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Editorial

This Special Issue on batch reactors is the result of a long process, too long perhaps.... May I mention, firstly, that it has been a major task to identify a pertinent number of research groups involved in batch reactors. With this in mind, distillation has been discarded, since originally we thought that batch distillation could be considered as a separate topic. We thus had the ambition to promote a great variety of applications for batch reactors, including fine chemistry, biotechnology and polymers.

We have, anyway, solicited[1] about thirty research centres, and a number of them agreed to contribute. After the classical review process, seven papers have been gathered in the present special issue. They illustrate a variety of views and applications of batch reactors, including one paper devoted to reactive batch distillation, which offers evident scientific similarities with the others.

As far as science is concerned, batch reactors are quite strange devices. From a technological point of view, they look like stirred tanks, perhaps, the oldest chemical engineering apparatus known. If mixed with a wooden spoon or a bone, they would certainly look like the oldest cooking devices. And in industries such as fine chemicals, the operation of batch reactors still follows recipes, which may be viewed as cooking recipes.

In multipurpose manufacturing plant, the general tendency is to adapt the process to existing equipment, and to derive from homothetic procedures ''standard'' operating conditions. The rule is then, ''do the same to get the same'', without paying much attention to scientific deficiencies, or to the fact that processes are not clearly understood and fully modelled.

This is particularly true for biotechnological processes where the behaviour of living organisms is not fully modelled, or hardly mastered, unless we consider strictly repeated procedures, and where the control of reactors has to be achieved despite very poor on-line measurements and information.

This is even true for polymers where a simple determination of on-line viscosity remains a challenge, even if it is necessary information for the final processing step. It is also true, of course, in the field of fine chemicals for a variety of reasons. These include the use of multipurpose facilities, commercial pressure to reduce time-to-market, and the need to check thousands of molecules to identify very few industrial successes.

In reality then, for chemical engineers, batch processes present complex challenges as they involve crucial needs in the fields of modelling, dynamic simulation, optimisation of time dependent operating conditions and process control of transient temperature or feeding profiles.

This contrast between the need for quick-to-obtain, safe, simple, reproducible, industrial operating conditions and the exacting scientific requirements for batch processes may result in discouragement. It is not surprising then that only a relatively small number of papers in the literature are devoted to batch reactors. So what are the common features and the different characteristics of the seven papers presented in the present special issue on batch reactors?

In four papers the application is clearly addressed: two of them are concerned with polymerisation, one other with fermentation and the last one with chemistry. For the others, the application is simply suggested and they may involve any chemical application. More emphasis is placed on theoretical aspects. All the papers deal with optimisation, optimal control, control, monitoring and supervision, but a small majority of them directly refer to experimental assessment and validation. And finally six different countries contribute to this special issue.

In the future, if we want to address the industrial problems linked to batch reactors with scientific tools, we have to consider several key points:

- rapid development of processes and products does not allow heavy, costly and long experimental and modelling efforts,
- under these circumstances, we have to develop intensive modelling studies in order to obtain the framework to validate scarce, incomplete and uncertain data and measurements,
- experimental procedures are aimed at direct optimisation and scale-up of processes. Thus, operating conditions used at the bench scale are not designed in order to obtain analytical or scientific information but to forecast future industrial operating conditions. They may, however, offer valuable information extracted via pertinent modelling efforts,

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– modern optimisation techniques allow us to design experimental conditions and operating modes aimed at maximising the information needed for model identification, assessment or discrimination. The question then arises: are the experiments which are designed for information, that far from experiments designed for process development? And what are the reasonable efforts needed to bridge the gap between them, in order to obtain both, under given time and economical constraints?
– in between the white and black box models are the grey box models. These may offer the most realistic route to fast and secure development of processes and the central key for batch reactors modelling, optimisation, scale up and automatic control.
– and finally, although there may be good reasons for selecting a batch reactor and more generally a batch process, in certain cases, the unique reason is that direct experimental scaling of the process from batch bench scale devices restricts us to a batch process. And it is well known that as far as safety is concerned, continuous processes are challenging.

Therefore, modelling, even with a grey box approach, would allow us to assess, at the same time, batch processes and continuous ones. A major criterion is the need to develop safe processes.

This may appear to be a strange conclusion for an introduction to special issue of CEJ on batch reactors. It emphasises the fact that chemical engineering sciences – amongst them computerised process modelling – play a major role, and have perhaps a key role to play in process development, should the ideal solution be batch or continuous operation.

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