

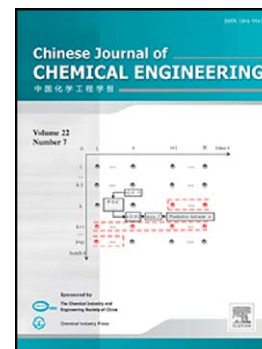
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Computational Chemical Engineering – Towards thorough understanding and precise application

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Computational Chemical Engineering – Towards thorough understanding and precise application

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Abstract The paradigms of chemical engineering discipline are discussed. The first paradigm of *Unit Operations* and the second paradigm of *Transport Phenomena* are well recognized among the chemical engineers all over the world, and what the next paradigm is remains still an open question. Several proposals such as *chemical product engineering*, *sustainable chemical engineering* and *multi-scale methodology* are considered as candidates for next paradigm. Might *Computational Chemical Engineering* be the next one, which is advancing the discipline of chemical engineering toward ultimate mechanism-based understanding of chemical processes? This possibility is comparatively expounded with other proposals, and the scope and depth of computational chemical engineering are shortly listed.

Keywords Paradigm, Unit operations, Transport phenomena, Chemical product engineering, Sustainable chemical engineering, Computational chemical engineering, Numerical simulation

1. Paradigms of Chemical Engineering

While chemical engineers are constantly striving to gain more thorough understanding of the discipline of chemical engineering and apply this knowledge efficiently to general process industries, they do look retrospectively from time to time at the history of the development of Chemical Engineering over more than a century. It is generally acknowledged that there are two paradigms in the early development of the chemical engineering discipline [1-3].

The first paradigm is *Unit Operations*. This term was first used in 1911 by A.D. Little in a report (see [2]), and also symbolized by George Davies's *Handbook of Chemical Engineering* published in 1901 and the textbook *Principles of Chemical Engineering* by H. Walker et al. in 1923 (see [4]). These works were essentially a systematic reduction of the to-date chemical production processes into their

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