

An expert system for a semi-batch pilot scale emulsion copolymerisation facility

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Abstract

A knowledge-based system (KBS) has been developed for a semi-batch pilot scale emulsion copolymerisation reactor facility. A simulation model was developed for the feed of styrene and MMA monomers as well as surfactant and initiator to control the particle size distribution (PSD) and molecular weight distribution (MWD) over the entire monomer conversion.

The expert system architecture provides continuous support and rectification of product off-specs, monitoring and maintaining safety functionality, as well as retaining process continuity. Process events such as the particle growth and secondary nucleation could be picked up by the rule-based expert system.

The knowledge-based system is built under multiple layers of a proposed supervisory architecture. This expert system was built using G2TM (Gensym Corp). The expert system provides diagnostic and decision support to the operator. The diagnostic module triggers alarm and send message queues whenever a process upset occurs. The decision support system (DSS) incorporates several features such as intelligent polymer recipe input interface to pre-select optimal pump controls.

The expert system was put to test on the actual facility and has been aiding the operator running the facility.

Keywords: Knowledge-based Systems, Supervisory Control, Emulsion Copolymerisation, Fault Diagnostic System

1. Introduction

Knowledge-based systems (KBS) or commonly known as expert systems are computer systems that assist the operator in making critical decisions under various operational scenarios with the capabilities of emulating the process behaviour based on knowledge of process characteristics. The KBS usually consists of a knowledge base, decision rules, and an inference engine. The knowledge base is comprised of facts pertaining to a specific process, while the decision rules are typically of the IF/THEN conditional statements.

Hopgood [1] states “Rules are an elegant, expressive, straightforward and flexible means of expressing knowledge” and in knowledge representation, Moore [2] pointed out that experts used their knowledge of plant structure, knowing how the connected process units affect each other. It is thus useful to use graphical form of knowledge representation, so experts can define the plant structure and interactions by connecting objects on a computer workstation. KBS development software such as G2 is designed to permit the process engineer to define the knowledge in natural forms with the capability of symbolic processing.

In this paper, the application of G2 is focused on a lab-scale semi-batch pilot scale emulsion copolymerisation facility. Supervision of an emulsion copolymerisation process is needed specifically for monitoring and control of monomer conversion as it is crucial both for proper process operation so as to aid the downstream separation, and for obtaining products with desired properties due to the influence of conversion on polymer molecular weight and particle size distributions [3]. Not only this, the decision support system (DSS) can easily be implemented by G2 and any other features to aid the operator.

2. Experiment

The laboratory setup of this facility consists of a 5 litre jacketed stirred reactor; a Julabo heating circulator provides heating/cooling water through the external jacket; 4 Prominent dosing pumps to introduce feed of the two monomers, surfactant and initiator; 3 RTDs for temperature monitoring; and 4 precision balances to determine the quantities of reactants used. Data acquisition is achieved via Honeywell’s PlantScape DCS. On-line control of process equipments can be done on the graphical-user-interface (GUI) which is developed on Honeywell’s system (see Figure 1). A schematic diagram of the reactor system built using G2’s Dynamic Display utility is shown in Figure 2. Semi-batch emulsion copolymerisation of styrene (99% purity) and MMA (99% purity) were carried out at 70, 75, 80 and 85°C under slight nitrogen pressure.

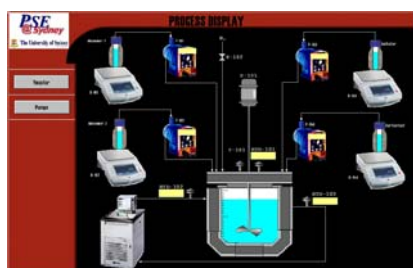


Figure 1. GUI in Honeywell DCS.

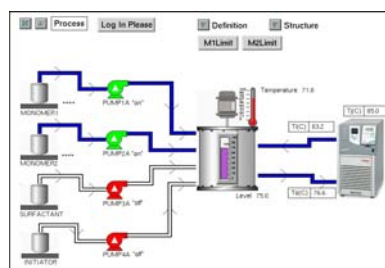


Figure 2. Process monitoring in G2.

3. Architecture of the supervisory KBS

The supervisory KBS is designed to embody expertise in a particular domain. It usually has two components; the knowledge module is called the knowledge base while the

control module is called the inference engine. The explicit separation of knowledge from control makes it easier to add new knowledge either during program development or in the light of experience during the program's lifetime, [1].

The proposed architecture or expert system shell is divided into four different domains, namely the operator/user domain, the expert supervisor domain, the simulation/processing domain and lastly the plant/action domain.

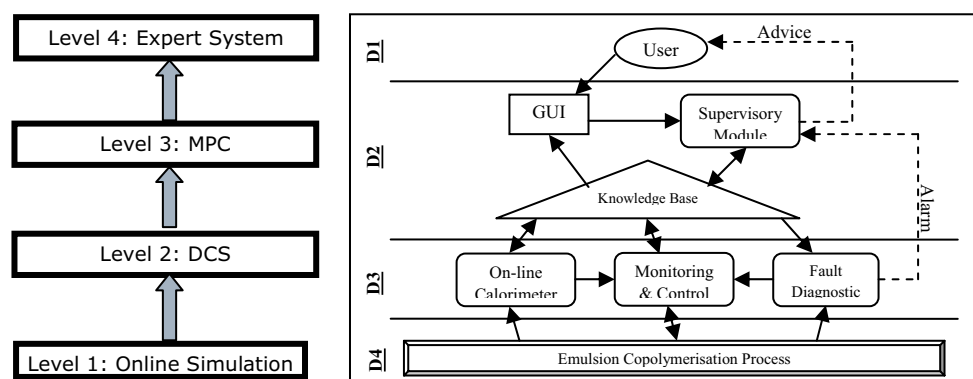


Figure 3. Scheme of the supervisory architecture.

- The operator domain comprises of a DCS workstation manned by the user which allows human intervention of the process. Advices, notifications and alarms can be read and acknowledged by the user.
- In the expert supervisor domain, the supervisory module acts as a manager of the distributed knowledge base as well as managing prioritised alarms if multiple errors appear. The artificial intelligence (AI) comes solely from the developer, who imparts the extensive knowledge and rules into the KB.
- For the simulation domain, the on-line calorimeter provides inferential conversion monitoring and control through calorimetric measurements of reaction temperature. An on-line diagnostic module is also added for processing detected faults, and to provide corrective control action to the plant.

4. Software

Four commercially available software have been utilised for the implementation of the architecture. These are outlined in this section.

gPROMS (Process Systems Enterprise, UK): For numerical simulation purposes, the sets of differential mass and energy balances, the kinetic equations and the population balance equation were solved using gPROMS.

Excel VBA (Microsoft Corporation, USA): MS-Excel was used extensively throughout the development of this KBS. The programming language was used to develop the communication bridge between G2 and the physical reactor. G2 utilises a tool called

“ActiveXLink” and is compliant with any Microsoft Windows based programs. Example of VB code fragments used in this application include:

Read data: **G2Gateway1.Call** (“*procedure-name*”, *arguments*);

Write data: **G2Gateway1_RpcStarted** (By Val *Name* As String, *InArgs* As Variant)

PlantScape r500 (Honeywell Corporation): The uploading and configuration of the control schemes to the controller is done using the software called Control Builder™. Control Builder allows analogue inputs of plant instruments for a series of conventional PID control over the plant.

G2 (Gensym Corporation, USA): This real-time expert system development tool uses several different knowledge representations: rules, object-oriented platform, connection stubs. These entities has classes and workspaces assigned, allowing the developer to define the knowledge in natural forms.

An example of how our metering pump (Prominent gamma/L) is defined in G2 is illustrated in Figure 4.



Figure 4. A workspace showing a pump definition.

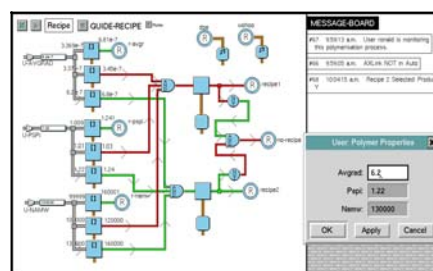


Figure 5. Screenshot of user interface for recipe selection

5. Features/Improvements

In order to allow the knowledge base to respond to various conditions, rules are used and they can be easily defined in plain text format. Rules describe knowledge in a manner that allows the KB to draw conclusions from existing knowledge, to react to certain kinds of events, and to monitor the passage of time. A total of 23 rules were by date updated into the KBS. Example of a rule used to investigate “secondary nucleation” by referencing historical data with present data is as follows:

whenever the conversion of soft-sensor receives a value and when the conversion of soft-sensor > 0.5 and the rate of change per minute of the polydispersity of soft-sensor during the last 15 seconds > 0 and the rate of change per minute of the

particle-number of soft-sensor during the last 15 seconds > 0 then post for the next 5 seconds "Secondary Nucleation".

In this paper, several added features were also presented. An automatic software launcher was developed in G2 which eliminates the complicated startup an operator has to face before running the experiment.

One of the key features that were developed would be the recipe scheduler. It was built based upon the graphical language component in G2 known as the G2 Diagnostic Assistant (GDA) tool. As with the above mentioned software launcher, this feature automates the task of selecting the optimal feed profile in Control Builder. The user/customer only needs to enter his/her preferred polymer properties press enter and the recipe formula would be selected accordingly to the matched logic structure developed in GDA. Figure 5 shows a screenshot of the user interface along with the structure of our feed recipe formula.

An experimental results logger was also implemented via GDA. An interface allows the user to key in a filename which will automatically record all process events and major alarm messages in a text format.

6. Results and Observations

The most obvious use for GDA would be the diagnostic support that would be utilised for early fault detection and perform corrective measures. Pre-analyses problems were targeted to test-run this prototype, which includes detection in pump flow deviations, pump/pipe blockages, product off-specs due to rate of reaction and abnormal reaction temperature and early detection of monomer feed run-out. An alarm panel appears when a process upset occurred.

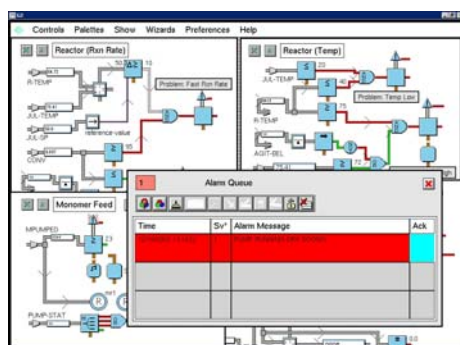


Figure 6. Screenshot of GDA structure and the alarm for "pump running dry".

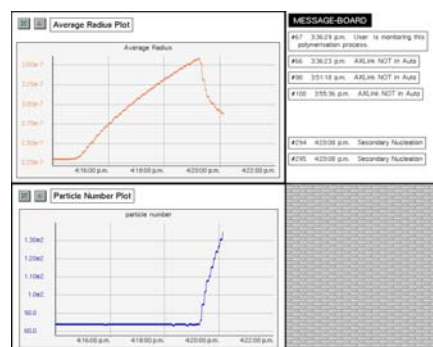


Figure 7. Screenshot of "Secondary Nucleation"

Example of a common fault that was purposely created is preventing the pumps from running dry. The user inputs in the amount of feed used, GDA will calculate the safe

level to be left in the feed bottle and when the safe level has been breached, GDA alarms and automatically shuts the pump. Figure 6 shows the pop-up of the alarm panel for this event.

To validate the above mentioned rule, 2 trend plots showed that the rule can be constructed to correctly identify “secondary nucleation”. Figure 7 clearly shows that at approximately 4.20pm, the rule initiates the message which coincides with the decrease in the particle size and the number of particle increases. The validation of optimal trajectories carried out with experimental runs is stated in literature, [4].

7. Discussions and Conclusion

A particle size distribution analyser (Polymer Laboratories) has recently been installed for the primary purpose of measuring PSD of samples from the batch. On-going research has been undertaken to enable online measurement during the batch process. A detailed (validated) mechanistic model has been developed to calculate set-point trajectories to ensure the production of a copolymer with a defined PSD [4]. In G2, an interface has been created to allow manual inputs of sampled PSD. This operator value will be validated with the current simulation, which will provide the eventual knowledge for rule generation and thus providing a more robust supervisory module when the analyser becomes online.

We tested this expert system and it has periodically been running for some experiments. The system gets periodic data and performs diagnostic support with no trouble. Recipe selection allows the GDA structure to target the Control Builder feed profile with exact precision. If a profile could not be matched, an online working model would be generated to find a new optimal profile/recipe for the user. This of course, would be included in our future work. Overall, this expert system maintains a continuous automated process, from the initial pre-run check, the less complicated software startup, the recipe selection step, the monitoring of secondary nucleation and particle growth events, the fault detection and corrective measures, to the eventual online sampling of PSD with G2 in an all-in-one package.

8. References

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