

Automation of Practice Problem Generation for Reactor Engineering

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Introduction

Reactor engineering is a fundamental paper in the chemical engineering curriculum. It forms part of the core knowledge of the degree and is required as part of accreditation by the Institution of Chemical Engineers, the body that accredits Chartered Chemical Engineers internationally. However, this paper is often difficult for the students, as it involves problem formulation using mathematics, and watching an instructor go through some problems in depth, as recommended by Woods et al. (2000), is insufficient to cement the knowledge. Learning how to solve these problems can only be properly done through repeat practice, by learning how to apply a common strategy (Woods et al., 2000).

To engage with these problems the students are encouraged to apply the Polya (1957) problem solving strategy, where the students need to understand the problem, devise a plan, carry out the plan and then look back. This is similar to the McMaster strategy (Woods et al., 2000) which involves engaging, defining the problem, exploring, doing it and looking back. However, these strategies require access to a large pool of practice problems, so that the students are not repeating the same problem over and over again, and thus not actually testing the strategy but rather memorising how to solve something very specific.

With the advent of computers there has been a shift to using technology to enhance learning. Some subjects have been fast adopters, such as simulations being used extensively in control theory with commercial packages such as ASPEN PLUS and Hysys Plant (Komulainen et al., 2012). However, there are other tailored examples, such as Cress et al. (2012), who developed a computational MATLAB tool to assist students with problem solving-skill development with specific course modules in mind, such as engineering biology and electrical engineering, which the students found helpful. Molina et al. (2018) also created a MATLAB based application with a graphical user interface for estimating parameters in chemical kinetic problems.

Another way that simulation has been integrated is through 'virtual laboratories', such as those presented by Naukkarinen and Sainio (2018), Domingeus et al. (2010) and Rafael et al. (2007), who have used it to overcome limitations of hands-on experiments. These simulation packages and virtual laboratories are often not intended to check solutions that can be worked through by hand, and are often used to simulate much more complex systems where the technology is mandatory (e.g. for simulating the dynamic operation of a plant).

Therefore, simulations and virtual laboratories do not necessarily guide you with respect to how to solve the problem, so much as allow you to explore the system and understand how it works. The aim of this work was to cement the problem solving strategy, and hence, this work focuses on the generation of a multitude of practice problems with guided solutions, similar to the work done by Lim (2017) for teaching fluid-solid systems. Lim created a friendly user interface to generate both the problems and the solutions, that the students can compare their hand-written ones against. The students found it useful and the marks were on average higher for the students that used the module.

The aim of this project was to augment the practice problem space available for students, so that they could learn through adequate practice. Currently, the students receive a nominal number of practice problems that are all paper based only, and there is often a call by the

students for more practice problems and worked solutions. However, the lecturer sees the problem structure and how they would approach it, making different problems appear the same to them through experience. This can be captured by creating a programme that can generate a variety of problems, automatically, using the same underlying structure.

The aim of this work was to investigate whether augmenting the available practice problems and detailed solutions, by automating their generation with MATLAB, would enhance the students' problem-solving ability and enable more effective learning. The hypothesis was that having more practice problems available would enable better learning of this subject, which can only be learnt by practice.

Methodology

Problem Generator Tool Development

The first part of this work was developing a tool that could be used to automatically generate problems and, optionally, detailed solutions to chemical reaction engineering problems. The scope of the tool was to include problems with the following specifications:

- Heterogeneous catalytic reactions only;
- Batch, packed bed and continuously stirred reactors;
- Five different types of reaction kinetics;
- Effect of internal catalyst mass transfer;
- Irreversible reactions only;

Effect of external mass transfer and catalyst deactivation were out of scope for this problem generator tool. The tool was created using the MATLAB LiveScript functionality. MATLAB was available to all the students, and they could install on their home computer, and thus use the module at their convenience. The automatic generator had to meet the following requirements:

- Be easy to use, such that no programming knowledge was required. This was to ensure that students were not put off using it if they were not confident with their programming skills;
- Be able to generate a variety of problems with detailed mathematical solutions and clear and easy to follow explanations;
- Be able to optionally select to give the answer only, so that the students can check against the answer first before asking for a detailed solution;
- Provide a large breadth of problems to practice with, including with quasi-randomly generated parameters so that the students focus on understanding the method rather than getting the numbers right.

Students' Feedback

Students' feedback was gathered in the form of an optional survey carried out at the end of the course. The survey was anonymous and confidential and ethics approval was obtained from the University of Auckland Human Participants Ethics Committee. The survey was carried out on-line using Qualtrics and sent out to the class of 65 students. The following questions were asked during the survey:

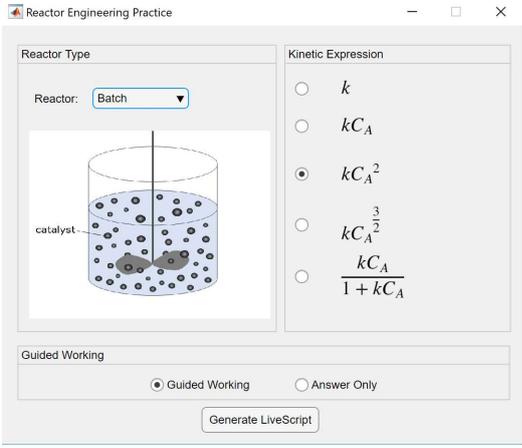
1. How would you rate your familiarity with Matlab?
2. Did you use the LiveScript Matlab module?
3. Approximately how many practice problems did you go through with the module?
4. How would you rate the useability of the module?
5. How would you rate the usefulness instructions for this module?
6. Did you try modifying the live scripts in order to create your own practice problems?
7. Did you require significant Matlab knowledge to be able to run this resource?
8. What did you like the most about these learning resources?

9. What did you dislike about these learning resources?
10. What improvements or changes would you like to see in the future that you think other students would find useful?

Results and Discussion

Problem Generating Tool

A practice module was developed, that could be run using an easy to use interface, as shown in Figure 1a. In the interface the student could select between five different reaction kinetics and three reactors (continuously stirred tank reactor, packed bed reactor and batch reactor), and could choose to have the answer only or have guided working provided.



(a)

Chemical Reactor Engineering Practice Problems

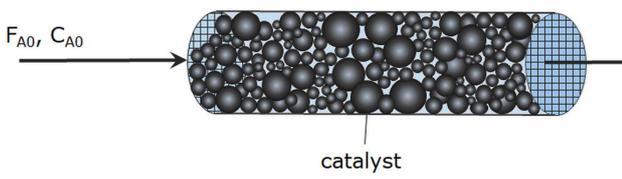
Problem Statement

What is the volume of catalyst required for a packed bed reactor that is converting A to product according to the following kinetics:

$$-r_A = 0.01 C_A^2 \frac{\text{mol}}{\text{m}^3 \text{cat.s}}$$

You have the following information:

- Initial concentration of A fed into the reactor of 150 mol/m³ at a rate of $F_{A0} = 20,000$ mol/hr.
- Conversion of 90 %.
- Internal catalyst diffusion coefficient, D_e , of $5.22 \times 10^{-6} \frac{\text{m}^2}{\text{s}}$.
- Catalyst pellet diameter of 3×10^{-3} m.
- Assume external mass transfer limitations are negligible.
- Assume the reaction is irreversible.



(b)

Figure 1: Snapshots of the (a) user interface for generating the problems (b) the LiveScript problem that is generated for the student to practice with.

Clicking on the 'Generate LiveScript' button would create a problem that is within the scope specified in the Methodology section, with quasi-randomised numbers, as shown in Figure 1b. Along with the generated problem, the script would contain a guided methodology for the solution, however the answer itself would not be available until the student ran the script. An example of the type of guided working that is provided to guide the student is shown in Figure 2. Both symbolic equations, populated with the specific problem numbers, and the code (programmed) solution, were provided.

The coded solution, shown in Figure 3, was at the very bottom so that the students were not distracted by the code implementation, but rather used the guided working to understand if they were approaching the problem in the correct way.

The tool is capable of generating over 100 different types of problems, with different numbers, unknowns, reaction and reactor types and with and without internal catalyst mass transfer limitations. The students can choose to omit the showing of the working, so that only the final answer is provided for them to check their working against.

Working

1. What is the design equation for a packed bed reactor?
2. Rearrange this equation in terms of V_s .
3. Is this reaction internally mass transfer limited? Explain.
4. What are the reaction kinetics?
5. Substitute in the reaction kinetics into the reactor design equation.
6. Convert the concentration, C_A , into conversion, X_A .
7. Substitute in the numerical values and integrate the equation to solve for V_s .

Answers.

1. The design equation for a packed bed reactor is:

$$\frac{dX_A}{-r_A} = \frac{dV_s}{F_{A0}}$$

2. The equation in terms of V_s is:

$$dV_s = \frac{F_{A0} dX_A}{-r_A}$$

3. Need to calculate the generalised Thiele Modulus to determine if the reaction is mass transfer limited:

$$M_T = \frac{-r_{As} L}{\sqrt{2De \int_{C_{Ac}}^{C_{As}} -r_A dC_A}}$$

We are assuming this is an irreversible reaction, therefore $C_{Ac} = 0$

$$\text{For } -r_A = k C_A^2, M_T = L \sqrt{\frac{3k C_{As}}{2De}}$$

We are also assuming external mass transfer is negligible, therefore $C_{As} = C_A$

$$M_T = L \sqrt{\frac{3k C_A}{2De}}$$

Figure 2: Guided working provided for the student to follow, in symbolic maths notation, as they would be expected to do the working by hand on paper.

6. Convert the concentration, C_A , into conversion, X_A :

$$C_A = C_{A0}(1 - X_A)$$

$$dV_s = \frac{F_{A0} dX_A}{0.01 C_{A0}^2 (1 - X_A)^2}$$

7. Substitute in the numerical values and integrate the equation to solve for V_s :

$$dV_s = \int_0^{0.9} \frac{2 \times 10^4}{0.01 C_{A0}^2 (1 - X_A)^2} dX_A$$

Matlab Code:

```
syms F_A0 X_A C_A C_A0 V_S dV_S % Define our symbolic variables
% Define concentration of A as a function of conversion
C_A = C_A0*(1-X_A)
% Define the design equation for calculating the volume of solids for a PBR
dV_S = F_A0/(0.01*C_A^2)
```

Now substitute the constants in

```
catalyst_vol = subs(dV_S, [F_A0, C_A0], [(20000/3600), 150])
```

Now integrate the expression

```
V_S = double(int(catalyst_vol, X_A, 0, 0.9)) % Definite integral
```

Now repeat numerically

```
V_S_numeric = subs(dV_S, [F_A0, C_A0], [(20000/3600), 150]);
f_integrand = matlabFunction(V_S_numeric, 'Vars', {'X_A'});
result = integral(f_integrand, 0, 0.9, 'ArrayValued', true)
```

$$C_A = -C_{A0} (X_A - 1)$$

$$dV_S =$$

$$\frac{100 F_{A0}}{C_{A0}^2 (X_A - 1)^2}$$

$$\text{catalyst_vol} =$$

$$\frac{2}{81 (X_A - 1)^2}$$

$$V_S = 0.2222$$

$$\text{result} = 0.2222$$

Figure 3: Snapshot of the solution that is calculated by the code.

Students' Feedback

The modules were made available to the students when the topics were covered, and for study before exams. This was a new resource not made available to the students before, and more could have been done to encourage engagement. The survey results cannot be analysed statistically because the number of responses was insufficient for assessing statistical significance, however some of the responses are discussed below. In this way, the survey ended up being more of an anonymous correspondence focus group.

Figure 4 shows how the students rated the useability of the module, and although ease of use was kept in mind during the design, none of the students rated it as 'very easy'. It is possible that part of this could be due to that to run this on your home computer you have to go through the MATLAB installation first. This creates an extra step. Additionally, most students in this chemical engineering department are not fluent with MATLAB, often having not used it since the first year course, whilst this is a third year course. However, 50% of the students specified that they required 'little' MATLAB knowledge to be able to use this resource, so this is unlikely to be a strong driving factor.

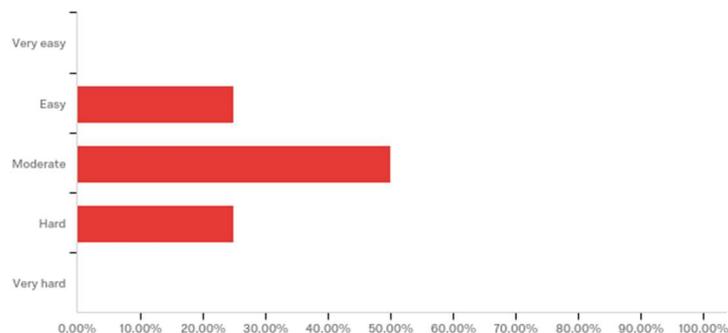


Figure 4: Students' rating of the useability of the module, answer to the question 'How would you rate the useability of the first module?'.

Figure 5 shows that a few students attempted to do a number of problems, with the greatest proportion of students attempting between 1 to 3 problems. There is insufficient information to determine whether the students did not attempt more problems because they found it more difficult to use, or whether the students only needed a smaller number of problems to have sufficient practice with the problem solving strategy.

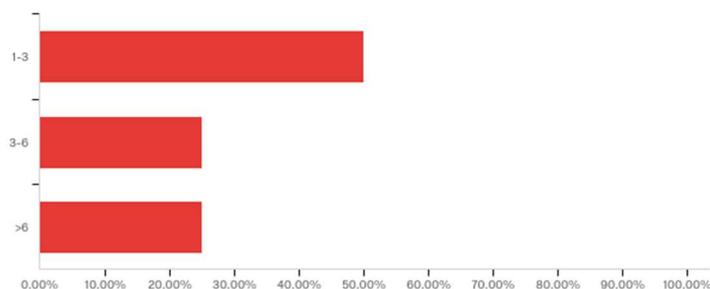


Figure 5: Number of problems attempted by students that tried to use the module, answer to the question 'Approximately how many practice problems did you go through with the first module?'.

There were several questions that were left open for the students to provide their own responses, and some examples of responses are provided in Table 1. It appears that the goal of providing a variety of practice problems and clear worked solutions was successful in as much as the students specifically commented on this. However, it was still not clear why

some of the students found the resource difficult to use, and different questions should have been asked to understand this part of the problem.

Overall, it would have been good to assess whether the students' performance improved in the corresponding tasks, however the response rate and adoption for this year was too low to be able to make this assessment.

Table 1: Responses to open questions in Qualtrics survey.

Question	Example responses
What did you like most about these learning resources?	<i>"The worked solutions showed me step by step what to do"</i> <i>"Variety of problems"</i> <i>"practice more questions"</i>
What did you dislike about these learning resources	<i>"hard to use"</i>
What improvements or changes would you like to see in the future that you think other students would find helpful?	<i>"Make a timed quiz of random problems – this might help as it is like an exam scenario"</i> <i>"providing more detail instructions on how to use the software"</i>

Conclusions and Future Work

An automatic problem generator tool was developed for creating a variety of practice problems and worked solutions for heterogeneous catalytic reaction engineering. The students found the variety of problems and worked solutions helpful, however some of the students found the resource difficult to use, and more work needs to be carried out to figure out the cause behind this. It is recommended the use of this resource be continued and it be introduced earlier in the course, with a demonstration of its use during a tutorial session to increase engagement. It was found that a key part of developing a resource such as this is not just the creation of it, but also integrating it well into the course and engaging the students with it to enable them to take advantage of it.

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