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APPLYING MULTISCALE SIMULATIONS IN EDUCATION OF CHEMICAL ENGINEERING FOR INTERNATIONAL STUDENTS

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ABSTRACT

Several examples of multiscale-simulations were introduced to international undergraduate students majored in chemical engineering in the classes of principles of chemical engineering. This improves the teaching practices of the course significantly, as the international undergrads pay much more attention to these examples than to the conventional lecturing. Moreover, those examples were easy to be visualized which can be suitable for distant education or SPOCs. This manuscript focuses on how to combine the various topics of the course with different simulation techniques to implement successful educational reform.

KEYWORDS: multi-scale simulations, educational reform, international students, engineering education

1. INTRODUCTION

More than one decade ago, MOOCs (Massive Open Online Courses) as well as SPOCs (Small Private Online Courses) were said to have revolutionized universities although distance learning was introduced even before the invention of TV (Kaplan & Haenlein, 2016). With the rapid development of information communication technologies (ICTs), MOOCs, which allow for unlimited participation of college students by cost-free independent learning, can support higher education worldwide, especially in developing countries (Corrado et al., 2021). However, only a fraction of students that enroll in a MOOC can fulfill the requirements of the course. And the sustainability of MOOCs is questionable, for the courses and study materials are typically provided free to the enrolled students. Hence, SPOCs emerge as the preferred model for specialized learning in universities, especially since the breakout of COVID-19 pandemic. Due to the closure of university buildings during the lockdown, a rapid shift from conventional teaching practice to distant education took place (Mac Domhnaill et al., 2021). Because student engagement during distance learning can be influenced by various factors (e.g., the availability of high-speed broadband (Mac Domhnaill et al., 2021), the lack of concentration for students due to the Internet's constant distractions), it is of great interest to find the effective strategy to deliver complicated information to overcome the inherent limitations of distance learning (Todhunter, 2013).

The interactive, web-based simulation and virtual tutoring system was introduced to higher education decades ago (Dorneich & Jones, 2001), while virtual reality (VR) technology as a cutting-edge technology in the information communication technologies became popular in engineering and medical education about a decade ago (Duan et al., 2019; Tao et al., 2011). With the help of these modern technologies, multiscale simulations (from quantum chemistry to continuum models) become possible even for remote education. For example, since the molecular simulations can lead to a better understanding of physical and chemical reactions at molecular level, it is widely used in teaching science and engineering students (e.g., molecular simulations were performed on interactive virtual laboratories (IVLs) to help engineering students learn thermodynamics (Cao & Koretsky, 2018)). Note that molecular simulation software is widely used in both industry and university (Marchand et al., 2014). Besides, as the biomolecular simulation works as a "computational microscope", which allow molecular biologist explore biological reactions with both high temporal resolution and space resolution (Dror et al., 2012; Guliaev, 2012), molecular dynamics simulations were applied to online biochemistry laboratory education (Costabile, 2020; Craig, 2020; Hati & Bhattacharyya, 2016; Spitznagel et al., 2016). In addition, molecular dynamics simulation can be used for frontier courses such as undergraduate nanoengineering course (Kilani et al., 2018). Simulations at coarser level also have broad applications in higher education. For students majored in mechanics, simulation-based learning modules were used for undergraduate engineering dynamics course (Karadoğan & Karadoğan, 2019). And the interactive machine simulation platform based on virtual reality technology (Sang et al., 2018) allows students to investigate the motion control mechanism of components of three coordinate measuring machine through distance learning. Moreover, industrial scale process simulations (Kuriyan et al., 2001) as well as computer aided design (CAD) (Hsu, 2005) become the standard tools for engineering students nowadays.

As technological skills development is one of the central topics for a country's educational policies, the integration of digital technologies in higher education in the teaching and learning processes is necessary (Rodrigues et al., 2021). The multiscale simulations discussed above can be introduced to undergraduate level courses by two approaches, i.e., programming approach and configuring approach (Magana et al., 2017). Although programming approach is more time-consuming compared to configuring approach, the programming skills of engineering students can be improved dramatically by introducing numerical techniques by programming approach (Mariano et al., 2019). Besides, for higher education, ideally, faculty members' research and teaching are interlinked (Dahlen et al., 2020), and some universities do provide such courses (Schot et al., 2021). Obviously, multiscale simulations have big advantages in this type of courses, for many simulation programs are open source software or freely available for different computing platforms (Linux/Unix, Windows, Mac) with detailed manuals and technical support (Chiang et al., 2013). Hence, it is fairly easy for undergraduate students to obtain and learn such software.

However, such multiscale simulation methods in various fields are not magic. Three decades ago, David N. Perkins of Harvard University proposed five facets of any learning environment which can

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be a good framework for evaluating educational technologies (Flori, 1997). Perkin's five facets are information banks, symbol pads, "phenomenaria", construction kits, and task manager, as shown in Figure 1a. R. E. Flori, Jr. (Flori, 1997) argued that although educational technologies might facilitate communication and promote cognition to some extent, it is difficult to develop software with task management capability which is considered to be the most important facet in achieving the aims of education. On the other hand, as demonstrated by M. Abdulwahed and Z. K. Nagy (Abdulwahed & Nagy, 2009), the learning outcomes can be enhanced significantly by introducing modern teaching technologies (such as remote or virtual lab sessions), since those activities can (e.g., virtual lab sessions) facilitate the active experimentation (AE) of Kolb's cycle (as demonstrated in Figure 1b). According to M. Abdulwahed and Z. K. Nagy's quantitative results of application of Kolb's experiential learning theory to laboratory courses, using the virtual lab in the preparation stage of a chemical engineering laboratory session can result in a better activation of the prehension dimension in Kolb's cycle. Therefore, the application of multiscale simulations to technical courses has a great potential in teaching practices, as they can contribute to the active experimentation ability of students which allow undergraduate students to realize the concrete experiences stage, based on Kolb's experiential learning theory.

In recent years, the number of enrolled international students increases significantly in China (Yu & Xie, 2021) before the breakout of COVID-19. However, the impacts of pandemic on international students are serious, since a large fraction of international students were locked out of the country. Therefore, it is of great importance to improve the efficiency of distance education by modern technologies (e.g., multiscale simulations), as many international undergraduate students solely rely on remote education. In this manuscript, several examples of applications of multiscale simulations to the teaching of principles of chemical engineering at undergraduate level were addressed. As broad topics on transport phenomena are covered by the principles of chemical engineering course, the selection of appropriate simulation examples is crucial due to the limited class hours. Hopefully, undergraduate students majored in chemical engineering can have a better understanding of fundamental laws of their important technical courses based on such introductory study materials of various simulations.

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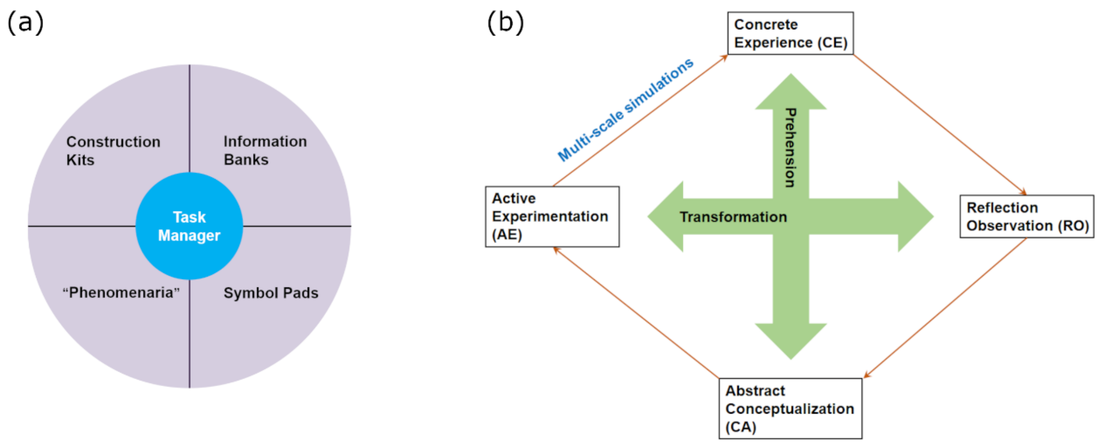

Figure 1: (a) Perkins' five facets of a learning environment. (b) Kolb's Experiential Learning Model.

2. METHODS AND DESIGN

As demonstrated in Figure 2a, using Google scholar and PubMed as the search engines, it is found that the number of publications per year which contain the keyword "molecular dynamics" increases dramatically during last three decades. And a schematic representation of various simulation methods is present in Figure 2b. Those methods not only become more widely used in academia and industry but can also elucidate complex physical and chemical reactions to engineering students. As shown in Figure 1b, multiscale simulations allow students to develop active experimentation capability. Traditionally, such capability is supposed to be achieved by engineering laboratory courses. Nevertheless, undergraduates usually only follow the protocols in the lab which might be very ineffective. By the way, some fundamental laws taught in principles of chemical engineering course such as the momentum/heat transfer phenomena at microscale can hardly be covered by common laboratory courses. Thus, the molecular scale simulations can be a good supplement to the traditional lab training. And these molecular scale simulations not only can be integrated with conventional chemical engineering experiments as described above, but can also be used independently in any theoretical lectures that would benefit from a quantitative approach to molecular dynamics – transport phenomenon relationships.

The principles of chemical engineering which is considered to be the most important core course for undergraduate students majored in chemical engineering, has covered both the fundamental laws behind transport phenomena and typical unit operations of chemical engineering. As a result, the processes addressed by this course range from molecular scale transportation (e.g., diffusion) to industrial scale operations (e.g., distillation). To provide direct impression of such processes to undergrads who have not been to any real chemical plants nor have used electronic microscopes can be a challenging job. As can be seen from Figure 2b, simulations at different scales might be the best

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approach for undergraduate students, since small scale simulations can be performed even on students' laptops.

The simulation activities described in this manuscript require no previous experiences with molecular dynamics simulation software (e.g., Lammps (Plimpton, 1995)) or visualization software such as VMD (Humphrey et al., 1996; Sung, 2011). We offer a step-by-step method to both domestic and international undergraduate students who are interested in molecular scale simulations and analysis. And we also encourage students to write simple code to simulate the simplest systems which might be helpful for their future careers.

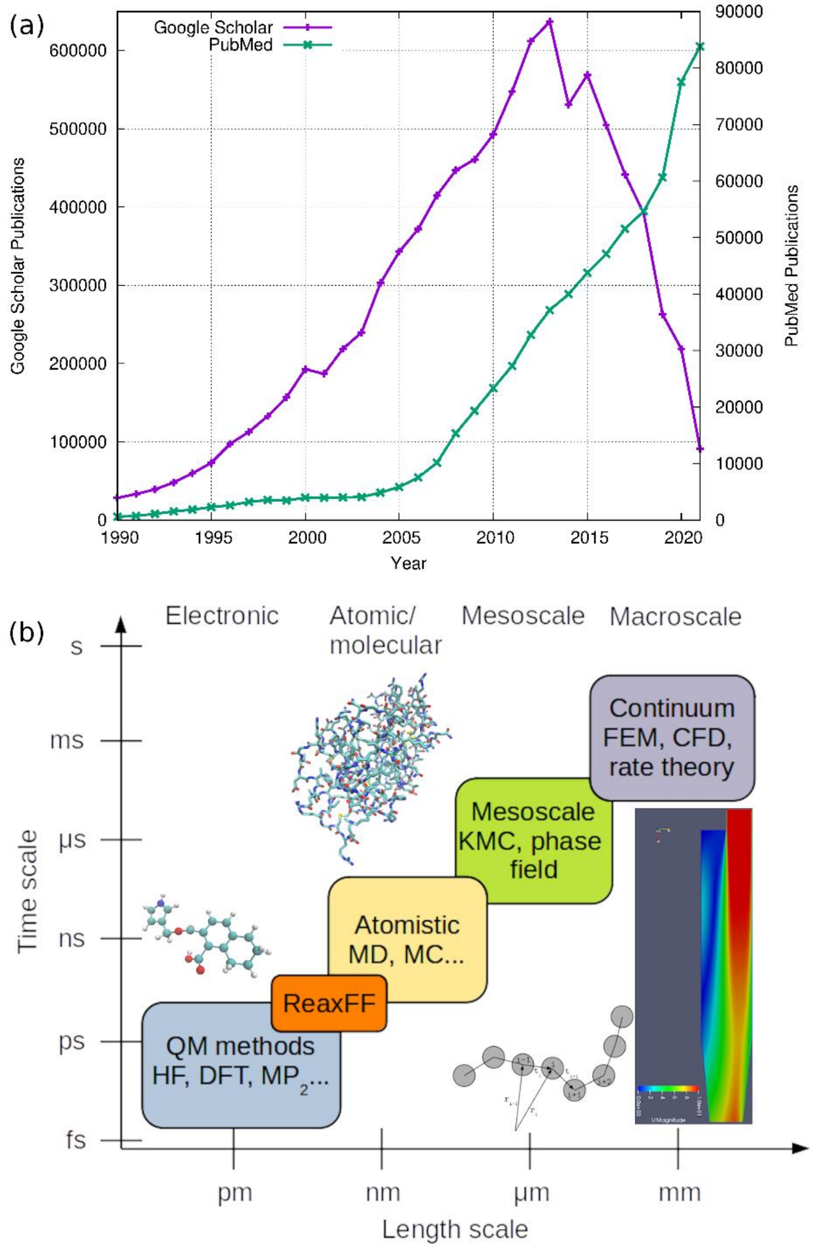

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Figure 2: (a) Number of research articles published per year with keyword "molecular dynamics" versus year (by Google scholar & PubMed). (b) Schematic representation of multiscale simulations.

3. DISCUSSIONS

3.1 Transport phenomena at molecular level

Any specific unit operation of chemical engineering is involved with the transport phenomena (momentum transfer, mass transfer, and heat transfer). The development of quantitative models of unit operations relies on deep understanding of transport phenomena at molecular level. For example, it might be difficult for some undergraduate students to understand the concept of control volume in fluid mechanics, which can be addressed in a simple fashion in molecular simulation. And before performing the Reynold's experiment in a laboratory course, a simple molecular dynamics simulation of shear using LAMMPS package can provide undergrads with direct impression of laminar flow and shear flow, as shown in Figure 3a. Such simulations allow students to achieve better activation of the prehension dimension in Kolb's cycle before taking a lab session. Moreover, some details of the molecular simulations were discussed in our course, specifically the Lees-Edwards boundary condition applied in common non-equilibrium molecular dynamics method (NEMD). The reason is that the Lees-Edwards boundary condition reflects the idea of laminar flow which can help students realize the difference between laminar flow and turbulent flow.

Another example of molecular transport phenomenon is molecular diffusion as demonstrated in Figure 3b. A build-in example of LAMMPS software of diffusion of colloidal particles with solvent particles was discussed in classes. The molecular diffusion is related to both mass transfer and heat transfer. Thus, this example can be integrated to different sessions of principles of chemical engineering course. Moreover, the example shown in Figure 3b can also be used for explaining Brownian motions to undergrads. With increasing size of colloidal particles, the Brownian motions of colloidal particles become weaker, which explains that during sedimentation process the Brownian motions of large particles can be neglected.

Other than these configuration approach examples; undergraduate students were encouraged to write simple code on simulate the random walks of particles/spheres. Firstly, the random walk of particles is easy to be realized, as those students usually took at least one course on programming language before taking the principles of chemical engineering course. And it is not too difficult to modify this simple piece of code to include multiple particles to simulate the momentum exchange between hard spheres at molecular scale. The students who finished this coding task can receive extra credits for their final grades.

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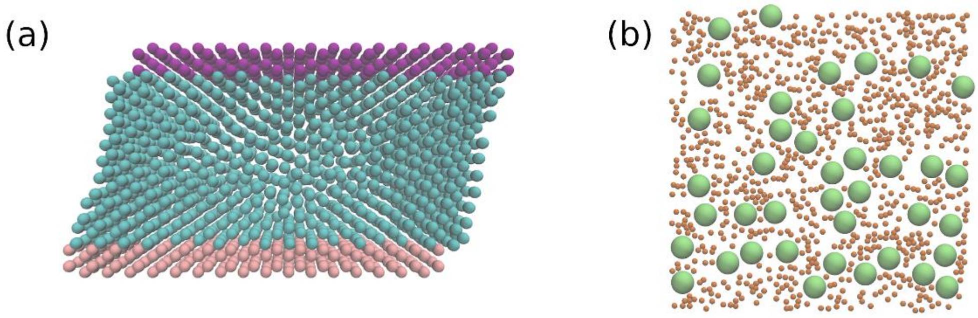

Figure 3: (a) The LAMMPS example of simulation of shear. (b) The LAMMPS example of simulation of colloidal particles with solvent particles

3.2 Chemical reactions by molecular dynamics

Chemical reactions, especially the kinetics of chemical reactions, are usually covered by chemical reaction engineering course instead of principles of chemical engineering course. Because the China University of Mining and Technology focuses on the research of coal industry, an example of investigating coal chemistry by molecular dynamics simulation was also introduced in principles of chemical engineering course, as it is the first chemical engineering course for undergrads. A. C. T. van Duin et al. proposed a reactive force field for molecular dynamics simulation (Duin et al., 2001) which can be used to study most common elements. For most classical force fields adopted in molecular dynamics simulations, chemical bonds which are usually modeled by harmonic springs cannot break even at high temperatures. Hence, the common empirical force fields cannot be used to simulate systems where chemical reactions take place. van Duin's ReaxFF force field which uses the bond order model is one of the most important exceptions. Recently, a large number of research articles have been published, investigating the kinetics of chemical reactions involved with coal at various temperatures. One example is combustion of lignite molecules at high temperatures as shown in Figure 4 (Yu et al., 2022). The reaction constant of lignite combustion increases rapidly as temperature increases so that undergraduate students can even tell the difference of simulations carried out at different temperatures by naked eyes. Although it is still extremely challenging to study chemical reactions by molecular scale simulations, the ReaxFF molecular dynamics simulation is an ideal tool for undergraduate students as it can bridge the gap between fundamental physics laws and laboratory scale chemical reactions observed by students.

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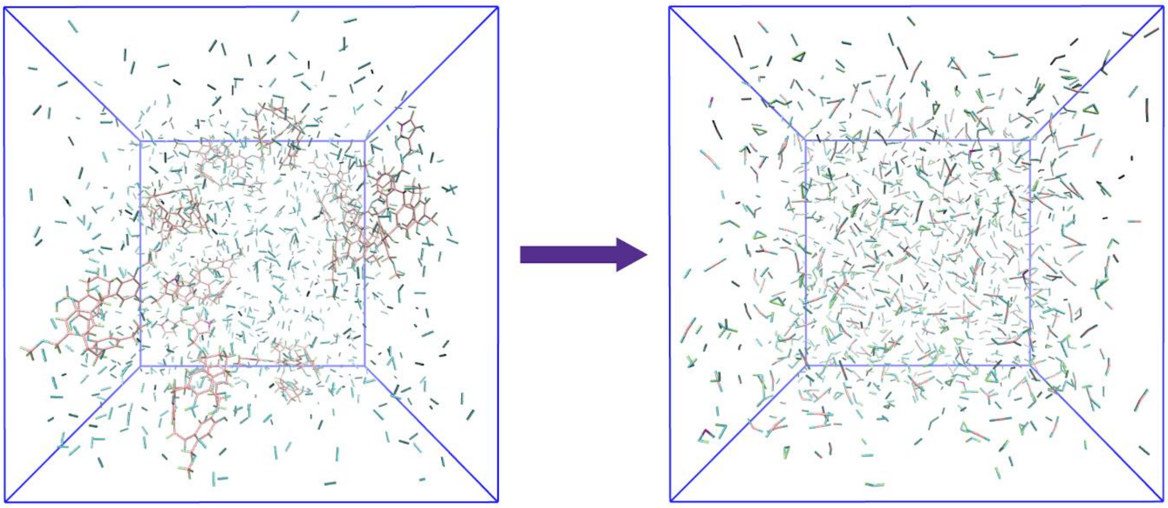

Figure 4: The combustion of brown coal at 3000 K (Yu et al., 2022).

3.3 Parabolic flow in pipe

The most common transportation phenomenon in chemical plant is fluid flow, which is covered in chapter one in many chemical engineering textbooks. With the help of computational fluid dynamics (CFD) software, the flow field can easily be simulated and visualized. The most commonly used CFD software Ansys Fluent is a commercial software. So, in this course, an open source CFD software – OpenFOAM was briefly introduced to students. It is not difficult to generate simple flow field such as parabolic flow by OpenFOAM package. Undergraduate students are encouraged to follow the instructions on the manuals to learn the basic commands for this software. Due to the numerical methods employed by CFD software is not as simple as that used in molecular dynamics simulations and cannot be related to prerequisite courses such as college physics and physical chemistry directly, the CFD simulation of fluid flow is not mandatory for undergraduate students. We hope that this brief introduction of CFD software can warm the students up if they decide to devote themselves into that specific area.

Usually, after taking the principles of chemical engineering course, undergraduate students are supposed to take course about performing process simulation (by AspenPlus or similar software) which is crucial for chemical engineering design. Many students just use the process simulation software as a black box. The introduction of CFD or some other numerical methods can help students partly understand the mechanism of the process simulation software.

3.4 Students' performance

After the breakout of COVID-19 pandemic, many international students cannot get back to campus as a result of various travel restrictions. A combination of SPOCs and traditional education was adopted for international students on campus and out of campus. Due to the disruption by pandemic, a large fraction of undergraduate students become less concentrated in class, especially the students locked out of campus. Traditional teaching practice seems to be very ineffective for those students, as they are not willing to pay attention to the lectures, since it is not convenient for the real-time communication between instructors and students. And many international students cannot follow the derivations of equations during the online study. The introduction of multiscale simulations examples eased this problem significantly, as both the attendance rate and grades were improved (Yu & Xie, 2021).

In addition, many international students were confused about how to use the programming language that they learned to solve the real engineering problem. Since several examples in the principles of chemical engineering course was introduced to students by programming approach, those students began to learn the wide applications of numerical methods in chemical engineering.

4. CONCLUSIONS

The distant education, or more specifically, SPOCs, becomes more and more important for universities nowadays. Due to the pandemic travel restrictions, the routine academic activities of undergraduate students, especially the international undergraduate students, are disrupted. Many novel teaching technologies are introduced which might help undergrads overcome the difficulties of remote education. In this manuscript, we focus on introducing multiscale simulations to an undergraduate course – principles of chemical engineering. The multiscale simulation examples not only allow the international students to obtain deeper understanding of transportation phenomena covered by principles of chemical engineering course, but also improve the programming skills of those undergraduate students. In addition. it is easy to visualized the computational results of the multiscale simulations which seems to be attractive to international students who have been locked out of campus and rely on SPOCs. In sum, even the simple simulation examples can be good supplementary study materials for engineering undergraduate students.

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