

Chemical Products for a Changed World from a PSE Perspective

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Abstract

Chemicals, in some form, can be found in all aspects of our daily life because we depend on chemicals-based products for our survival on earth. Regardless of geographical location, society needs to use a variety of products that are directly or indirectly connected to chemicals. We design and operate manufacturing processes for single species products like bulk-chemicals, specialty chemicals, and many more for Business to Business (B2B) options, which we then use to design and operate manufacturing processes for chemicals-based products (single species, blends, formulations, etc.) to satisfy our daily needs for Business to Consumer (B2C) options. An important issue is what to make, both for B2B and B2C, before we decide on how to make. The former is related to product design, while the later is related to process design (Gani and Ng, 2015, Zhang et al., 2020). Both are related to product and/or process development. As the number of chemicals being used and their applications in processes and/or products grow, their implications on human health and environment as well as the economy need to be understood and analysed (Syeda et al., 2021; Syeda et al., 2022).

The issue of what to make is also closely related to why to make, because as we know, only a small percentage of chemical product ideas or concepts actually end-up being produced for B2C options. Therefore, it is important to make the right decisions related to what and why to make as early as possible so that the product development time and costs can be reduced. The current challenges that we are facing related to energy-water-food-health-environment and together with the pandemic due to COVID-19 have changed many of the factors influencing our decision making related to chemicals based product design and development. Factors such as recycle, re-use, replace need to be considered together with requirements of sustainable development (Gani et al., 2022). A closer look at the chemicals we use in our products is also necessary. For example, while some chemicals have no safety, health or environmental issues, others have issues that are well-documented and are usually monitored and controlled. Yet, there are others for which we have little information and could potentially be very dangerous, unless their uses are strictly monitored. It is necessary to identify the likely problems from uses of these dangerous chemicals and take necessary steps to prevent future problems, rather than cure them later. These are difficult, multi-disciplinary problems where Process Systems Engineering can play an important role to manage the complexity (Pistikopoulos et al., 2021).

The goal of this presentation is to give an overview of some of the issues that need to be considered in chemicals-based product design and development and how advances in methods and computer-aided tools from the PSE community can contribute to help tackle them efficiently and reliably. It is necessary to look beyond the process simulators as we know them. What about a chemicals-based product simulator? What about integration of B2B and B2C options as in simultaneous design of catalysts, solvent, adsorbents together with processes to manufacture them as well as processes that use them for B2C options? A general framework for tackling chemicals-based product design and development problem is necessary together with associated methods and tools that could be used in different work-flows within the framework. Perspectives on interesting new developments in the area of chemicals-based products related to PSE methods and computer-aided tools will be highlighted.

References

- Gani, R., Ng, K.M., 2015, product design – Molecules, devices, functional products, and formulated products, *Computers & Chemical Engineering*, 81, 70-79
- Gani, R., Chen, X., Eden, M.R., Mansouri, S.S., Martin, M., Mujtaba, I.M., Padungwatanaroj, O., Roh, K., Ricardez-Sandoval, L., Sugiyama, H., Zhao, J., Zondervan, E., 2022, Challenges and Opportunities for Process Systems Engineering in a Changed World, *Computer Aided Chemical Engineering*, 49, 7-20
- Pistikopoulos, E.N., Barbosa-Povoa, A., Lee, J.H., Misener, R., Mitsos, A., Reklaitis, G.V., Venkatasubramanian, V., You, F., Gani, R., 2021, Process systems engineering – The generation next? *Computers & Chemical Engineering*, 147, 107252.
- Syeda, S.R., Khan, E.A., Padungwatanaroj, O., Kuprasertwong, N., Tula, A.K., 2022, A perspective on hazardous chemical substitution in consumer products, *Current Opinion in Chemical Engineering*, 36, 100748.
- Syeda, S.R., Khan, E.A., Padungwatanaroj, O., Kuprasertwong, N., Gani, R., 2022, A Model-Data Driven Chemical Analysis System for Products and Associated Processes, *Computer Aided Chemical Engineering*, 49, 181-186.
- Zhang, L., Mao, H., Liu, Q., Gani, R., 2020, Chemical product design—recent advances and perspectives, *Current Opinion in Chemical Engineering*, 27, 22-34



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