usable and customisable derived function blocks (DFBs). These DFBs (integro-differential-algebraic expressions) are built by making use of *Concept*'s primitive function blocks, according to the simple observation that these expressions can be represented by binary operators corresponding to the five basic operations of arithmetic, and unary operators corresponding to the transcendental functions of a single variable. With this approach, the idea of hierarchical sub-model decomposition can easily be exploited to maximise the interconnectivity among software components. Material, energy and information data is transferred between components by connections, variable references and switches that define what elementary blocks are enabled, and how process and simulated data flows between them.

The implementation of the general mass balance (Equation 1) in the control system, according to the ideas above, is shown in Figure 9. A number of DIVision, INTegration, SUBstraction, MULtiplication and ADDition blocks perform mathematical operations between measured process variables (IFC01_PV, volumetric flow-rate at the inlet of reactor #1; IFC03_PV, outlet flow-rate; ILV001, liquid level) and PLC system variables (eg IVsPi_R1_CV, calculated specific volume of the process fluid at the inlet of reactor #1; IMrPo_R1_CV, calculated outlet mass rate; IMqPh_R1_IH, calculated mass hold-up of liquid).

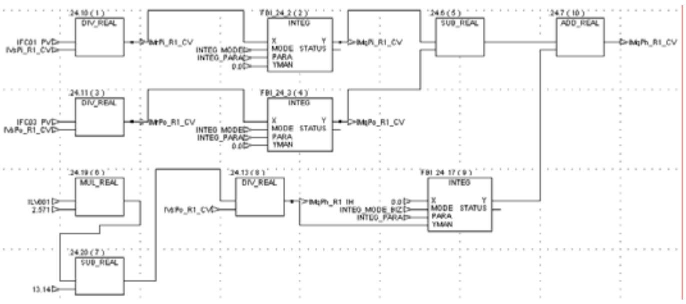

Figure 9: Snapshot showing the implementation of the mass balance in the control system.

Due to the sequential processing nature of elementary instructions of the controller CPU, plus the intrinsically simultaneous nature of the fundamental laws of conservation, special attention had to be devoted to the development of a tailored initialisation procedure. For this purpose, a series of switches are also used to initialise the hybrid simulation from user-defined values (eg the initial concentration of reactants in the system) and process-related magnitudes (eg the measured hold-up of liquid in the CSTRs).

Most of the *virtual* information generated by the *soft-reaction* hybrid simulation, which is useful from the perspective of experiential education, is conveyed to the user by HMIs. When the hybrid process data is presented to students via these HMIs, the distinction between *virtual* and *real* information on the behaviour of the reaction system is irrelevant to the user. However, it must be stressed that this extended software-based information of output and state process variables was obtained exclusively by implementing *soft-reactions* in a state-of-the-art fully instrumented WP laboratory facility running continuously with a safe and inexpensive process fluid (water).

CONCLUSION

This hybrid facility provides students with a dynamic and interactive learning environment and a positive experience with enhanced learning for high achieving students through extension programmes. Key features of the pilot WP are:

- Multi-functional equipment: Pilot scale plant can be physically configured to operate in a number of modes;
- Flexible learning environment: Simulated reaction modules can be selected to study reaction engineering, process modelling, energy and momentum conservation, heat and mass transfer, process optimisation, and process control under various plant conditions;
- Industrial environment: Students are exposed to industrial training where key elements of plant dynamics, control and operation are learned using standard industrial equipment;
- Web-based access: Expanded teaching programmes include long distance learning with practical modules;
- Vocational training: Learning modules as accredited industrial courses can be mixed as part of an MES programme.

A key challenge remains increasing the level of interaction between the remote student and the physical plant. This can be achieved by establishing clever learning modules to deliver learning outcomes based on the experimental facility, and by extending the modelling to simulate faults and conditions in the equipment, such as the presence of a sticky valve. Another important challenge is to develop modules that are aligned with the leaning outcomes at different levels of the degree programme, thus optimising and enhancing learning. This requires the exploitation of such a facility to its fullest. As a developing research area, distance experiential education can facilitate the learning of practical engineering education components in an economic, safe, flexible and multi-user environment.

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