A TExT for Engineering Education in the 21st Century

2. A Sample Study Unit

The traditional lecture format is the predominant teaching method employed in undergraduate engineering education in the United States\(^1,2\). At the same time, concerns are being raised that the effectiveness of engineering education needs to be improved\(^3,4\), and consequently, it has been suggested that teaching methods need to be changed\(^2\). Research shows that when active learning is properly implemented and used as a teaching method, it is much more effective than the conventional lecture format\(^4-10\). However, most undergraduate engineering instructors do not have much, if any, experience with non-traditional teaching methods such as active learning, either as student or as instructor. As a result, and in light of significant non-teaching demands on their time, many engineering instructors continue to use the traditional lecture approach.

For engineering instructors in many fields and areas, the most readily available teaching resource is the textbook they select for use in their course. Textbooks provide for information transfer to the students, assuming the students actually read them. Textbooks usually also provide a wealth of problems and examples that can be used for learning and in assessment. Many also provide tools like computer codes that are useful in solving problems in the field. In most cases, however, textbooks fail to provide resources for teaching the subject in the classroom, and particularly so in the case of teaching approaches such as active learning. Such resources are available from other sources, particularly via the internet, but this imposes upon the instructor the additional burdens of locating suitable teaching resources, modifying them to fit their specific course, ensuring that pre-requisites are incorporated earlier in the course, and deciding exactly how to implement their use in the classroom.

An alternative to this situation would be to replace current day textbooks with toolkits for exceptional teaching (TExTs)\(^11\). A TExT would provide all the same resources currently provided by textbooks along with additional resources for both the student and the instructor. For students, in addition to written objectives, information and examples, the TExT would provide videos with content corresponding to the lectures of the traditional teaching approach. However, these video lectures would be used by the students outside of the classroom, ideally just prior to the corresponding class meeting. For the instructor, the TExT would provide (a) slides and notes that could be used in class to briefly review the material from the readings and videos assigned for that day, (b) a catalog of learning activities from which to choose for in-class use on the assigned topic, and (c) any necessary simulators, etc. that are needed for the learning activities. Most importantly, each learning activity would include a lesson plan describing how to implement its use in the classroom and a listing of additional supplies, if any, that are needed. These learning activities would be completely integrated with the readings and lecture videos so that the nomenclature is the same, and the students would already have gained any pre-requisite knowledge for the activities in prior classes, readings and lectures. Of course the TExT would also provide the instructor with solutions for all the examples and problems. It would additionally provide a grading rubric for each example and problem that indicates relative credit.
Replacing conventional textbooks with such TExTs, or supplementing textbooks so that they become TExTs, could pave the way for a widespread transition in engineering education away from the traditional lecture approach toward more effective active learning approaches. This bold statement presupposes several untested hypotheses to be true. Specifically, in order for TExTs to effectively facilitate the widespread adoption of active learning in engineering education, the following must first be demonstrated:

- that an instructor would be able to implement active learning via the resources supplied with the TExT without investing significantly more time than would be invested in teaching via the traditional lecture
- that by providing lesson plans and teaching instructions for each learning activity, an instructor without an education background or prior experience involving active learning, will be able to implement active learning effectively (i.e. so that student learning improves relative to the situation where the same instructor used traditional lectures)
- that engineering instructors who currently teach using conventional lectures will be willing to change to active learning via a TExT (assuming the first two points are successfully demonstrated)

Through an NSF Award from the Division of Undergraduate Education entitled “TExTs for the 21st Century” (DUE Award No. 0736495), a prototype TExT in the area of chemical kinetics and reaction engineering is being developed in order to test the three postulates enumerated above. An overview and a more thorough exposition of the objectives have been presented previously along with a description of how a course in kinetics and reaction engineering is being taught using the available parts of this prototype. The purpose of this poster presentation and conference proceedings contribution is to demonstrate and describe each of the components of a representative study unit from the prototype kinetics and reaction engineering TExT.

The content of the prototype TExT derives from the undergraduate course on chemical kinetics and reaction engineering taught by the author. The course content was divided into four parts, and each part was further divided into multiple sections. The sections are then comprised of “Study Units” that correspond roughly to 20 minutes of a traditional lecture. The subject matter of parts I through III (see below) is included in most first courses in kinetics and reaction engineering nationwide, while the inclusion of the topics in the fourth part is more varied. Therefore, while the ultimate plan is to create all four parts of the TExT, it was determined that completion of the first three will suffice for the purpose of creating a prototype that can be used for testing the hypotheses above. The following is an outline of the four parts of the TExT and their sections (in the interest of space, the individual Study Units are listed for part I, but only the number of Study Units is given for parts II through IV):

I. Chemical Reactions
A. Introduction
  1. Definitions
B. Review
  1. Stoichiometry
  2. Quantifying Reaction Progress
  3. Reaction Energetics
  4. Reaction Equilibrium

II. Chemical Reaction Rates
  A. Introduction (2 Study Units)
  B. Generating Kinetic Data (9 Study Units)
  C. Proposing a Rate Expression (12 Study Units)
  D. Validating a Rate Expression (5 Study Units)

III. Engineering of Ideal Chemical Reactors
  A. Introduction (3 Study Units)
  B. Perfectly Mixed Batch Reactors (4 Study Units)
  C. Continuous Flow Stirred Tank Reactors (7 Study Units)
  D. Plug Flow Reactors (4 Study Units)
  E. Matching Reactors to Reactions (9 Study Units)

IV. Non-Ideal Reactions and Reactors
  A. Alternatives to the Ideal Reactor Models (5 Study Units)
  B. Coupled Chemical and Physical Kinetics (10 Study Units)

The Study Unit on “Reaction Equilibrium” from part I, section B (Study Unit 4) is representative of a typical Study Unit and has been selected for use here. Students taking the course using the TExT would have the following resources available to them for this Study Unit: a list of learning objectives, an information reading, an information video, an examples reading, an examples video, and several additional problems (some with and some without solutions). All provided solutions include a grading rubric, as already mentioned.

As the outline shows, the “Reaction Equilibrium” study unit is encountered early in the course. Prior to this unit, the students will have learned how to quantify the composition of reacting mixtures through the use of reaction progress variables including the fractional conversion and the extent of reaction. They will also have learned how to calculate the enthalpy, entropy and Gibbs free energy changes accompanying a chemical reaction by making use of the fact that these are state functions.

TExT Components for the Students

In the “Reaction Equilibrium” study unit, the students are provided with the following objectives:

After completing this unit, the student should be able to
1. write and use the equation for the equilibrium constant at 298 K in terms of the standard Gibbs free energy change at 298 K.
2. write and use the equation for the equilibrium constant at any temperature T in terms of the equilibrium constant at 298 K and the (temperature-dependent) standard heat of reaction.
3. write and use the equation relating the equilibrium constant for a reaction to the thermodynamic activities of the participant species.
4. write and use equations relating the thermodynamic activity of gases, liquids and solids to the composition of a mixture containing them.
5. calculate the final equilibrium composition of a reacting mixture given the initial composition, temperature and pressure.
6. analyze a chemical reaction to determine how the final equilibrium composition will be affected by a change in temperature, pressure or the initial composition.

The information reading and information video lecture are similar to material found in almost any undergraduate chemical engineering thermodynamics textbook, so only a brief overview will be offered here. The information reading and video discuss the theory and equations necessary for meeting the objectives set forth above. Equations (1) through (9) are among those that are presented and discussed.

\[ K_{j(T)} = \exp \left( \frac{-\Delta G^0_{j(T)}}{R(T)} \right) \]  

(1)

\[ K_{j(T)} = K_{j(298 \text{K})} \exp \left\{ \int_{298 \text{K}}^{T} \frac{\Delta H^0_{j(T)}}{RT^2} dT \right\} \]  

(2)

\[ K_{j(T)} = \prod_{i=\text{all species}} a_{i,j}^{\text{v}_{i,j}} \]  

(3)

\[ a_i = \frac{y_i P}{1 \text{ atm}} \]  

(ideal gases)  

(4)

\[ a_i = \frac{y_i \phi_i P}{1 \text{ atm}} \]  

(non-ideal gases)  

(5)

\[ a_i = x_i \]  

(ideal solutions)  

(6)

\[ a_i = h_i x_i \]  

(non-ideal solutions where \( i \) obeys Henry’s law)  

(7)

\[ a_i = \gamma_i x_i \]  

(non-ideal solutions)  

(8)

\[ a_i = 1 \]  

(solids)  

(9)

The examples reading and video present three example problems that illustrate how the information presented in the unit can be used to meet the stated objectives of the study unit. More specifically, the solutions presented in the examples reading and video illustrate calculation of the equilibrium constant at 298 K and at other temperatures, expression of the thermodynamic activity in terms of composition, and solving for the equilibrium composition. The examples involve different phases (gas and/or liquid), and they illustrate calculations where reaction progress variables are used and those where atom balances are used. For each problem, the solution also includes a rubric that relates each step of the solution back to a learning objective from the TExT and that suggests the relative point value for completion of that step of the overall solution.
In this particular unit, the students are also provided with three equilibrium simulators. These are JAVA applications that calculate the equilibrium composition and conversion. Each simulator is specific to a single chemical reaction: methanol synthesis, reverse water-gas shift, and methyl chloride formation from methanol and hydrochloric acid. These particular reactions were chosen because in two of them, the total moles remain constant, but one reaction is exothermic while the other is endothermic. The third reaction involves a change in the total moles. These simulators are used in one of the learning activities for the unit as will be described presently.

When a simulator is launched, it initially displays a splash screen, Figure 1a, while the program loads, and then presents the user interface shown in Figure 1b. After the students enter values for the initial conditions and click on the “Equilibrate” button, the thermodynamic properties for those conditions are presented in the upper

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**Figure 1.** User interface of the TExT simulator for the equilibration of the methanol - HCl reaction including (a) the splash screen, (b) the initial interface, (c) interface showing the results, (d) the “User Guide” and (e) the “About Box.”
right along with the equilibrium composition information at the lower right and the equilibrium conversion information at the bottom, Figure 1c. The students can access a “User Guide,” Figure 1d, and an “About Box,” Figure 1e, from the menu labeled “Help.”

An instructor using the TExT to teach kinetics and reaction engineering would typically give the class the assignment of reading the information and examples readings and watching the corresponding videos prior to class. They would be told to bring any questions or points for clarification with them to class. If the instructor planned to use an in-class learning activity that involved use of the simulators, then the assignment would also ask the students to familiarize themselves with how the simulators work. (Alternatively, the simulators might be used as part of an after-class assignment, or they could simply be provided for the students’ self-use.)

Depending on the length of the class period, the instructor might assign one or more additional study units in a similar manner.

Thus, in principle, when the students arrive for class, they have already experienced a traditional lecture on the subject at hand via the assigned videos, and they have also read the corresponding written materials. In the author’s experience, though, the majority of students are not in the habit of arriving for class in such an advanced state of readiness. However, as the class progresses and the students accommodate to the active learning approach, the author has found that this situation improves. In addition, if some of the learning activities also serve as quizzes or otherwise count toward the final grade, this sometimes motivates students to complete the assignment prior to class.

**TExT Components for the Instructor**

Figure 2 shows the review slides that the TExT provides for the instructor to use in class. They follow a pattern that is repeated in every set of review slides. The first slide enumerates the learning objectives for the study unit. This is followed by a slide that attempts to place the study unit in context within the course and the field. This second slide also seeks to motivate the students to meet the stated objectives by pointing out the relevance of the information and how they will need to use it in the future. The remaining slides present a concise summary of the information that was presented in the readings and videos for the unit.

Typically the instructor would use these slides at the start of the class session for which the readings and videos had been assigned. While most instructors will be able to use these slides without additional instruction, the TExT does provide a set of notes that highlight important points that can be made during the review. The review would typically consume the first 5 to 10 minutes of the class meeting, and at the end of the review, the instructor would ask the class whether anyone had identified questions or points of clarification during their reading and viewing and would answer or clarify, as appropriate.

At this point, the instructor might give a very brief quiz, or alternatively could initiate the first learning activity to be used in the class. The author often uses short quizzes at this point,
After Studying this Unit, You Should be Able to

- Write the equation for the equilibrium constant at 298 K in terms of the standard Gibbs free energy change at 298 K.
- Write the equation for the equilibrium constant at any temperature T in terms of the equilibrium constant at 298 K and the (temperature-dependent) standard heat of reaction.
- Write the equation relating the equilibrium constant for a reaction to the thermodynamic activities of the participant species.
- Write equations relating the thermodynamic activity of gases, liquids, and solids to the composition of a mixture containing them.
- Calculate the equilibrium constant and the final equilibrium composition of a reacting mixture given the initial composition, temperature, and pressure.
- Analyze a chemical reaction to determine how the final equilibrium composition will be affected by a change in temperature, pressure, or the initial composition.

Context and Relevance

- Kinetics involves mathematical modeling of the rates of chemical reactions.
  - As a reacting chemical system approaches thermodynamic equilibrium, the net rates of all the reactions must approach zero.
  - Thus, reaction equilibrium imposes constraints upon reaction kinetics.
  - One must understand those constraints if one wishes to understand kinetics.
- Equilibrium "constants" often appear in rate expressions, and therefore you will need to know how to calculate them as a function of temperature.
- The equilibrium composition represents the best you can hope to achieve in a purely reactive chemical system.
  - You should know how to calculate the equilibrium composition so that you can do so each time you begin the design of a new reactor.
  - If you don’t know how to calculate the equilibrium composition, or if you don’t bother to do so, you may waste a lot of time and effort trying to design a reactor that does the impossible (i.e., goes beyond equilibrium).

Calculating the Equilibrium Constant for a Reaction

<table>
<thead>
<tr>
<th>Step</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Calculate the change in the standard Gibbs free energy for the reaction at 298K.</td>
</tr>
<tr>
<td>( \Delta G_{f}^{0} = \sum_{\text{species}} v_i \Delta G_{f}^{0}(i) )</td>
<td></td>
</tr>
<tr>
<td>2.</td>
<td>Calculate the equilibrium constant at 298K.</td>
</tr>
<tr>
<td>( K_{(298K)} = e^{\frac{\Delta G_{f}^{0}(i)}{R(298K)}} )</td>
<td></td>
</tr>
<tr>
<td>3.</td>
<td>Generate an expression for the standard heat of reaction as a function of temperature.</td>
</tr>
<tr>
<td>( \Delta H_{r}^{0} = \sum_{\text{species}} v_i \int_{298}^{T} \hat{c}_i , dT )</td>
<td></td>
</tr>
<tr>
<td>4.</td>
<td>Calculate the equilibrium constant at the desired temperature.</td>
</tr>
<tr>
<td>( K_{(T)} = K_{(298K)} e^{\frac{\Delta H_{r}^{0}(i)}{RT}} )</td>
<td></td>
</tr>
</tbody>
</table>

The Equilibrium Expression

- Write an equilibrium expression for each of the independent reactions:
  \( K_{(j)} = \prod_{\text{species}} a_i^{\gamma_i} \)
- Convert the thermodynamic activities in the equilibrium expressions into composition variables
  - For gases (assuming the standard state is an ideal gas at 1 atm):
    \( a_i = \frac{\gamma_i P}{1 \text{ atm}} \)
  - For liquids (ideal, Henry’s Law, non-ideal):
    \( a_i = x_i \quad a_i = \bar{R}_i x_i \quad a_i = \gamma_i x_i \)

Figure 2. Review Slides for the TExT study unit on “Reaction Equilibrium.”

particularly at the start of the semester, to further motivate the students to properly prepare prior to class. In fact, the review slides and the quiz that will be administered are posted on the course web site prior to the class meeting. The students are encouraged to print out these materials prior to class and to use them for recording notes, etc. during class. If the learning activities for the class also include written materials, they are also posted.

The TExT also provides the instructor with learning activities that can be used in the classroom. In any one offering of the course, the instructor would not use every activity that is provided, but instead would typically select one for use. The activities are of varied types that will appeal to students with differing learning styles or preferences. The different kinds of activities include object lessons that teach by analogy, inquiry activities (often using simulations), “one minute” papers or memos, contests, individual or group problem solving, debate, panel discussion, role playing, and more. Some involve physical activity, some are more auditory and some more visual. In some cases students begin working independently and then progress to group collaboration where they can “better” their individual solutions. In each case, the TExT provides the instructor with a list of the resources that will be needed, any computer simulations that will be required, and a lesson plan describing how to implement the activity in the classroom. The
prototype TExT provides three activities for the “Reaction Equilibrium” study unit, and these will now be briefly described.

The first activity begins with the students individually examining an equilibrium composition calculation that has “gone wrong.” In the calculations presented to the students, there are multiple reactions taking place, but not all the reactions are mathematically independent. The equations have been set up using all the reactions, and as a consequence it is not possible to solve for all the variables that have been introduced. In addition, some of the equations have been written incorrectly, and there are a few algebra errors, too. The students are asked to examine the calculations and determine why the equations can’t be solved. They are given some time to do this, after which they are formed into small groups (three students per group is suggested) to compare and reconcile their findings. They are required to come to agreement on what is wrong and what needs to be done to fix it. During this phase of the activity, it is not uncommon for the students to be teaching each other the information from the readings and videos.

There are a few alternative endings for the activity. One is to have a group volunteer to present their finding, and if other groups disagree, have them also present, followed by discussion/debate to resolve the issue. Another is to assign the correct solution of the problem in question as homework, letting the groups continue to work together outside of class and turn in a single solution. Yet another is to assign the students to summarize their deliberations in the form of a memo where they present all the possibilities they considered and explain why some were eliminated leading to their final analysis.

The second activity provided for this unit in the prototype TExT entails use of the equilibrium simulators. The activity begins with the students working in groups of three. Each group works with only one simulator, but within the class as a whole, all three simulators are being used. The students are told to identify through simulation as many trends as they can with respect to the equilibrium of the reaction they have been assigned. After they have had time to complete this task, the students are re-grouped so that members of each group have studied different reactions. The new groups are asked to determine whether the trends observed by each member are consistent or not, to reconcile or explain any inconsistencies, and to write a brief memo describing trends in equilibrium conversion with temperature, pressure, initial composition, and any other factors they identified. In doing so, they will find that the temperature trends differ for endothermic versus exothermic reactions, that pressure only has an effect when total moles change, etc. They will then need to explain these phenomena.

The third activity entails in-class problem solving. The students will be told to work individually on the calculation of the equilibrium composition for a reaction involving a solid phase. None of the examples for the unit involve a solid, but the activity of solids is presented in the information reading and video. Many of the students will not know how to proceed. After the students have had sufficient time either set up the calculation (if they know how) or to realize that they are stuck, their work is interrupted. Those students who have set the calculation up correctly are then identified, and they are assigned to teach the remaining students how to calculate equilibrium
compositions when a solid phase is present. (The students who were not able to solve the problem are broken into groups so that each “teacher” works with one group.) To conclude the activity, the students are told to prepare, as homework, a three-slide presentation on how to calculate equilibrium compositions when a solid phase is present. At the next class meeting, one of two of the students are called upon to present their slides.

After class, the instructor can assign homework problems involving reaction equilibrium. The TExT provides a set of problems to choose from. It also provides a rubric for each problem which can be made available to teaching assistants for grading purposes and to the students (after the assignment has been turned in).

Summary

A prototype Toolkit for Exceptional Teaching (TExT) is being developed in the area of chemical engineering kinetics and reaction engineering. The TExT is designed to provide the same resources as are normally supplied by textbooks along with a fully integrated set of classroom teaching resources. The motivation for producing a TExT is to make it very easy for an engineering instructor who is not accustomed to using active learning to begin doing so effectively. Later, the prototype discussed here will be used to test whether it actually accomplishes this goal. This document has described the different types of components provided by the TExT by examining a representative unit from the prototype. At the poster presentation of this paper, the actual components will be available for examination and demonstration.

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Bibliography


