The Potential of Process Informatics

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Needless to say, "what to make" as well as "how to make it" are important issues in chemistry and chemical engineering. Furthermore, the physical properties of materials are influenced by the way they are made. This has given rise to the concept of 'process informatics', which is concerned with the successful use of informatics to closely relate the development of materials with desired properties with the conditions of their synthesis and manufacturing processes. The basic idea is to put the entire manufacturing process on the informatics stage by linking material design and process design and expanding the concept to quality control in production.

This 'process informatics' is a term and concept that I first proposed about eight years ago through lectures and writings[1]. Since then, the meaning of the term has been explored from different perspectives in industry, government, and academia. In industry, I have often heard people say that things related to process informatics have been implicitly done even before that time. However, looking at it again, it seems that "what to make" and "how to make" were not necessarily linked, but only in the sense of studying or controlling manufacturing conditions. Again, what is important for process informatics is to closely link "what to make" and "how to make it", and to consider the overall picture of the use of informatics, including quality control (how to make it as a product). It is to design the basic manufacturing conditions for materials with the desired properties and to formulate the correspondence between the process variables obtained from the synthesis and manufacturing equipment and changes in properties.

With the penetration of the basic concept of process informatics, synthesis, and manufacturing process variables have been introduced during materials design, so that 'what to make' and 'how to make it' are now considered in conjunction with each other as a matter of course. In addition, the use of real-time monitoring tools (soft sensors) built to include the process variables used there makes it possible to manufacture products with stable quality by using some of the process variables as operating variables.

As a supplementary note, the use of process variables such as temperature and pressure as modeling parameters in synthesis and production is the usual practice, but the use of various spectral data that can be measured in real-time is also beginning to be used in combination. Spectra are a reflection of the material structure and are therefore linked to physical properties. If we can thus monitor changes in physical properties and structure during synthesis and production, we may be able to get closer to the essence of the expression of physical properties. In the case of linking physical properties and synthesis, the construction and operation of multimodal models using process variables and spectral data will open up new process informatics in the future. The concept of process informatics is sure to provide new perspectives for the development of new materials in the future.

Bibliography:

[1] Kimito Funatsu, Special issue on AI-based manufacturing, a Paradigm shift towards data-driven chemistry, Chemical Economics, November 2017. (Published in Japanese)