Technical Notes

Plant-Independent Process Representation

K. Wall,* P. N. Sharratt, N. Sadr-Kazemi, and J. N. Borland

Department of Chemical Engineering, UMIST, P.O. Box 88, Manchester, M60 1QD, UK

Abstract:

Of the traditional process representations commonly used by chemical engineers, flow diagrams or Process and Instrumentation Diagrams represent the interconnections between plant items, and mass and energy balances present the flow, composition, and conditions at the inlets and outlets of the plant items. It is only during detailed modelling of particular unit operations does the engineer normally address the physicochemical processes that are happening inside the equipment. The rapid leap from process to plant considerations creates a language barrier between engineers and chemists that potentially slows down process development and gives rise to scale-up problems as the controlling processes are overlooked. A simple representation of chemical processes has been devised that focuses on the controlling phenomena that ultimately should allow processes to be scaled-up much more easily.

Introduction

The usual approach to process design adopted by chemical engineers is predicated on the assignment of "unit operations". This phrase was coined by Arthur D. Little in 1916 although the concept was clearly recognised by George E. Davis, as can seen from inspection of his "Handbook".[1] As far as the modern chemical engineer is concerned, there are many cases where an obvious unit operation exists to achieve a particular process step, and consequently, most process developers think directly in terms of equipment when they are developing conceptual process designs.[2]

Prior to the concept of unit operations, each process was represented by drawings and descriptions of the equipment as it related to the particular chemical under consideration, emphasising the mechanical aspects of the plant. Many of the drawings are works of art (see for example Knapp[3]). For a chemist however, process design is focused on the composition and conditions of his laboratory experiments. A completed process description done by a chemist is, in effect, a recipe, detailing quantities and order of addition and the temperatures and pressures to which the chemicals are subjected. Other processing conditions are largely ignored. Thus, there is a language barrier that must be overcome.

There have been attempts at other representations of process, although these have usually been devised to address particular issues such as representing the mass balance,[4] the cost structure,[5] energy flows,[6] Hazop information,[7] and process/operating sequence structure.[8] Mahalec and Motard[9] did present a more general representation in their analysis of the process of synthesising separation flowsheets, although even this was very equipment- rather than operation-focused. Block diagrams are commonly used (e.g., for depicting mass and energy balance data[10]) although the assignment of the blocks is almost always by unit operations. The block diagram has been developed into a State Task Network[11] for the analysis of the scheduling of batch process operations.

A number of problems arise from the focus on equipment:

• Batch processes, particularly those that reuse equipment for multiple operations during the batch are very poorly represented.

• Opportunities to combine operations are not readily identified (for example reactive distillation or reactive crystallisation) because commonality of driving forces or conditions are not clearly shown.

• Process flowsheets are only valid for the specific equipment shown on the diagram both in terms of size and type. Increasing or decreasing the designed plant output requires the whole flowsheet to be redrawn to compensate for the nonlinear scaling of key parameters.

* To whom correspondence should be addressed. Telephone: +44 161 200 8854. Fax: +44 161 200 4399. E-mail: Kevin.wall@umist.ac.uk.

(1) Davis, G. E. *A Handbook of Chemical Engineering*; Davis Brothers: Manchester, 1901.

(2) Siirola, J. J. An Industrial Perspective on Process Synthesis. *Proceedings of FOCAPD 1994*; Snowmass, Colorado, July 10−15, 1994.

(3) Knapp, F. *Chemical Technology; or, Chemistry Applied to the Arts and Manufactures*, [Tr. with numerous notes and additions]; Ronalds, E., Richardson, T.; Eds. Hippolyte Bailliere: London, 1848.

(4) Flower, J. R.; Bikos, S. C.; Johnson, S. W. The Graphical Mass Balance in the Early Design of Clean Processes. *Trans I. Chem. E* **1993**, *71*(B), 194−202.

(5) Douglas, J. M.; Woodcock, D. C. Cost Diagrams and the Quick Screening of Process Alternatives. *Ind. Eng. Chem. Process Des. Dev*. **1985**, *24*, 970−976.

(6) Linnhof, B.; Townsend, D.; Boland, D.; Hewitt, G. F.; Thomas, B. E. A.; Guy, A. R.; Marsland, R. H. *User Guide on Process Integration for the Efficient Use of Energy*; The Institution of Chemical Engineers: Rugby, 1983.

(7) Srinivasan, R.; Ventatasubramian, V. Petri Net-Digraph Models for Automating HAZOP Analysis of Batch Process Plants. *Comput. Chem. Eng*. **1996**, *20*, S719−S725.

(8) Naka, Y.; Lu, M. L.; Takiyama, H. Operatoinal Design for Start-up of Chemical Processes. *Comput. Chem. Eng.* **1997**, *21*(9), 997−1007.

(9) Mahalec, V.; Motard, R. L. Procedures for the Initial Design of Chemical Processing Systems. *Comput. Chem. Eng*. **1977**, *1*, 57−68.

(10) *Chemical Engineering Practise*; Cremer, H. W., Davies, T., Eds.; Butterworths: London, 1956; Vol. 1, p 438.

(11) Kondili, E.; Pantelides, C. C.; Sargent, R. W. H. A General Algorithm for the Short-Term Scheduling of Batch Operations -I. MILP Formulation. *Comput. Chem. Eng.* **1993**, *17*(2) 211−227.

 10.1021/op010002j CCC: $20.00
Published on Web 05/23/2001

• Opportunities for the use of innovative equipment to enhance desirable aspects of the process may be lost (for example the use of microwave or ultrasound energy).

• Poor equipment selection may result from inadequate understanding of the controlling process parameters.

This work is being carried out as part of the 3-year £1.3m *Britest* Project.[12]

The Project has identified that some development time was wasted because key experimental data were not being passed on to the process development engineers because its significance was not apparent to the development chemists. Thus, the objective was set to develop a process representation that:

• provides a common language between chemists and chemical engineers,

• focuses on the fundamental physicochemical processes associated with any particular task,

• is useful in the early stages of process development where data is limited,

• becomes increasingly sophisticated as the process development activity proceeds, and

• is amenable to computerised storage and manipulation.

Furthermore, in adopting a process rather than equipment-based representation we recognise that the selection of a particular piece of equipment for a duty may impose some limitations on the process. However, by determining the needs of the process, the mapping of the process onto the plant may be done in the light of quantitative knowledge concerning the potential performance-limiting phenomena, and thus, the designer is able to explicitly make any tradeoffs between process performance and plant costs.

Plant-Independent Process Representation

A process is a linked feasible sequence of tasks, where the function of the tasks is to manipulate the concentrations and conditions of the process materials in such a way to convert the raw materials into the desired products and treat or recycle any coproducts. A good process representation should present in pictorial form the operations performed and the consequential flows of mass and energy. Key variables that must be controlled for safety, quality, or environmental reasons or that would otherwise potentially limit the performance of the process should be readily identified.

Recognising that State Task Networks are well suited to the representation of task sequences, we used this form of representation as the basis of the diagrams which we have termed "Process Definition Diagrams" (PDDs). In the PDD representation, as the level of knowledge about the process increases, the tasks are broken down into sub-tasks, with special symbols denoting specific sub-tasks. The development is best illustrated by way of an example:

(12) **B**atch **R**oute **I**nnovative **T**echnology **E**valuation and **S**election **T**echniques. *Britest* has set itself the challenging targets of halving the total time from the start of process development to manufacture, reducing manufacturing time (work in progress)—with a subsequent 50% reduction in working capital, reducing total plant capital cost by 30−40% and producing a plant that has a higher occupancy and is inherently more flexible than a traditional unit. [http:/www.britest.co.uk/].

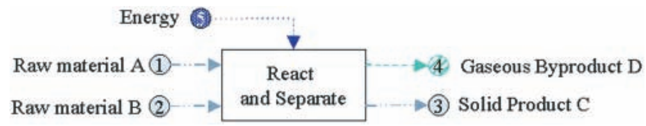

Figure 1. **Level 0 PDD representation of process.**

Table 1. **Data for level 0 PDD of process**

		state ID				
		1	**2**	**3**	**4**	**5**
form		solid	solid	solid	gas	energy
material	mol wt.	stream concentration (mass fraction) and amount (kg/kg of A)				
A (base)	302.9	1	0	0	0	
		1	0	0	0	
B	138.1	0	1	0	0	
		0	0.456	0	0	
C	404.5	0	0	1	0	
		0	0	1.335	0	
D	36.5	0	0	0	1	
		0	0	0	0.121	
heat kJ/kg A						−2000
T (°C)		ambient	ambient	ambient	ambient	
P (atm)		1	1	1	1	
max size (μm)				200		
color (hazen)				<5		
odor				none		

When a chemist first devises a route to a product, all that is explicitly known initially is the reaction stoichiometry, and some facts about the products and raw materials. For example:

$$A + B \rightarrow C + D \qquad (1)$$

A, B, and C are solids, and D is a gas. This whole process can be represented by a single task box (Figure 1) where the circles represent the initial and final states of the materials. The diagram is accompanied by a table that gives the conditions, amounts, composition, and any other relevant data on the "states" of the materials at those points.

At this level of resolution, the diagram itself has only limited value, but the accompanying table (Table 1) permits the calculation of the best possible raw material usage (and hence lowest possible operating cost) and specifies the product requirements that must be met. One of the reactants is selected as the "base" material to which the numeric quantities of the process are scaled—in this case material A has been arbitrarily chosen. Note that the estimated heat of reaction (calculated by a group contribution method) is significant, with subsequent implications both for the final reactor design and the plant infrastructure.

The process is developed in the laboratory—perhaps when using a solvent, an excess of one raw material (e.g., B), it is found that the traces of water in commercially available material B would cause a loss of yield and therefore would need to be removed. Environmental constraints impose limits on the gaseous emissions of D. The specification of C would no doubt be expanded to include residues of B and possible contamination from D. The raw material specifications would also be under development with some initial values entered.

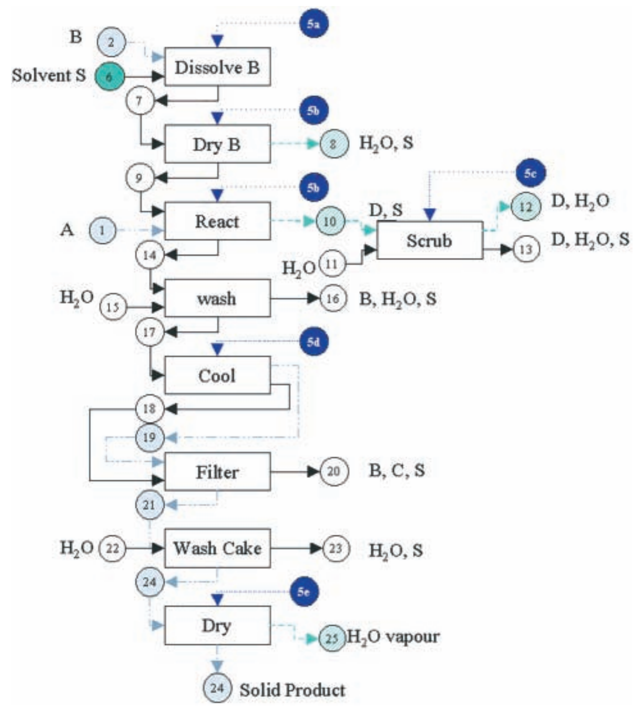

Figure 2. **Level 1 PDD representation of proposed process.**

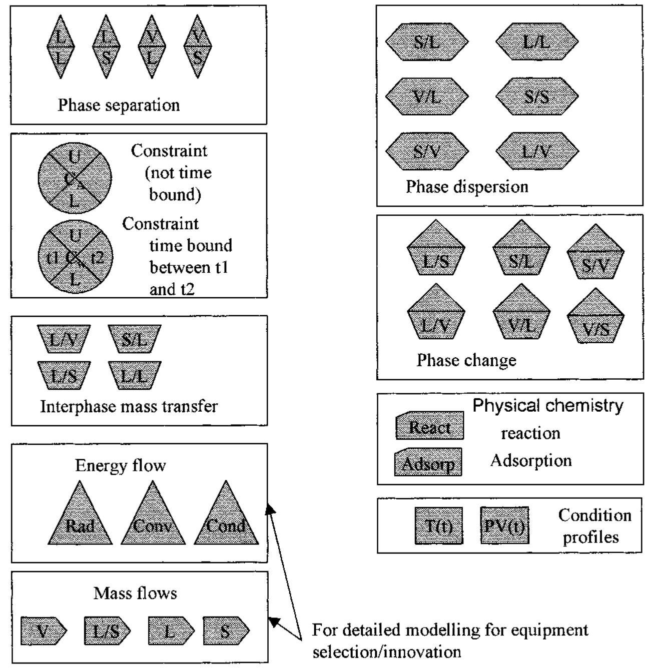

Figure 3. **Symbols representing physiochemical sub-tasks.**

The Process Definition Diagram at this stage looks like an expanded mass or energy balance block diagram (Figure 2 shows the graphical part), although there is no pre-requirement for the assignment of tasks to be conventional unit operations, but rather simply process steps that are recognizable both to the chemists and chemical engineers.

We use different colours to fill in the state circles to signify the different phases present (grey for solid, white for aqueous liquids, green for organic liquids, and light green/hatched for vapour). Different line types help to differentiate the phases (solid for liquids, dashed for vapours, and chain dot–dash for solids). The energy flows (with dotted lines and blue-filled states) on this diagram are usually only available as estimates at this stage. The composition of many of the streams may also be estimated but nonetheless provides the engineer and chemist some basis on which to converse. It is likely that several variations will exist, utilising different technologies to achieve the tasks, but it can be envisioned that much of the data to resolve which are the preferred options should already exist within the PDD, either as measured values or else as estimates.

Development work in the laboratory will have been continuing with aim of providing the information for the next level of PDD, where each of the tasks is sub-divided into its major physiochemical sub-tasks. Here we need to define the phenomena in which we are interested and the symbols that we use to represent them.

All the phenomena that we have needed to represent thus far fall into one of nine categories (Figure 3). Within each category there is only a relatively small number of combinations—for example there are only four phase separations possible (assuming that supercritical fluids do not need to be identified explicitly). Mass- and energy flows are generally only considered when representing specific embodiments of a process step, for example where the optimum mechanical design features are sought, although mass flow may be important in some membrane processes. The constraint symbols represent the action of monitoring and controlling process variables—generally these are values that must be measured during the process to ensure proper operation, although some may be implied from other process variables. Eventually, a number of these will be identified by the instrumentation engineer as the variables by which the plant will actually be controlled.

The condition profile symbols represent the imposition of temperature, pressure, and phase-volume profiles on the process step. Their "action" may extend into the subsequent sub-tasks, and they may be simple or complex functions of time. It is through the use of these functions that the residence and hold-up times in the system are represented. These sub-tasks and the ones directly above them in Figure 3 all may involve significant energy flows. Although only two physical chemistry sub-tasks are shown, it is recognised that there are others that may be relevant to particular situations (for example surface phenomena), but these are usually much less significant than those shown. The convention adopted for dispersion is that the line representing the continuous phase passes through the symbol horizontally, and the line representing the dispersed phase passes through the symbol vertically.

When the PDD is first drawn with the sub-tasks included, most of the values are not known—optimisation of the sub-tasks by experiments or modelling should determine the values to use. For example, when only the reaction step is taken, the PDD at the sub-task level would look something like Figure 4.

This representation says that stream 9 (dry B in solvent) is subjected to a temperature profile for the reactor and has dispersed in it solid A. Both the solvent and the solid have pressure–volume–time profiles that in this instance simply reflect the hold-up of the two phases. A dissolves (a phase

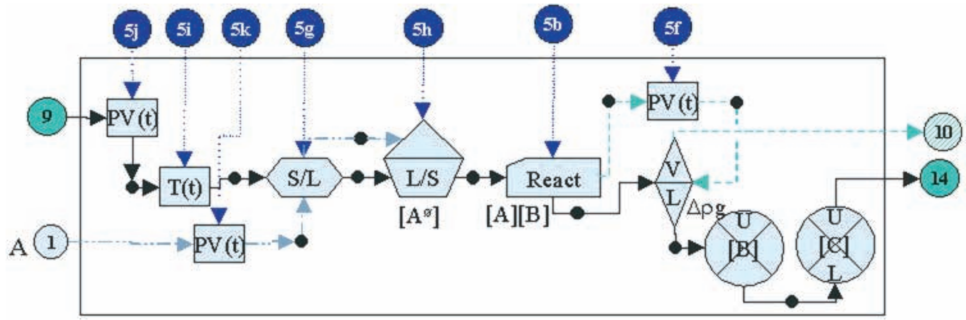

Figure 4. **Sub-task level PDD of reaction step from Figure 2 (diagram only).**

change with driving force that is a function of the relative degree of saturation of A in the solvent [A$^{\varnothing}$]) and immediately reacts (under the influence of the reaction driving forces—the concentrations of A and B ([A] and [B]) to form an additional gas phase that must be separated from the liquid phase. The generated gas phase has its own pressure—volume profile with time. The concentrations of B and C in the liquid phase must be constrained (the former to provide some excess, the latter defines the required product concentration in the reactor outlet). There are thermal energy flows associated with the maintenance of the temperature profile, the phase change (heat of dissolution), and the reaction exotherm. In addition there are mechanical energy flows associated with the dispersion of the solid in the liquid and possibly for the maintenance of the correct pressure. The small black nodes in the diagram represent "virtual states"—that is, ones for which it may not be possible to complete a state property table and may be omitted if desired.

Even without entering quantitative data into the PDD, it is possible to apply qualitative modelling to the process to design experiments that would prove the validity of the model and hence quickly home in on the parameters that are vital to effective functioning of the process. Thus, the number of experiments performed should be minimised, whilst the chances of obtaining a process that will be robust and easily scaled-up are greatly increased.

So far we have applied the representation at a qualitative level to seven different batch processes and have found it a useful tool in increasing the understanding of the factors that control the process. The provision of quantitative data is proving a little more difficult as companies are currently not geared up to measure the parameters in the form that is required for this representation (rates of dispersion for example). However, we recognise that this tool is in its early stages of development, and this is one of many aspects to be resolved before full use can be made of it. One of the major tasks to be addressed is the quantification of the process performance that standard pieces of process plant can actually deliver so that the process-need may be mapped onto equipment-capability. More processes need to be represented so that potential problems may be identified and remedied.

Conclusions

We have devised a process representation that is focused on the phenomena taking place within the process and not centered on equipment or unit operations. The representation highlights the important process variables, driving forces, and constraints in a pictorial form, but this is backed up by tables of data that present information such as material specifications and mass- and energy balances. Experiments need to be devised to provide the information for the quantification of the sub-tasks, and plant performance needs to be reviewed in terms of its capabilities to deliver the sub-tasks.

Acknowledgment

The contribution of EPSRC (Grant number GR/L65956) and the industrial sponsors of the *Britest* project is acknowledged. *Britest* aims to develop tools to achieve step change improvements in process development time, manufacturing time, working capital, plant capital cost, occupancy, and flexibility over traditional approaches.

Received for review January 10, 2001.

OP010002J