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Computational Science in Chemical Engineering

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As a chemical engineer, it has always been a surprise to me when my friends ask me whether my job is to deal with petroleum or not. Well, that was the chemical engineering one century ago. It is very interesting to read the definition of chemical engineering nowadays on Wikipedia:

"Chemical engineering is a branch of engineering that applies the natural (or experimental) sciences (e.g., chemistry and physics) and life sciences (e.g. biology, microbiology and biochemistry) together with *mathematics* and economics to production, transformation, transportation and proper usage of chemicals, materials and energy".

In 1960, R. Byron Bird published his ground-breaking textbook entitled "Transport Phenomena", which has then become the classical in classrooms and been translated into many different foreign languages. This book was a milestone in the classroom for generations of chemical engineers to come, bridging chemical engineering from an empirical practice into a rigorous science. I still remember how shocked I was when I first deep dived into this book: I considered this book as the "Mathematical Principles of Natural Philosophy" in chemical engineering. For the first time, I clearly saw how those complicated phenomena in chemical engineering could be explained mathematically based on a few elegant fundamental equations. We all know that if we have a model complex enough to capture the essentials of the system that we are interested in, and a computer powerful enough to produce a result within an acceptable time frame, we could essentially run our experiments in our virtual laboratory: the computer. In the 1960s, what a computer could achieve seems to be trivial by the standard of modern computers. However, scientists and engineers clearly saw that this was the future: tomorrow most of our experiments conducted in the laboratory would happen in the virtual world of a computer.

Perhaps nowadays the mass media haven't realized what the true implication of computational science is to our society. It is much more than a pure scientific tool floating in the hefty academic cloud. Computational science already began to benefit our society and increase our productivity in a very profound way. In the semiconductor industry, the design cycle time has been dramatically reduced thanks to various powerful automated design tools. In the aviation industry, the improvement of accuracy of predictions in aerodynamics has allowed us to rely more on our calculations instead of experimenting with extremely expensive machinery. In the medical industry, bioinformatics is wildly spreading and growing, helping the doctors in diagnosis in an unimaginable way. From the perspective of this editorial, the time has never been better to launch the *Journal of Theoretical and Computational Chemistry*. Open access (like open source software) makes sure that our knowledge could propagate as fast as possible to avoid the old story of re-invention of the wheel. I believe that with more and more open access journals launched, we will see the next round of our knowledge blooming and flourishing like never before.

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