# The Use of Computer-Aided Process Design and Simulation Tools in Undergraduate Research Projects

Sivakumar Kumaresan[a], Dominic C. Y. Foo[b], Ramlan A. Aziz[a,*], Mohamad Roji Sarmidi[a]

[a]*Chemical Engineering Pilot Plant, Universiti Teknologi Malaysia, 81310 UTM Skudai, Johor, MALAYSIA.*
[b]*School of Chemical and Environmental Engineering, University of Nottingham Malaysia Campus
Jalan Broga, 43500 Semenyih, Selangor, MALAYSIA.*

## Abstract

This paper demonstrates the use of computer-aided process design (CAPD) tools in guiding undergraduate research projects. Over the past two years, SuperPro Designer, a batch process simulation software has been integrated into the one-year undergraduate research projects at the Chemical Engineering Pilot Plant, Universiti Teknologi Malaysia (CEPP, UTM). Four different research projects were successfully carried out and it was found out that the CAPD tools serve as good educational concept in delivering different modes of learning. It was also found that through the use of simulation software that the students underwent all six levels of Blooms Hierarchy of learning.

*Keywords: Engineering Education, Blooms Hierarchy, computer-aided design, undergraduate research project.*

## 1. Introduction

Computer Aided Process Design (CAPD) tools have been widely used in the bulk and petrochemical industries since the early 1960's. It involves the use of computers to perform steady-state heat and mass balancing as well as sizing and costing calculations for a process [1]. However, these CAPD tools have only emerged for batch chemical production in the past decade [2]-[7], many works remain to be done on this relatively new area.

In this work, we focus on how using a process simulation software can help in the students' learning of batch process modelling, optimisation and engineering economics. From our point of view, the aim of higher education in engineering can be summed in the saying by Confucius, "The essence of knowledge is in having it to apply". Thus when we embarked upon these student research projects, our aim was to ensure that they were able to apply the knowledge they received through classroom teaching into the real life industrial case studies via the use of a process simulation software.

The batch process simulation software used in the various student research projects is SuperPro Designer (SPD) developed by Intelligen, Inc. SPD is an integrated software for the modelling and optimisation of biochemical, pharmaceutical, food and environmental processes, which are operated either in batch or continuous mode. It can also handle economic evaluation for a given process design.

One factor that was used to evaluate the effectiveness of the method was to see if it allowed the students to go through most of the levels of Bloom's hierarchy of learning [8]. To recap, Bloom categorised learning achievement by the following six ascending levels and its associated abilities.

i. *Knowledge* - recall of data
ii. *Comprehension* - understanding information
iii. *Application* - applying knowledge to a new situation
iv. *Analysis* - separates information into part for better understanding
v. *Synthesis* - builds a pattern from diverse elements
vi. *Evaluation* - judges the value of information

Four different undergraduate research projects were successfully carried out and the educational aspects gained by each individual student are summarised in the following sections.

## 2. Simulation in pharmaceutical process debottlenecking

* *Corresponding author. Tel: 607-5531571; Fax: 607-5569706; Email: ramlan@cepp.utm.my*

Tan [9] applied batch process modelling to the decision making strategy for a local pharmaceutical plant in their expansion planning. The modelling was carried out on an anti-allergic cream production process as shown in Figure 1. The initial process was limited by the extremely long cooling time required in the main blending section, which is also quite fully occupied in size (90% size utilisation).
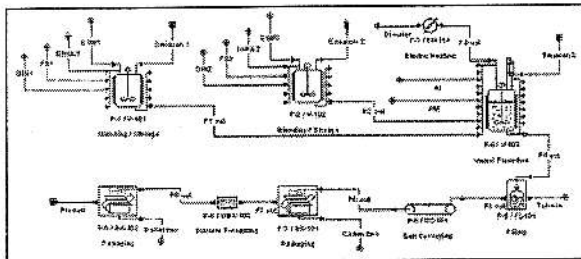


Figure 1. Anti-allergic cream production of a local pharmaceutical plant

Five alternatives were considered by the company to address the time and throughput bottleneck such as incorporating a intermediate storage tank, changing the main blending tank into a multifunctional tank with heating and cooking functions, and adding a new filling machine. The final chosen alternative in Figure 2 had the highest cost-benefit ration (CBR), lower processing time and higher production rate.
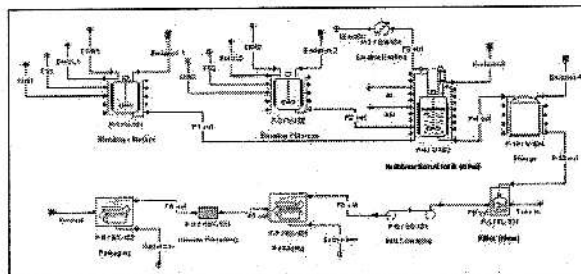


Figure 2. Debottlenecking scheme for cream production

From an educational point of view, the educational aspects gained by the student include:

i. Real process modelling i.e. collecting process data and working within a company environment to do so
ii. Applying economic indexes such as CBR in comparing various process debottlenecking alternatives
iii. Coming up with multiple differing alternatives based on available vendor equipment supplies

## 3. Simulation in feasibility studies

Athimulam [10] applied batch process modelling to the production of Tongkat Ali (*Eurycoma longifolia*) water extract. In his work, he modelled a pilot plant scale operation run at the UTM, CEPP (Figure 3). The objective of his project was to model the current process and propose alternative schemes that would render the process economically attractive as the current process was not economically viable and would not attract technology investors nor build up small to medium enterprises.
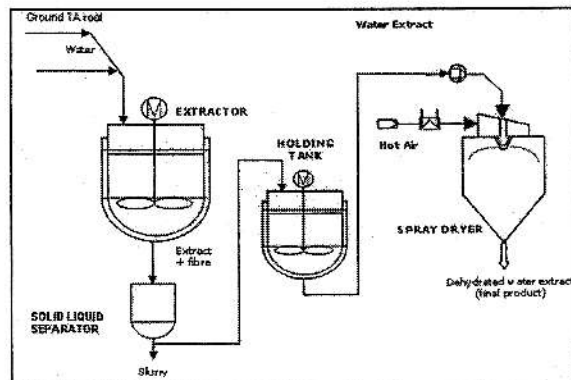


Figure 3. Pilot scale *Eurycoma longifolia* water extract production of CEPP, UTM

The initial production process shown in Figure 3 produced a semi complete product with lower value with extremely long operating time (due to the long duration of spray drying operation). Batch process debottlenecking techniques and engineering economic evaluation were applied and five alternatives were developed. The alternative shown in Figure 4 with the highest rate of investment (ROI) due to the value added step of producing the final product of bottled extract capsules as well as shorter operating time was chosen.

From an educational point of view, the educational aspects gained by the student include:

i. Real process modelling i.e. the student had to gather real process and economic data to integrate into the simulation
ii. Applying engineering economics to the alternatives thus making the student aware of the real applications of economic evaluation

## 4. Process simulation in life cycle analysis

Kuan [11] later extended the work of Athimulam [10] by looking at the environmental aspect on the Tongkat Ali water extract production, via life cycle analysis (LCA)

tool. Based on the optimal manufacturing scheme in Figure 5 [10], Kuan [11] further developed two alternative schemes to consider for the reuse of Tongkat Ali root residue. In Alternative 1, the root residue is used as a feedstock for electricity and/or steam production to supplement fossil fuel. In Alternative 2, the residue is used as feedstock for bio-ethanol production via fermentation route.

Both schemes are modelled using the simulation software and data from the simulation are used in the LCA study. A comparative environmental life cycle inventory assessment was conducted to quantify and compare the comprehensive sets of environmental flows of the two schemes over the water extract production life cycle. Results of the LCA show that Alternative 1 (Figure 5) is the most "environmental friendly" option, with the least environmental emissions, as compared to the energy intensive alternative of Alternative 2.

From an educational point of view, the educational aspects gained by the student include:

i. How to relate the two separate areas of simulation and LCA, which are conventionally usually treated as two different topics.
ii. Simulation software was a good source to obtain emissions data as well as evaluating alternatives.

## 5. Process simulation in process synthesis

Figure 6 show the simulation flowsheet of the polyvinyl chloride (PVC) manufacturing process developed by Chan [12]. This simulation model has been developed based on the operating condition of an existing PVC manufacturing facility. It consists of 10 parallel batch polymerisation reactors, blow-down vessel, and two parallel trains of downstream processing equipment. Each downstream processing train consists of a stripper, two decanters and a fluid bed dryer. The plant is operated in a semi-batch mode where upstream reactors are scheduled to match the downstream processing trains that are operated in continuous mode.

The simulation model was later used as the case study on water minimisation (via water pinch analysis). Water flowrates and the corresponding start and end time of each water-using operation were extracted from the simulation model. Two scenarios were considered, i.e. network with and without water storage systems. Flowrate targeting for both scenarios were conducted using the recent developed water pinch technique [13].

From an educational point of view, the educational aspects gained by the student include:

i. How to model an existing batch PVC manufacturing plant based on the plant operating condition.
ii. The interaction between process analysis (simulation) and synthesis (water pinch analysis) tools

## 6. Conclusion

In the four projects undertaken by the students it was clear that they all went through the six levels of the Bloom hierarchy. Through the use of the simulation software, they had to recall their knowledge such as critical process parameters as well as have clear comprehension of the knowledge and the real industrial data they were seeking such as operating conditions. They then applied their knowledge to the problem at hand, such as when they drew the flowsheets, or analysed the findings from the simulator, etc. The synthesis and evaluation of the proposed alternatives then followed.

In essence the process simulation software served to strengthen their understanding and application of the knowledge received during the undergraduate education. We believe that the incorporation of simulation tools as early as possible within the undergraduate career would further enhance their ability to comprehend process information, design feasible alternatives and evaluate process viability.

A similar conclusion can also be made for the professional training run by CEPP for practising engineers, where the same software tool was used to guide engineers in modelling and optimising batch process operations [14, 15] and wastewater treatment facilities [16]. Participants who attended the training were from the biochemical, polymer, pharmaceutical, and wastewater treatment sector.

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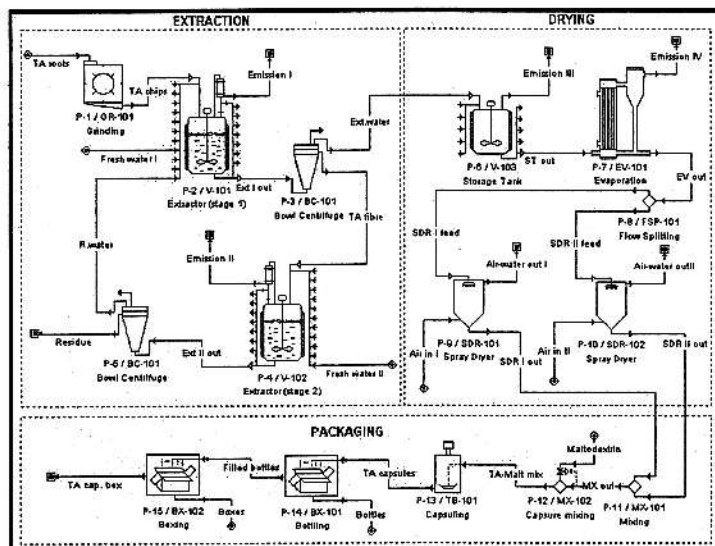
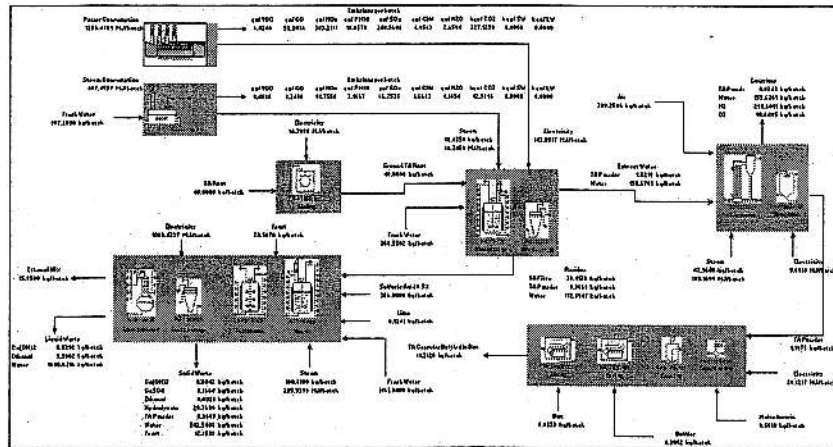Figure 4. Optimal Tongkat Ali water extraction production with highest ROI value
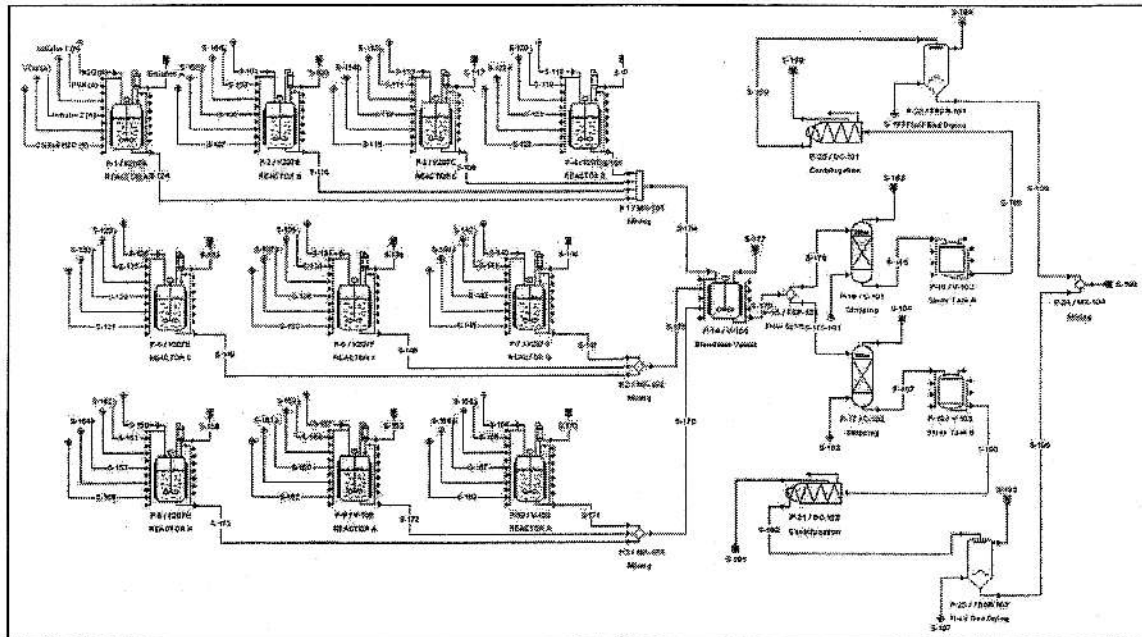
Figure 5. LCA of Tongkat Ali production [11]



Figure 6. Simulation flowsheet for PVC production