Process simulation: when programming is easier than user-friendly packages

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Abstract

This paper presents the comparison of progress trends between the use of programming languages with all its complications for user and commercial packages despite of its ease to application, as well, limitations and obstacles, which could face in simulation procedure. Besides, the aim of this study is to show in practice the opposite derivative trends in chemical engineering education for undergraduate and graduate students.

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1. Introduction

To provide the highest level of successful results in research, scientific and industrial advances, students of engineering disciplines should be trained by expert users who have prior experiences in programming and simulation packages. Thus, education and training must be properly assessed in advance looking forward to the future activity of trainee(s). For instance, future PhD students and R&D engineers should strongly benefit from an early education in programming, despite of future chemical engineers for industry and management, who need less deep but more widespread and general skills. As it is evident, the application of commercial packages and also programming languages, depends on the field of use in industrial and academic areas, which have undergone the most development in recent years, is

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the most dominant, as the lack of use of them in research area, would make invalid and incomplete fate for case study [1-3].

2. Programming

The roles of programming in chemical engineering may not be taking into account less. Although programming skills are not critical to chemical engineering as a final goal, instead are a means to the end of developing engineers capable of solving complicated real problem. Chemical engineers are called upon to prepare the students for the wide variety of computer related issues that may arise in their engineering details, should be an important approach to develop programming [1]. Programming to solve the complicated problems especially in professional level is a complex and precise task for researcher and students. Then, the steps to meet the level of efficiency and usability for user should be scheduled in advance. In this level of learning and training for researchers, who are interested in developing their requirements by programming, the basic programming skills may be inadequate. They should also be trained that how to develop GUI, UAM and other applications focusing on the professional aspects of chemical engineering programming. The necessity of broaden their understanding and training level in programming in prior levels than PhD or being industrial researcher, makes sense [2]. Although first steps of programming almost face with relatively high unsuccessful results, also user is confronted with complex programming design, which would need to have a strong background of mathematics, it is preferable to insist applying programming languages as the key to solve the core problems that is much more time spending procedure. Learning to program is known to be more problematic than learning to package among students and researches. This causes by not comprehend a range of fundamental programming concepts or carry misunderstandings and misconceptions about programming well [2].

3. Commercial package issues

Although simulation packages are based on professional programming language(s), their application is so easy for novice users. It means there is no necessity for user to have deep knowledge about the structure or/and the solving methods, which have been implemented in the package. In other words, it is the definition of user friendly interface that it can be used by anyone who is familiar with the package in his/her field. Some advantageous of the use of commercial packages are undeniable. It can be mentioned their effectiveness and efficiency which make them so clear and easy to learn and use, also would make the situation to user to do what she/he is supposed quickly and in the least time, also the most important property of them, being user friendly interface which creates more intuitive atmosphere, in some case to encourage the user to apply it without any ambiguous or confusing points. Eventually, it can be stated that the package with focus on process engineering applications is included the general properties such as: physic-chemical properties databases, component databases, thermodynamic databases, general models, validated models in thousands of applications which is no need to know numeric concepts of them.

4. Combination of programming and simulation tools

These days, using the simulation packages available commercially for application of industrial and academic purposes is becoming widespread. It depends on the nature, precise, speed and purposes of the effort for simulation that chooses the preferred package. Being familiar with the programming language(s) and also simulation method, which coupled with the package in critical situations in the case of facing with some limitations that simulations are not able to show the real results, is indubitable. The model used in the package, as common, is the basic model that it is not included the models in detail as it
is desirable for user. In this point, the limitation of application of package is evident. To troubleshoot, the following step should be adding the model provided by user which, would be so detailed and more complicated due to its dynamic nature and the methods would be solved the equations (PDE). Although the procedure of the programming, which is included the planning, testing, trying to correct the grammatical and structural errors of codes, selecting the best mathematical method to solve the equations, in the case of optimization, decide on the appropriate optimizing method which is efficient and also time saver, makes the process of using the programming language problematic, it would be assured consistent and precise results for favorite conditions of user. On the other hand, to approach the programming goals, possessing the profound knowledge of programming language, problem solving and methodologies to implement, with all basic concepts is necessary. No doubt, in the case of developing the code, the user would consume more time and precision to gain the desired results. In parallel training of package and programming, students should be given more motivation to deepen their skills of broader programming concepts to extend their own program and not make them confused for facing the limitation in package as unsolvable problem. To evaluate the desired level of results, the user is expected to design an equipment with his/her own models and parameters, including all specification of variables, parameters, conditions, implement model equations such as material and energy balances, adequate numerical methods to solve and execute them. In the case of using the package, the progress is so fulfilled until reaching to the limitation level, which is not able to adjust the parameters to access reasonable results. The alternative option would be programming and using UAM to link into the package. The package in this study is able to predict the behavior of the process by time.

![Diagram](image-url)

**Fig. 1. Programming embedded with commercial package**

It provides the option to add the user model inside the package with his/her own graphical interface. Actually, the option of user added model (UAM) should overcome all difficulties including definition of parameters, which in some cases, are exceeded more than hundred parameters, specification of them one by one to identify for package by name, description..., specifying data types, optional initialization or default value, add the equations as the user models, model algorithm, methods to solve the equations with optional programming languages, which would make it so complicated. In the case of thermo interface,
the user should add the list of his/her components as pure components and their properties which should be supported by package along with all calculation methods. Also it needs to specify the structure of model class in advanced steps [see for example 4, 5].

5. Case Study

Methanol synthesis already presented elsewhere [6] has been selected as the case study in this work. The main cause of this selection is related to the complexity of fixed–bed tubular reactor for methanol synthesis from syngas. Methanol synthesis plant is known as a key chemical process on account of its application in production of numerous raw materials, solvents and also its potential in energy saving and use as the alternative fuel. Therefore, focusing on optimization of its production is so interesting for industrial purposes, in aspect of energy sector, try to increasing the profit and also, environmental goals. In this work, it has been simulated the methanol synthesis process by simulation package and presented the results in following to discuss more and compare with the results of programming which it has been done in previous work of authors. No more details are given about the model, for the sake of conciseness. Some relevant profiles resulted of methanol synthesis reactor simulation by commercial package are presented in the Figure 2-3.

![Fig. 2. (a) yield of methanol; (b) reactor temperature through the reaction](image1)

![Fig. 3. (a) yield of methanol; (b) reactor temperature through the reaction](image2)

In spite of the acceptable results from simulation package for this methanol production in different flow rates of reactants passing through the reactor per unit of time, it is observed that in higher flow pass the production increases (Figure 2a). However, increasing the production more may cause exceeding the
temperature of reaction from hot spot due to its exothermic nature (See Figure 2b). As it shown in Fig. 3., Lifetime of the catalyst in high porosity which fresh catalyst is applied in packed-bed, the amount of production is reasonably more than the case its void fraction is smaller (Figure 3a-b). According to the basic model that simulation package is benefited from, the possibility of providing the improved results with consideration of extra functional factors declines. For example, some limitations which user faces to apply such as: specification of the catalyst (its shape, material, porosity, density, etc.) is highlighted. In contrast, the use of programming solely to model and simulate the process would be resulted in according to the thresholds and high controllability of the process. It can be also pointed to the limitation in the selection of the reactor configuration as one of the most important factors to meet the higher methanol production. To overcome all of these lacks and problems, it would be required the skills of analyzing data and results derived from package and then developing by strategy of coupling the user added mode (UAM), which could be effective to rectify the limitation of the package. Analysis the results with the proposed models which has been presented based on programming in the work in methanol synthesis reactor, illumines the abovementioned differences between programming and commercial results.

5.1. Analysis of educational level

The outline of learning procedure and its final results by covered limitations, which is focused in commercial package and programming in progress trend, is presented in Figure 4. After some criteria period which lasts almost 2-3 months and also depends on the speed of training procedure, in learning step, programming skills qualitatively would be augmented abruptly.

As it indicated in the results of the survey, although, there is no exact statistical samples to present the precise training trend quantitatively, it has been qualitatively obtained that the progress of learning and applying the programming languages after 2-3 months with non-stopped and severe attempts would be
satisfied and the growth in higher standard rises up sharply, however, in this period, the progress in the skill of simulation package remains in the same level, smoothly.

6. Conclusion

It is worth stating that the selection of simulation package or programming language must be weighted expecting to the final target to apply, deliverable, time to achieve the results and the availability for training. Engineers, especially the ones close to our fields such as chemical, process, and energy engineers, should be skillful in programming in some cases to solve their model problems directly. After approaching to limitation boundary in commercial packages, which basic model in package couldn’t prepare satisfied feedback, the user immerses into the deep process that he/she must essentially apply a programming language. Engineers could be able to break down their own problems into the probable phases or periods in programming languages and develop the required. Basically it would be essential to strengthen their education, experience and skills in programming and solving methods, which are challengeable concepts in programming to conduct into cope the problems.

References

[1] Silverstein D. Template based programming in chemical engineering courses. Proceeding of the 2001, American society for engineering education 2001; session 3513.

[2] Shuhidan S, Hamilton M, D’Souza D. Understanding novice programmer difficulties via guided learning. Proceeding of the 16th ITiCSE. New York: 2011; p.213–217

[3] Tan P, Ting C, Ling S. Learning difficulties in programming courses: undergraduates’ perspective and preception. IEEE, Kota Kinabalu 2009; p. 42–46

[4] Manenti F, Buzzi-Ferraris G, Pierucci S, Rovaglio M, Gulati H. Process Dynamic Optimization Using ROMeo.. Comp Aided Chem Eng 2011;29:452-456.

[5] Signor S, Manenti F, Grottoli MG, Fabbri P, Pierucci S. Sulfur Recovery Units: Adaptive Simulation and Model Validation on Industrial Plant. Ind Eng Chem Res 2010;49:5714-5724.

[6] Manenti F, Cieri S, Restelli M. Considerations on the steady-state modeling of methanol synthesis fixed-bed reactor. Chem Eng Sci 2011, p.152-162