

# EDUCATION IN PROCESS SYNTHESIS

## *Application to Inorganic Processes*

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The first task in process design is selecting the raw materials and the reactions and operations needed to manufacture the desired product. Process synthesis accomplishes this task by generating different process alternatives and selecting the best ones.

Taking into account the void existing in the literature about inorganic process synthesis, this paper is an attempt to show, in a simple and summarized manner, how the principles of process synthesis can be applied to inorganic processes. These principles can also be applied in other fields of chemical engineering.

Process synthesis uses heuristics, or "rules-of-thumb" based on experience, for the generation and selection of process alternatives. Education in process synthesis implies that students will acquire, in a systematic way, the necessary experience to enable them to apply heuristics, or even to "invent" them when the situation demands it. Douglas<sup>1,2</sup> propounded a systematic application of heuristics to process synthesis of organic processes and also indicated the possibility of using the procedure in chemical engineering instruction.

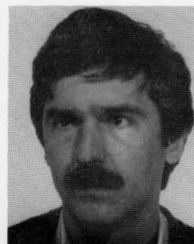
The application of process synthesis methods to inorganic processes requires specific considerations due to the different chemistry and properties of inorganic compounds. However, it seems possible to give heuristics which will permit the student to acquire systematic knowledge about the processes.

Raw materials are very important in inorganic processes. Natural compounds are the raw material for one (or a very reduced number) of the derived compounds of every element, and from this (or these) all the other compounds of the element are obtained. The natural raw material for an element and its derived compounds is selected according to the ele-

ment concentration, ease of mineral extraction, ease of separation of the desired compounds, associated impurities, etc. The most frequent natural raw materials are sulfides, oxides and hydroxides, chlorides, carbonates, and silicates.

The next step in process synthesis of inorganic processes is the selection of the reaction path. Three types of reactions can be considered in inorganic processes: redox, displacement (exchange of ions between compounds), and change of crystal structure.

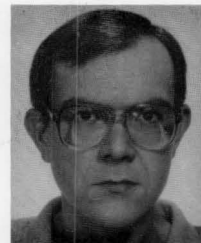
For redox reactions, the general rules are: oxidations must be made at the beginning of the process; reductions will, if possible, be the latest steps of the process; and electrochemical reactions will be the last step. The oxidant or reductor selection can be made using Ellingham's (or a similar) diagram and taking into account the price of the reactants and the ease of reaction-products separation. Air for oxidations, and H<sub>2</sub>, C, or CO for reductions, will be considered first. Displacement reactions are closely



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related with separation steps and are generally used when a precipitate or an easily separable gas is formed. When a change of crystal structure is required, the corresponding reaction will be the latest step in the process.

Following the scheme given for organic processes, the next step in process synthesis is to decide the species allocation, *i.e.*, the route of each species through the process. Thus, quantity and reactivity of impurities permit one to decide if they are processed or not. If there are ions in the solution, every valuable product or by-product and every group of species with waste destination and similar solubility will constitute an outlet. Recirculation of the mother liquor, with a purge to avoid the build-up of impurities, can be convenient.

The general structure of the separation system depends upon the phases leaving the reactor. In every case, first separation is a phase split, and after that the stream of each phase is driven to the corresponding separation system (solid, liquid, or gas). From each separation system, streams of different phases are normally produced and driven again to the corresponding separation system.

The same heuristics as in organic processes can be applied when choosing the separation task. Crystallization and precipitation operations, followed by solid-liquid separations (sedimentation or filtration, by example) are used in many cases. In inorganic processes there are normally not a great number of separations and the sequencing problem is not difficult. In all cases, heuristics such as the removal of corrosive and dangerous species first, removal of the most abundant species, making difficult separations last, etc., can be applied.

The last step in process synthesis is the integration of operations. In the inorganic processes, the same general criteria are valid as in organic processes.

It can thus be concluded that the student's education in process synthesis can consist of transmission of the necessary experience together with heuristics or rules-of-thumb. This instruction in process synthesis can be an advantageous substitute for the exhaustive descriptions of chemical processes which is given to students in subjects such as industrial chemistry.

## REFERENCES

1. Douglas, J.M., " Hierarchical Decision Procedure for Process Synthesis," *AIChE J.*, **31**, 253 (1985)
2. Douglas, J.M., *Conceptual Design of Chemical Processes*, McGraw-Hill, New York (1988) □

Winter, 1992

## LETTER: Langmuir's Isotherm

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And from Eqs. (4) to (6)

$$\begin{aligned}\theta_j &= K_j c_j \theta_{\text{free}} = K_j c_j \left( 1 - \sum_{i=1}^m \theta_i \right) \\ &= K_j c_j \left( 1 - \frac{\theta_j}{K_j c_j} \sum_{i=1}^m (K_i c_i) \right) = K_j c_j - \theta_j \sum_{i=1}^m K_i c_i\end{aligned}$$

Solved for  $\theta_j$

$$\theta_j = \frac{K_j c_j}{1 + \sum_{i=1}^m (K_i c_i)}$$

The concentration of  $j$  on the adsorbent is proportional to the surface fraction occupied by  $j$ , so that

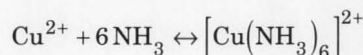
$$q_j = k_j \theta_j = \frac{k_j K_j c_j}{1 + \sum_{i=1}^m (K_i c_i)} \quad (7)$$

where  $k_j$  is another constant. This is of the form of Eq. (1), with  $k_j K_j$  corresponding to  $a_j$  and the  $K_i$  to the  $b_i$ .

This derivation also gives the same result as Langmuir's for adsorption of a dissociating molecule, for instance, of  $H_2$  as 2 H occupying two sites.

Langmuir-type adsorption is seen to result from "ideal" thermodynamic behavior, that is, from the absence of any specific interactions that would result in activity-coefficient corrections or call for the definition of additional species. This is a more germane reason than are the adsorption and desorption rates. That adsorption *equilibrium* has a basis in thermodynamics will be easier for the student to accept and will convey better insight into why many adsorbents behave in this manner, and why some do not.

When I went to school, more years ago than I care to count, textbooks still derived the mass-action law for reactions with the kinetic argument of equal forward and reverse rates at equilibrium—one of them even with the reaction



postulating a single-step mechanism with hepta-molecular formation and decay into seven fragments! Happily, we have long outgrown such nonsense and have put the mass-action law for reactions on a sounder basis. Is it not time that we accord the Langmuir isotherm the same courtesy?

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1. Langmuir, I., *J. Am. Chem. Soc.*, **38**, 2221 (1916)
2. For instance, see Fogler, H.S., *Elements of Chemical Reaction Engineering*, Prentice-Hall, Englewood Cliffs, NJ, p. 241 (1986) □