

Modeling, Design and Optimisation of Industrial Phosphoric Acid Production Processes

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In the present work we address the systematic and effective design of industrial scale phosphoric acid production processes through a generic modelling and optimization framework. Available research efforts focus on phosphoric acid process modelling issues while overlooking the prospect for improvements in the existing processes through optimization approaches. In view of this, we develop a framework that aims to facilitate the modelling, design and optimization of phosphoric acid production processes in order to propose solutions that improve the performance of the existing production technologies. The proposed framework is built upon an iterative procedure where design detail is added to the developed models based on evaluation of model results against industrial data. The framework allows the models to be independent of the processes they are expected to emulate as it is developed through use of generic process modules, thus facilitating design variability and flowsheet interconnectivity. The proposed modelling and optimization approach is implemented on the phosphoric acid production process employed by our industrial partner.

1. Introduction

The technology currently utilized for the production of phosphoric acid in industrial scale involves processes that fail to account for modern design considerations. Existing processes produce aqueous solutions of low phosphoric acid concentration and high energy consumption is required in order to produce commercially viable phosphoric acid products. Furthermore, the consumption of raw material in such processes is increased, process losses can be high and low product recovery is noticed, depending on the employed production process.

Despite the obvious need to effectively address the above shortcomings through efficient process design methods, the currently available research on the industrial production of phosphoric acid (Abu-Eishah and Nizar, 2001; Mathias et al., 2000; Yeo et al., 1991) is largely concerned with process modeling issues. The models presented in published literature manage to capture major phenomena occurring during the phosphoric acid production process to a sufficient extent, regardless of the design detail level employed. However, they fail to provide design flexibility as they are oriented towards the real-life case they are expected to emulate. Furthermore, the few reported attempts to address design issues in the existing production methods are limited to the haphazard study of a reduced number of design factors. No methods have yet been

proposed that are able to systematically explore and identify design targets of optimum performance for the production of phosphoric acid.

In this context, we develop a generic design framework that is able to transparently capture the process phenomena involved regardless of the modelled process task. It provides design flexibility and allows design options leading to performance improvements to be revealed. It is based upon an iterative design strategy and employs generic process modules for the representation of the processes involved. The following sections discuss the above features.

2. Modelling and optimization framework

2.1 Iterative strategy

The aim of the modelling and optimization framework is to allow the simplification of the model-related mathematical calculations while a detailed and realistic representation of the phosphoric acid production process is maintained. As the developed model is expected to become the basis for optimization of the existing phosphoric acid production process technology, the proposed framework should provide venues towards optimal design options without adding to the increased computational requirements. It should account for all the interactions among the different design elements that affect the decision making process, thus providing the designer engineer with insights that can reliably lead to the emergence of optimum decision paths.

In view of the above, an iterative modeling and optimization procedure is utilized. At first, simplified/conceptual process models of reduced detail can be developed that will allow the fast screening of the design alternatives as well as evaluation of the drawn design insights against industrial/experimental data. The evaluation will allow the identification of those features of the designed processes that provide valid results and lead to improved process performance. Features resulting to poor model performance will become the target for further improvement. Furthermore, features that might lead to design insights deemed unnecessary for the scope of the investigation could be excluded from the iterations that follow. The iterative procedure will continue until a desired match between the obtained results and design problem objectives is achieved.

2.2 Modular Design

The mathematical representation of the phosphoric acid production process should be sufficiently generic in order to encompass any of the existing phosphoric acid process flowsheets or the flowsheets that will potentially be designed through optimization. This is achieved through the use of modular design.

In general, modular design addresses the organization of a complex system as a set of distinct components. The components are developed independently and are then interconnected through a common interface. Although the idea of modular design appears to be simple, it does not follow from the automatic subdivision of the process tasks at hand. An appropriate implementation of modular development in a complex flowsheet is essential for the effectiveness of the design as well as for computational efficiency. It has the advantage of decoupling the components from each other, thus facilitating component interactions, simplifying computer calculations and providing opportunities for incorporating third-party components.

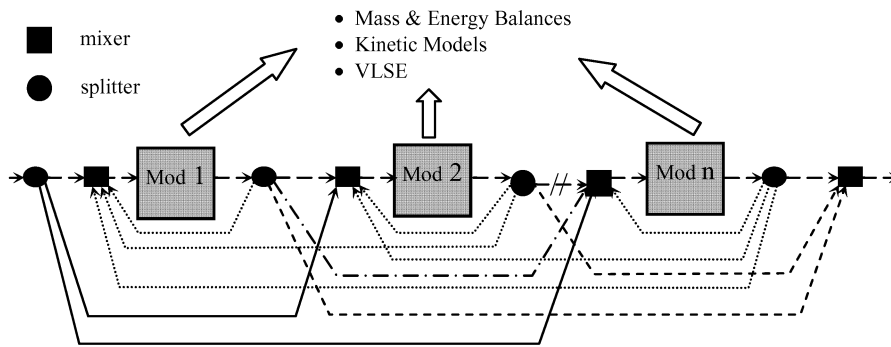


Figure 1: Modular design concept of the process flowsheet

Figure 1 demonstrates a generic concept of the implementation of modular design in process modeling, based on the concept of the RMX unit proposed by Linke and Kokossis (2003). A certain module consists of an inclusive set of equations representing mass or heat balances for all the processes involved in a flowsheet. Several terms of the equations are linked to kinetic, thermodynamic or other phenomena taking place in the processes. By activating the appropriate terms of the equations it is possible to simulate different processes of the flowsheet through the available set of equations. The mixers and splitters preceding and following the modules, respectively, act as mathematical sinks and sources of incoming and outgoing process streams, thus facilitating the interconnectivity of the modules.

Based on the above concept we develop process modules that can provide a conceptual or rigorous representation of all possible reaction or mass/heat exchange phenomena taking place during the process. All possible contacting and mixing pattern combinations between streams can be generated and all possible interconnectivity scenarios and flowrate distribution policies can be implemented. All inlet streams are connected to all mixers prior to each module. Each module effluent stream is split and connected to the subsequent module as well as the final product mixer.

3. Industrial case study

3.1 Phosphoric acid production flowsheet

Phosphoric Fertilizers Industry (PFI) has provided the design problem for the implementation of the proposed modelling and optimization framework. The conceptual process flowsheet employed by PFI is shown in Figure 2. The feed (Feed 1,2) entering the reactors (R1, R2) consists of phosphate rock, sulphuric acid and dilute phosphoric acid that is recycled (Recycle 1,2) from the filter (F). The main product stream of the reactor is a slurry stream containing gypsum mixed with the phosphoric acid produced. The slurry stream is lead to a filter where the solid phase (gypsum) is separated from the liquid phase (phosphoric acid, sulphuric acid, water). Streams exiting the filter unit consist either of solid gypsum (CaSO_4) with a certain fraction of moisture or liquid phosphoric acid at a certain concentration.

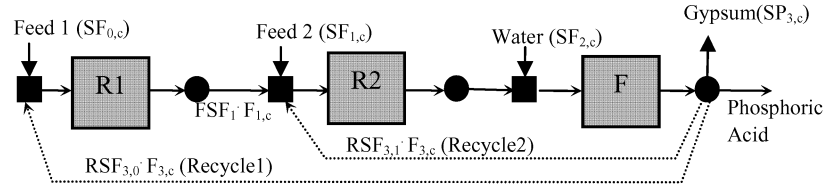
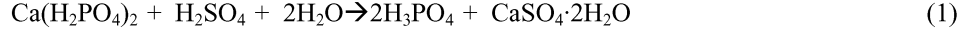


Figure 2: Phosphoric acid production flowsheet employed by PFI

3.2 Flowsheet Model

Phosphoric acid is produced in a reactor that facilitates the mixing and contact of phosphate rock with an aqueous solution of sulphuric and phosphoric acid. The phenomenon can be described by the following two-stage reaction (Abu-Eishah, Nazir 2001):



A set of generic mass balance equations is used in order to model the flowsheet of Figure 2, based on the modular design concept presented in section 2.2. Let *SECOMP* be the set of components (c_1, c_2, \dots, c_n) in the system and *SEM* be the set of modules. The equations describing the system are the following:

Mass balance:

$$\begin{aligned} FSF_i \cdot F_{i,c} + \sum_{j \neq i, j=1}^{SEM} RSF_{i,j} \cdot F_{j,c} + SP_{i,c} &= (FSF_{i-1} \cdot F_{i-1,c} + \sum_{j \neq i, j=1}^{SEM} RSF_{j,i-1} \cdot F_{j,c} \\ &+ SF_{i-1,c}) \cdot (1 + r_c \cdot X_i \cdot \frac{a_c}{a_c^{LR}} \cdot \frac{M_c}{M_c^{LR}}) \quad \forall i, j \in SEM, \forall c \in SECOMP, i \neq j \end{aligned} \quad (2)$$

Sum of split and mass fractions:

$$FSF_i + \sum_{j \neq i, j=1}^{SEM} RSF_{i,j} = 1, \quad \sum_{c=1}^{SECOMP} x_{i,c} = 1, \quad \forall i, j \in SEM, \forall c \in SECOMP, i \neq j \quad (3)$$

Volumetric flowrate and component concentration:

$$Q_{i,c} = \frac{Fi,c}{\rho_i}, \quad C_{i,c} = \frac{Fi,c}{\sum_{k=c}^{SECOMP} Q_{i-1,k}}, \quad \forall i \in SEM, \forall c \in SECOMP \quad (4)$$

The phenomena associated with the kinetics of the reactor involve the dissolution of the phosphate rock into the reactor and the nucleation and crystal growth of the gypsum crystals. The equations used for the mathematical representation of the above phenomena are taken from Abu-Eishah and Nizar (2001) and Becker (1989). The design equations utilised in the filtering section are available in Richardson (2002).

3.3 Optimization algorithm and objective function

Simulated Annealing (SA) has proved to be an efficient algorithm for optimization in separation (Papadopoulos and Linke, 2004) and reaction-separation (Linke and Kokkosis, 2003) process synthesis problems. It is a statistical cooling optimization technique that generates a biased random search and employs Monte Carlo simulations under a variable probability schedule. SA is used in order to evaluate the objective function associated with the problem at hand. In our case, the phosphoric acid exiting the process is diluted in water and energy intensive evaporation is required in order to reach the specification limits imposed for commercial use. As a result, the objective is to maximize the amount of phosphoric acid produced while minimizing the amount of water in which the product phosphoric acid is diluted.

3.4 Results and Discussion

In Table 1 we present the results obtained using the modelling equations of section 3.2. These results are compared with the available industrial data in terms of key process stream flowrates and compositions. Results show a relative difference in the range of 0.21-3.6%, with most values being in the range of 0.2-1.5%. It appears that there is a close match between the industrial and model calculated data. A similar relative difference range (0.42-3.46%) between model calculated and phosphoric acid pilot plant data is reported by Abu-Eishah and Nizar (2001), who use similar reaction kinetic models to the ones employed in this work.

Table 1: Comparison of model calculations and industrial data

	Industrial data	Model calculated data	Relative difference (%)
P ₂ O ₅ % in product	30.5	31.6	3.6
P ₂ O ₅ % output of Reactor 1	16	15.5	3.1
P ₂ O ₅ % output of Reactor 2	19.8	20.2	2.02
Total flowrate of product stream (tn/hr)	59.41	60.23	1.38
Total flowrate of gypsum stream (tn/hr)	111.41	111.65	0.21
Total flowrate output of Reactor 1 (tn/hr)	154.08	152.07	1.30
Total flowrate output of Reactor 2 (tn/hr)	222.62	223.14	0.23
Total flowrate output of Recycle stream 1 (tn/hr)	101.16	102.62	1.44
Total flowrate output of Recycle stream 2 (tn/hr)	41.6	41.73	0.31

Table 2 shows the results of a design case where the degree of freedom for optimisation is represented by the percentage of the filtrate stream (filter liquid outlet stream consisting of phosphoric acid, water and minor amounts of sulphuric acid) recycled in reactors 1 and 2 of Figure 2. The optimized case results indicate that it is possible to obtain a higher value for the mass fraction of the product stream phosphoric acid by slightly reducing the amount of filtrate directed to the product stream, while increasing the amount of filtrate recycled into reactor 2. The proposed optimum solution allows the produced phosphoric acid to remain at the same quantity as in the industrial case but significantly reduces the amount of water directed to the product stream. This is a solution that can be easily implemented in the existing process and will lead to a reduced evaporation load.

As this is ongoing work, the study of the flowsheet has led to the identification of further design scenarios that will potentially benefit the existing process. One such case

is the addition of a recycle stream between reactors 1 and 2. This will result to an increase in the reaction time and is expected to lead to minimization of the unreacted rock exiting the two reactors. The proposed design option will be coupled with determination of the optimum recycle flowrate as well as with re-determination of the filter recycle flowrates entering the reactors. An additional identified point of interest is the effect of the alteration of certain operational parameters such as the sulphuric acid excess currently utilised in the production process and the flowrate of the washing water used in the filtering section.

Table 2: Proposed optimization scenario and comparison with industrial case

	% Filtrate recycled in Reactor 1	% Filtrate recycled in Reactor 2	% Filtrate lead to product	% P ₂ O ₅ in product
Industrial case	50.2	20.4	29.4	31.6
Optimized case	49	25	26	35.5

4. Concluding remarks

This work proposes a generic framework that facilitates the modelling, design and optimization of phosphoric acid production processes. The main aim of the framework is to provide design flexibility and to allow the systematic identification of improved design options of optimum performance in the existing processes. The presented work has outlined the design philosophy of the proposed framework and presented its successful application to the development of a model for the phosphoric acid production flowsheet provided by our industrial partners. Furthermore, we presented an optimization case that leads to higher concentration of the phosphoric acid in the product stream and identified certain design options that will become the target for exploration through optimization.

Acknowledgments

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