Pergamon

Computers chem. Engng Vol. 19, Suppl., pp. S571–S576, 1995
Elsevier Science Ltd. Printed in Great Britain
0098-1354(95)00121-2

MODELLING AND SIMULATION OF THE OPERATION OF AN INDUSTRIAL BATCH PLANT USING *gPROMS*

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ABSTRACT

The complex operating sequences of integrated batch plants involve many discrete operations. This renders their simulation using current process modelling tools.particularly difficult. The *gPROMS* (generalised PRocess Modelling System) package is an equation oriented modelling tool for combined discrete and continuous processes, which makes it particularly suitable for the modelling and simulation of batch plant operations. This paper summarises the results of a project in which *gPROMS* was evaluated using a realistic industrial case study. The simulated process consists of a series of batch operations carried out in sequence in a plant comprising three reactors, one buffer tank, and two distillation units. Utilities include steam, hot and cold water and a flue gas vent. Each unit operates according to a precise schedule. Our objective was to simulate the exact load on the utilities during a typical production cycle (about 50 hours from raw materials to products). *gPROMS* was also used to carry out parametric studies on the effect of equipment size on plant performance. Finally, we analyse the performance of *gPROMS* in an industrial environment and judge its potential for further widespread industrial applications.

KEYWORDS

Dynamic simulation; batch processes; discrete event simulation; equation-oriented simulation.

INTRODUCTION

Traditionally simulation systems have been classified as either discrete event or continuous. The simulation of systems which belong to either category has a long history which dates back to the 1950's. However systems where both continuous and discrete changes take place and interact to a significant extent are not uncommon in chemical engineering applications such as multistage batch plants and continuous plants undergoing shut-down and start-up. For many years, the direct analysis of this type of problems was considered marginal and their behaviour was usually abstracted until it conformed strictly to one of the two main categories.

General purpose dynamic simulators (Marquardt, 1991) have found wide application in the process industry. These packages often have sophisticated languages and formalisms for model development that allow the description of complex differential/algebraic models. However the complete dynamic modelling of batch operations is more complicated because of the need to model not only the physical behaviour of individual units, but also the complex sets of discrete control actions imposed onto them and the logic which co-ordinates their actions . For these reasons, special packages have been designed for batch process simulation (Joglekar and Reklaitis, 1984), but their flexibility in supporting model development is often limited, especially in comparison with the facilities made available by equivalent packages for continuous processes. The necessity of integrating these two separate areas of simulation led to the development of *gPROMS* (Barton, 1991; Barton and Pantelides, 1994). In *gPROMS*, the process is described in terms of both the physico-chemical behaviour of the plant (the MODELs) and the external actions imposed on it (the TASKs). Mechanisms are provided to enable these two types of entity to interact.

PLANT DESCRIPTION AND AIM OF SIMULATION

We decided to carry out an evaluation of *gPROMS* using a realistic case study from industrial practice. The process consists of a sequence of batch operations. The plant comprises three reactors (R1, R2 and R5), two distillation vessels (R3 and R4), and a buffer tank (BU), as shown in Fig. 1. Each unit operates according to a specific schedule. At the end of the cycle of each unit, the hold-up is

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discharged to the next unit for further processing. Each unit is immediately utilised as soon as it is available.

Cooling and heating are provided by cold (25 ^{o}C) and hot (70 ^{o}C) water and saturated steam (1.2 bar). Before discharging a reactor's hold-up, the gas cap is flushed with nitrogen to the vent line to avoid release of noxious fumes. R5 has a different vent system because of potentially more toxic fumes.

Fig. 2 shows the schedules for the various units. The reaction starts in R1. The products are then moved into R2 where hydrochloric acid and iso-octane are added. Two phases form and a settling period is allowed to separate the organic and the aqueous layers. The aqueous layer is disposed whereas the organic one is sent to the buffer tank BU. The latter accommodates differences in cycle time and capacity between the reactors and the distillation vessels. In R3 and R4, iso-octane is removed via distillation in two stages at different pressure. Finally, in R5 the last reaction takes place and the final product is removed.

Although the schedule of Fig. 2 provides a rather complete definition of operations, changes may occur which in turn affect the operation of the plant. Certain events are not triggered at specific times but rather by other events. As an example, the flow of cooling water in a reactor starts when a certain temperature is reached. Also changes in steam or hot water availability, or in the specific heat capacity of reactor contents will alter the system behaviour and ultimately cause deviation from the original schedule. With *gPROMS*, one is able to study the interactions between the physico-chemical behaviour of the system on one hand, and the schedule and the operating sequence on the other. In this study we are particularly interested in:

- the load to the vent system during a typical cycle of operation,
- the demand profile for water and steam.

It is worth noting that plant designers usually oversize utilities. For the specific plant under consideration, this would normally correspond to simply sizing the utilities to the combined maximum loads and demands of all units. This rather conservative approach is costly and not always feasible. As the vent must be treated before being released in the atmosphere, a better understanding of the load would allow adequate sizing of the associated downstream equipment (scrubbers, absorbers, *etc.*) without compromising the safety of the plant while possibly achieving substantial capital savings. Furthermore, at the design phase, such a simulation would allow early consideration of load levelling and flexibility issues.

MODELLING in *gPROMS*

The *gPROMS* modelling language employs concepts from object oriented programming , in particular allowing the construction of MODEL and TASK hierarchies of arbitrary depth. Each reactor model is made up of five sub-models describing respectively feed conditions, the stirred tank, the condenser, the physical properties of the liquid phase and the physical properties of the vapour phase. Fig. 3 shows the model hierarchy for the first three vessels in the plant. *gPROMS* uses the concept of TASK to model the external actions imposed on the system. Tasks can also be decomposed according to a hierarchy, the lowest level of which involves elementary operations such as the opening of a valve to allow the flow of a reactant in the stirred tank. Generally, the lower a task is in the hierarchy, the closer it relates to the plant hardware. At higher levels, several of these elementary tasks can be combined to form a complete description of the reactor operation. Considering R2 as an example, the elementary tasks are:

- Add iso-octane
- Add HCl
- Receive the content of R1
- Reaction
- Allow phase separation to take place
- Dispose of the aqueous layer
- Add more water and HCl
- Allow phase separation to take place
- Dispose of the aqueous layer
- Transfer rest of reactor contents to BU.

These events form the frame of a higher level task describing the operation of R2. Also note that some tasks are repeated. In *gPROMS*, these naturally share the same primitive definition. The higher level task manages the co-ordination and sequencing of these events. In doing this, one can include set conditions (*e.g.* iso-octane is added for a fixed amount of time and with a certain flow rate), or impose dependencies on the physical system (*e.g.* the reaction is terminated when a certain pressure is reached inside the reactor) and on other events (*e.g.* the transfer to BU does not take place until enough capacity is available). Finally, these tasks are further combined to describe the operation of entire plant sections.

The plant model comprises 36 elementary task descriptions. These are used in 5 tasks for the operation of the vessels and 3 more tasks describing transfer of fluid between vessels. Finally, these 8 middle-level tasks are combined in two plant-wide tasks which fully describe the plant operations. A complete description of the tasks and their structure is given by Winkel (1993).

SIMULATION RESULTS

The plant operation was simulated over several cycles. Here we report the results from two cycles, starting from an empty plant. Fig. 4 shows the vent flowrates from R1, R2, and BU. Peaks are observed every time fluid is moved into or out of the vessels These are due to the pressurisation of the vessel and to the nitrogen flush. Fig. 5 shows the vent flowrates from the two distillation columns R3 and R4, while the vent from the entire plant is shown in Fig. 6. It is evident that the largest peaks are due to the distillation and cannot be reduced by changes in schedule and/or plant design. However, the simulation is valuable in leading to a better understanding of the constraints affecting the plant. If, for instance, a number of similar plants were operating in parallel, we could shift their relative schedule so as to avoid any coincidence of peaks from different plants. In general, such peaks could lead to a large overdesign of the vent treating system; however, this analysis suggests that it might be preferable to direct these large but short peaks to a different system (*e.g.* a flare).

Fig. 7, 8, and 9 show the plant-wide demand for cold water, hot water and steam. In many sites, these utilities are drawn from a common pool, and the simulation provides the engineer with insight as to how a certain schedule affects the demands, and how to achieve better load levelling and utilisation.

Finally, Fig. 10 shows the space available in the buffer tank using a vessel of nominal size or a smaller one. As expected, the larger vessel always allows for more residual capacity. It also appears that filling and emptying are not carried out at the same time as the smaller vessel induces larger waiting periods.

CONCLUDING REMARKS

This case study involved a modelling and simulation exercise which cannot be performed with commercial dynamic simulators without extensive use of user-written FORTRAN subroutines and the loss of abstraction allowed by the concept of TASK. Purely discrete-event simulation packages would also be inappropriate for this application given the importance of the continuous aspects of this system.

gPROMS enabled us to write a reusable model of the process, and to perform the necessary simulations. The solution of the differential/algebraic system is carried out by well proven state of the art algorithms (Pantelides and Barton, 1993), and the novel internal architecture of the package (see Barton, 1991) makes it easy to develop large models without being slowed down by compilation and linking of executables.

With the currently on-going development of diagnostic and data management facilities required by all but the most expert model builders, we believe *gPROMS* will become a mature tool of widespread industrial applicability. Compared to the common industrial application of equation oriented dynamic simulation, the package opens process simulation to new industrial applications and new research challenges. However, it is worth noting that the ease of description of discrete events makes it easier to define simulations in which frequent discontinuities lead to very substantial computational times. Novel methods to tackle this emerging class of problems are needed and actively sought.

ACKNOWLEDGEMENT

One of the authors (MLW) acknowledges the financial support from Shell Research B.V. during the course of this project.

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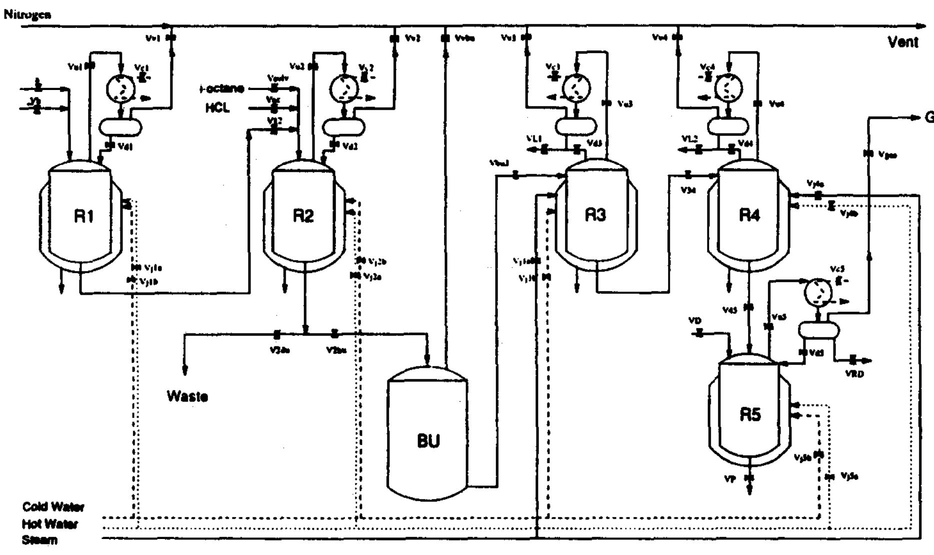

Fig. 1: Plant flow sheet

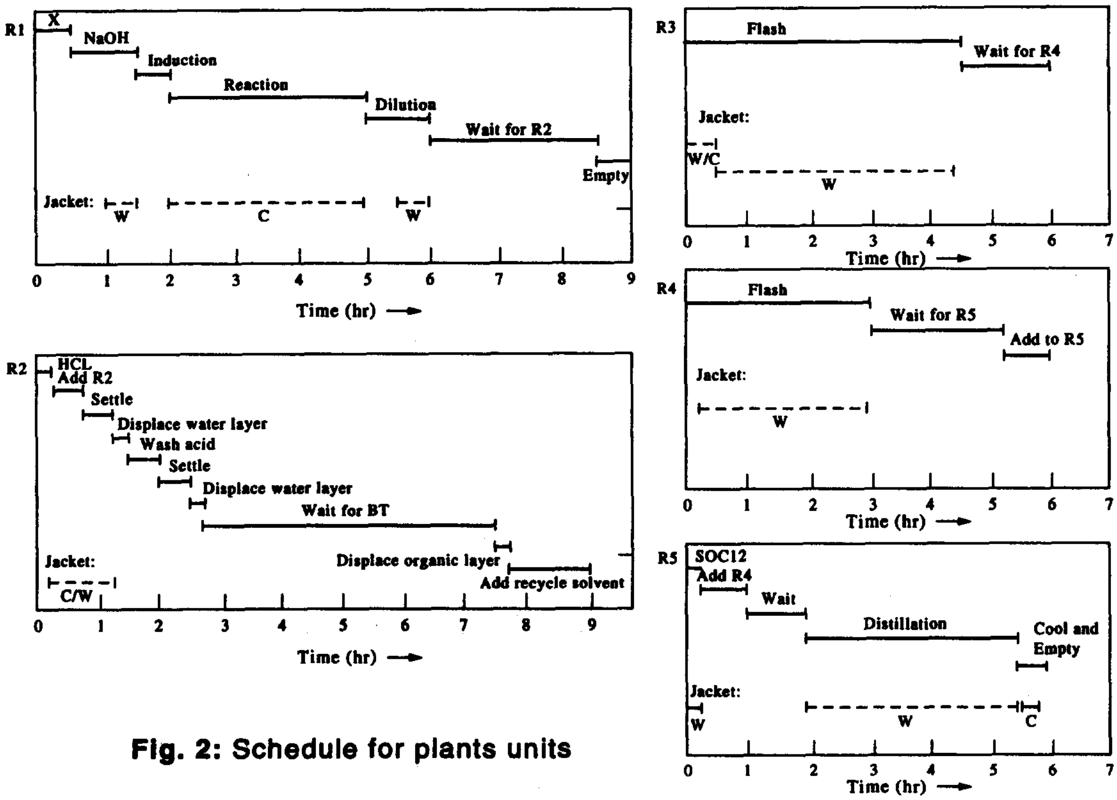

Fig. 2: Schedule for plants units

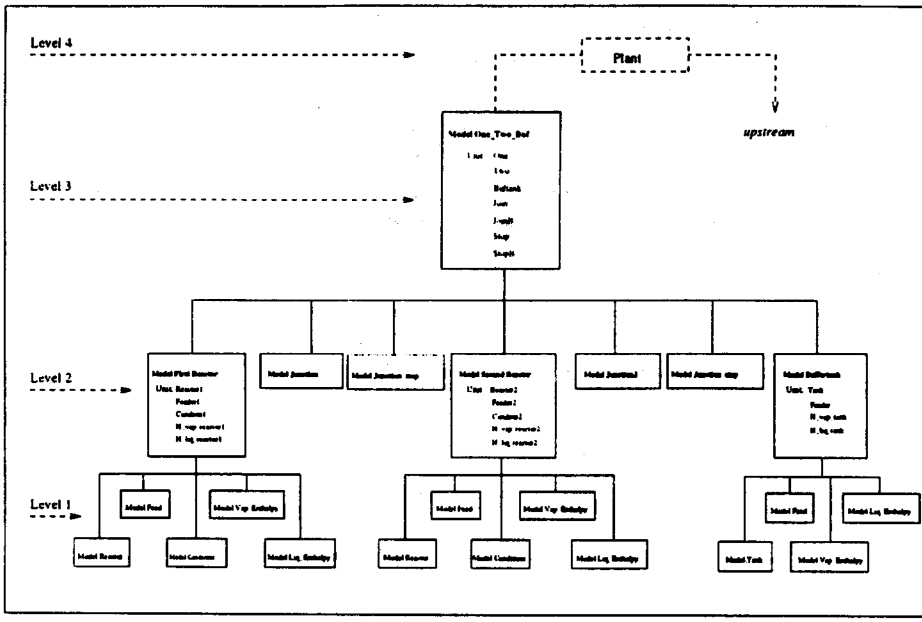

Fig. 3: Model hierarchy for the first three vessel in the plant