SPECIAL FEATURE SECTION: SOFTWARE FOR APPLICATION IN CHEMICAL DEVELOPMENT AND SCALE-UP

Editorial

When I am asked a question about what the Process Research and Development Laboratory of the future will look like, my biggest level of uncertainty is in the area of computational-assisted process development. As computing power has increased exponentially over the last 20 years, we have seen some tremendous advances in the way software can aid Process Research and Development chemists. Those of you who are not old enough to remember the days before SciFinder and Crossfire may find it hard to imagine how chemists were ever able to do their job prior to the arrival of such software. The ability to be able to store and retrieve huge amounts of data is potentially very powerful, but it also has a darker side in terms of the propensity to confuse data with information and knowledge. This raises what to me has been, and always will be, the key issue in this area. How effectively does software interface with the working scientist? It is clear that we can change software more rapidly than we can change human behaviour. I feel that this aspect has only gained significance amongst the software community during the past few years; however, I think that adopting an approach that supports and liberates the laboratory chemist, rather than that which endeavours to replace him, will reap future benefits that few of us can really imagine today. In this special edition I have tried to pull together several different applications of software, from e-notebooks to databases, as well as an article that tries to anticipate where the future challenges and benefits might lie.

I thank all of the authors for their time to contribute these articles. It will be interesting to speculate what a future special issue in 2020 might look like.

David Lathbury*

AstraZeneca R&D Charnwood, Bakewell Road, Loughborough, Leicestershire LE11 5RH, UK OP0498215