APPS FOR CHEMICAL ENGINEERING EDUCATION: OFF-THE-SHELF AND DO-IT-YOURSELF DEVELOPMENT OPTIONS

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INTRODUCTION

CACHE (Computer Aids for Chemical Engineering) is a nonprofit organization that promotes the development and distribution of computer-related and/or technology-based educational aids for chemical engineering. Recently, at its 50th Anniversary Conference, CACHE brought together leaders in chemical engineering to review the history of the organization, explore current state of the art, and discuss future directions. A group of young faculty was invited to give presentations related to their innovations in developing educational media, exploring novel ways of organizing student-instructor interactions to enhance learning, and experimenting with alternative knowledge delivery modes. This manuscript reports on one major topic discussed at the conference — integrating computation into the chemical engineering curriculum using various pre-compiled applications or "apps" as teaching and learning aids. Apps can be used as cyber-assisted educational tools for instructing and engaging chemical engineering students, conducting computational research, and introducing lay audiences to chemical engineering concepts in informal learning environments outside of the classroom. Here, we refer to apps as packaged versions of graphical user interfaces (GUIs), which encapsulate computational software within a visual environment where users can provide interactive input through brief text or point-and-click controls and display query or simulation results through an automated process without needing to learn a programming language or a sizeable set of commands.

Although programmable calculators have been in existence for decades and online engineering tools are ubiquitous, the recent proliferation of mobile devices (i.e. smartphones and tablets) and their seamless integration of convenience, connectivity, and processing power have enabled revolutionary educational tools. While the majority of students' mobile device usage likely revolves around social media, texting, photography, and shopping, the opportunities to include education within this mix remain largely untapped. Chemical engineering educators are in a key position to guide, shape, and lead how chemical engineering concepts are packaged and delivered in this new era. Previous publications have described apps for chemical engineering education covering a range of specific topics: AIChE Concept Warehouse,[1] technical writing,[2] solution colorimetry,[3] unsteady-state heat conduction,[4] thermodynamics,[5] process controls,[6] and materials science.[7] Additionally, chemistry-related apps have been reviewed elsewhere,[8] and a number of interactive simulations for chemical engineering are archived by CACHE.[9] Here, we survey apps for chemical engineering education developed for iOS®, Mathematica®, Microsoft Excel®, R®, WebMO®, MATLAB®, and COMSOL® that have been used and/or developed by the authors for use in chemical engineering classrooms.

This paper is organized by software and progresses from off-the-shelf apps towards fully customizable simulation environments. We use "off-the-shelf" to describe any of the apps that educators and students can use without investing time in customization or development. The ChemE App for iOS is the result of hundreds of work hours coding (original code and implementing frameworks) in Objective-C, data collection/curation, and graphical design; it is intended to be used off-the-shelf. Many Mathematica-based Wolfram Demonstrations are available as off-the-shelf resources, but can be created or customized by educators or students with a work-

ing knowledge of Mathematica. Custom R Shiny® Apps can be created by users familiar with the software, but the apps described here are intended for off-the-shelf use. WebMO is publicly available with a suite of accompanying YouTube video tutorials illustrating how to set up, submit, and analyze the WebMO simulations. These are intended to be used with the off-the-shelf framework. MATLAB and COMSOL apps for some examples have been provided as off-the-shelf learning tools by the authors. Additionally, the software tools described can be used to develop custom do-it-yourself apps. The app generation and packaging steps are relatively straightforward and typically take a few hours for each project.

Figure 1. Screenshots from application provided on CD-ROM included with Himmelblau and Riggs. [10]

The rate limiting step is building the model for the underlying scientific topic or engineering principle. This could be straightforward for a typical homework or example problem, or time-intensive for a sophisticated ongoing research project. Undergraduate and graduate students can readily develop a MATLAB or COMSOL app as a homework assignment if the underlying model is provided or well-defined. A more complicated GUI leveraging simulations of a research-grade code may be more appropriate as a term project and often requires a substantial time investment.

iOS

Electronic learning resources have been gradually growing since internet access became widely available in the 1990s and as digital media began being distributed. However, the majority of these resources represent one-way communication mechanisms, such as online documentation, video lectures, and general course content delivery. An important area where mobile apps can be used within the chemical engineering curriculum is to modernize textbook appendices from static text and diagrams to dynamic tools that enable chemical engineers to work smarter, faster, and better. The digitization of textbook appendices into an integrated set of calculators and data repositories first became feasible in the 1990s with the advent of optical storage. Mass and energy balance textbooks[10, 11] included CD-ROMs that facilitated access to calculations and data (Figure 1).

The major limitation of distributing and using CD-ROM software, downloaded software, or web-based applets and other content is the requirement to work on a desktop or laptop computer. The "inertia" associated with working on a desktop or laptop makes it inconvenient for "on-the-fly" calculations and informal learning. These limitations persisted for nearly two decades and were only disrupted by the widespread adoption of smartphones and mobile devices. Now, this core of the chemical engineering curriculum can be reached through the powerful, intuitive, and broadly accessible iOS (i.e. iPad and iPhone) platform. Thus, providing tools for chemical engineering problem solving has not only become much easier with the ability to reach users globally, but the barriers to using these tools are greatly diminished.

Chemical Engineering AppSuite, or the "ChemE App," has been available for iPhone® since January 2012 with an enhanced iPad® version released in May 2012. Since usage tracking began in May 2013, users in at least 185 countries have launched the app more than 500,000 times to perform over 1,000,000 calculations. ChemE App provides a number of tools for chemical engineering students and professionals including unit converters, thermophysical properties for 1000+ compounds, steam properties, equation of state calculators, and a variety of reference tables and charts provided via PDF files (Figure 2). The ChemE App is available through Apple's App Store.[12] The iPad version of the ChemE App provides additional content and an enhanced experience that is enabled by the larger screen size. Additional features include graphing of many properties relative to temperature and several additional problem solving tools such as the "Combustion Analyzer," which facilitates the routine, yet tedious and formulaic, determination of reactive mass balances involving combustion of hydrocarbons. Feedback on the ChemE App has been highly positive, garnering a 4.4/5 rating in the App Store. Students, educators, and professionals have appreciated
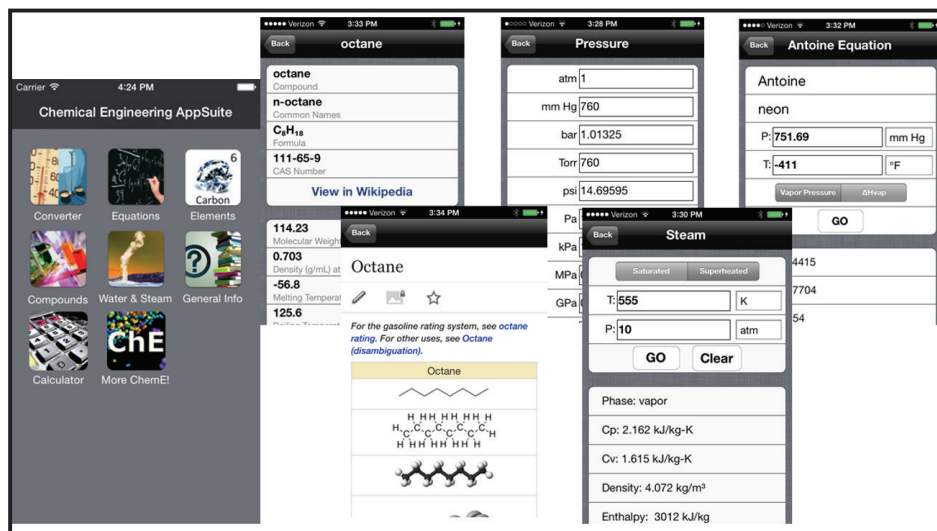
Figure 2. Screenshots of the ChemE App's main iPhone interface (far left) and selected modules (right) created by Prof. Bara.

the features of the app. Those not fully satisfied with the app found bugs in the code which were taken as valuable feedback, and these issues were typically corrected in the next update. Selected comments publicly posted to the App Store include:

- OMG! Best app ever! As a scientist, I use units, chemicals, and equations everyday. This app has surprised me everyday with something it has that I didn't know about. This app makes it easy for me to do quick unit conversions, learn chemistry, and review science. I love this app and I would highly recommend it to anyone who lives on the planet earth or anywhere in the universe!

- Very handy. I used this all through college as a student at The University of Alabama. Now that I'm out and have a job, I find myself still coming back to this app time and time again. It's great, it's free, and always very useful in and out of school. If you're a chemical engineer, this is a must-have.

- I wish I found this freshman year. This app has everything you could need studying chemical engineering. If you're studying chemical engineering, get it. Now. You'll thank this app for saving you from so many awful charts and paper cuts.

MATHEMATICA

Thousands of Wolfram Demonstrations, interactive illustrations built on Mathematica, have been archived online.[13] A suite of Wolfram Demonstrations have been developed specifically for chemical engineering applications across several courses: fluid mechanics, heat transfer, kinetics, mass and energy balances, materials science, process control, separation,

statistics, thermodynamics, and physical chemistry.[14, 15] These programs are freely available on the LearnChemE website[16] as a combination of browser-based simulations and downloadable files that can be played with the Wolfram CDF player. Additionally, Wolfram Demonstrations files for worked examples from Fogler's kinetics textbooks[17, 18] are distributed online.[19]

EXCEL

Besides its widespread adoption, Microsoft Excel's built-in tools make the software amenable to development of simple app-like simulations. The random number generator can be used to simulate variability, and the Data Table function allows Sheets within a Workbook to be simulated multiple times without explicitly programming the cells. Using these two features, users can perform many (tens of thousands) snapshots of a chemical engineering calculation on a standard laptop in seconds. For example, students can use this approach in estimating the risk of investment of their senior design projects. As another example, the random number and Data Table functions can be used to perform 25,000 estimates of the temperature in a non-isothermal CSTR (Figure 3). Each estimate uses reactor variables that are randomly generated between upper and lower bounds. Students are tasked with modifying the set points for the different variables until the number of cases where the reactor temperature exceeds a threshold is equal to zero.This Excel simulation app (Figure 3) is available on Canvas Commons™ for off-the-shelf use.

R

Online educational tools can be powerful resources, inside and outside of the classroom, as they are easily accessible (platform independence) and require little effort to setup and use. One approach for accelerating the development of online applications is R Shiny.[20] Shiny is an open source package for the R statistical language that streamlines the process of making interactive R code available online. One of the advantages of the R Shiny framework is the trove of open source R libraries that can be easily be incorporated into the R Shiny apps that cover topics from differential equations[21] to interactive plots.[22] R Shiny is most often used to generate interactive interfaces for data analysis and other statistics-
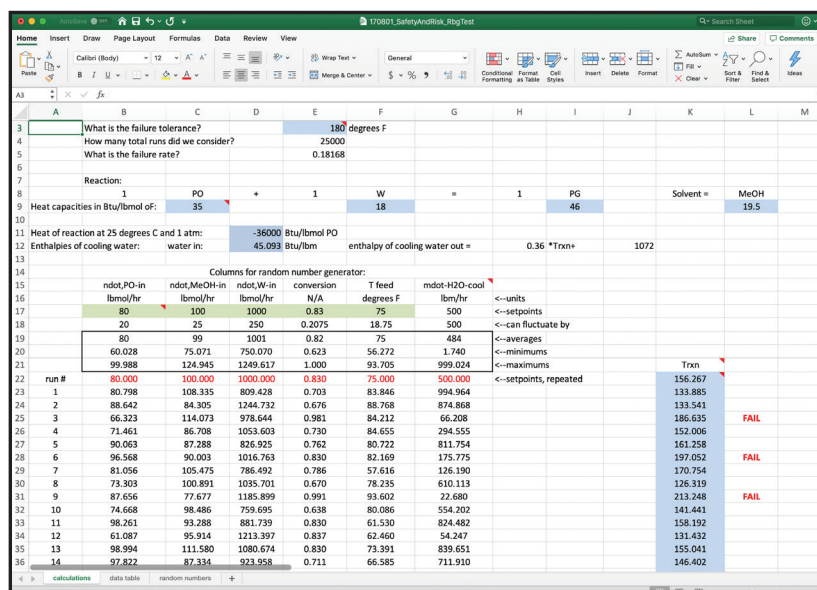
Figure 3. *Screenshot of Excel simulation app created by Prof. Getman that uses the random number generator to calculate the temperature in a CSTR with different combinations of randomly distributed variables.*
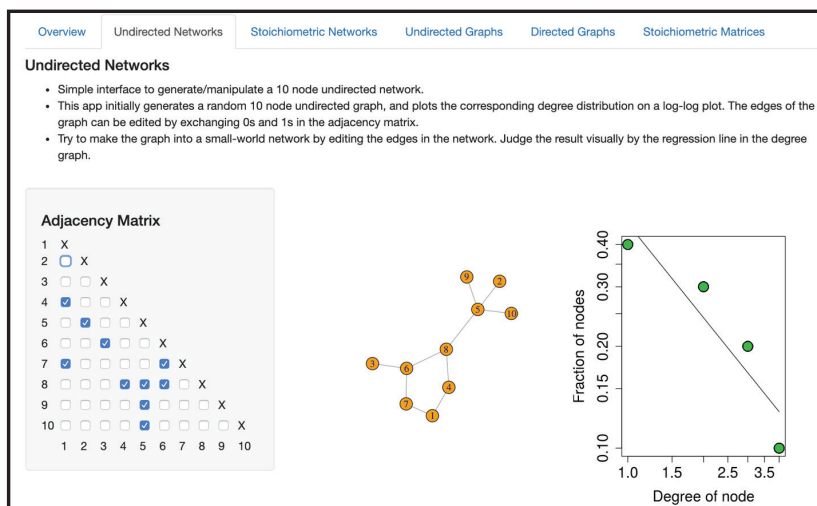
Figure 4. *Screenshot of the R Shiny app created by Prof. Kieslich for teaching undirected networks and their properties from Module 2: Static Network Models. This app allows a user to manipulate a 10-node undirected graph by adding or removing edges in the adjacency matrix, while the graph and its corresponding properties are automatically updated. Shown here (from left to right) are three interactive objects: a clickable interface for adding or removing edges of the graph, a schematic illustrating the graph defined by the current adjacency matrix, and a log-log plot of the degree distribution of the graph with a linear trendline.*

oriented projects and has been previously used to develop educational applications for teaching probability and statistics,[23, 24] including applications for research-informed learning. Prof. Kieslich has been involved in an effort to develop online teaching modules using R Shiny that cover various modeling topics in systems biology. Some of the R Shiny apps included in the modules provide the students with simple ways to manipulate example systems without requiring coding (Figure 4), while other apps are aimed at providing a large number of practice problems for challenging concepts. The systems biology modules developed using R Shiny are hosted online.[25]

WebMO

While topics in the chemical engineering curriculum generally involve the macroscale, many of the grand challenges facing chemical engineers today involve molecular level chemistry. Having an appreciation for molecular-level phenomena will better prepare chemical engineers to handle problems in energy, water, food, catalysis, advanced materials, and other fields. A barrier to creating assignments that involve the molecular level is the large learning curves associated with molecular simulation software. However, this is greatly reduced with web-based GUIs such as WebMO.[26] Anyone can use WebMO to set up and run a short quantum chemical simulation for free. The software includes a GUI that lets the user make straightforward choices about their simulation. The software translates these into an appropriate input file and submits it to a high performance computer in just a few button clicks. Further, WebMO summarizes the key output within the GUI. Chemical engineering students can use WebMO to find the transition state for an isomerization reaction, calculate the energy of interaction between two physically bonded molecules, and find the energy levels for a 3d transition metal atom to illustrate quantization of energy. Prof. Getman's poster from the CACHE 50th Anniversary Conference is archived in the Living Archive for Process Systems Engineering (LAPSE),[27] and the poster includes screenshots of some of these computational exercises in WebMO and

information about how one can access her course materials through the Canvas learning management system.

MATLAB

MATLAB is a popular software environment for science and engineering computation used in many university chemical engineering programs worldwide. MATLAB provides excellent user support for rapid development of professional-quality GUIs by engineering educators, academic researchers, and science and engineering undergraduate and graduate students. MATLAB GUIs can be packaged as apps to be shared as .mlappinstall files that work much like zip files that seamlessly install into the Apps menu in MATLAB or as standalone executable files with the MATLAB runtime environments included. The latter are suited for users without MATLAB installed on their computers, but the files take longer to install and use. MATLAB provides a tool called GUI Development Environment (GUIDE), which provides a visual canvas for constructing GUIs from scratch or from templates. The MATLAB documentation and sample scripts for building these GUIs using GUIDE[28] are approachable for undergraduate engineering students, and case studies of converting traditional MATLAB functions and scripts into functioning GUIs that can be distributed as apps are included in a clear textbook.[29] Undergraduate and graduate students in Prof. Ford Versypt's research lab and classes have assisted her in developing customized GUIs for further use in the chemical engineering curriculum (specifically mass and energy balances, heat transfer, and chemical kinetics), in an interdisciplinary upper division/graduate elective titled Applied Numerical Computing for Scientists and Engineers,[30, 31] and in several informal learning environments. The team has made the code

available[32] for their MATLAB app to simulate drug dosing to introduce chemical engineering design, kinetics, and mass balances concepts to novices or non-chemical engineering audiences through first-year engineering and outreach experiences.[33-35] Prof. Ford Versypt's poster from the CACHE 50th Anniversary Conference is archived in LAPSE,[36] and the poster includes an image gallery of her MATLAB GUIs that are available upon request from educators.

COMSOL

COMSOL Multiphysics is a powerful cross-platform finite element analysis and simulation software package with an intuitive user interface, which makes it an attractive visual accessory for teaching physical phenomena to students. Several textbooks use COMSOL for both undergraduate[17, 37-39] and graduate[40] chemical engineering courses. Tutorials for using COMSOL for solving chemical kinetics problems have been distributed online.[41, 42] Recently, COMSOL introduced a compiler add-on that allows one to create stand-alone executables of apps built using the Application Builder tool. These compiled apps include the full runtime libraries so that the recipients do not need to purchase any software in order to execute the apps. This enables instructors to share their knowledge and expertise in the form of standalone modeling and simulation apps that can be deployed to anyone through cloud computing environments. Prof. Voronov created a sample "Laminar Flow in a Pipe" COMSOL app (Figure 5), which is designed to illustrate a parabolic velocity flow profile for a fluid mechanics course. This example COMSOL App and others can be found at Prof. Voronov's website,[43] and his poster from the CACHE 50th Anniversary Conference is archived in LAPSE.[44]
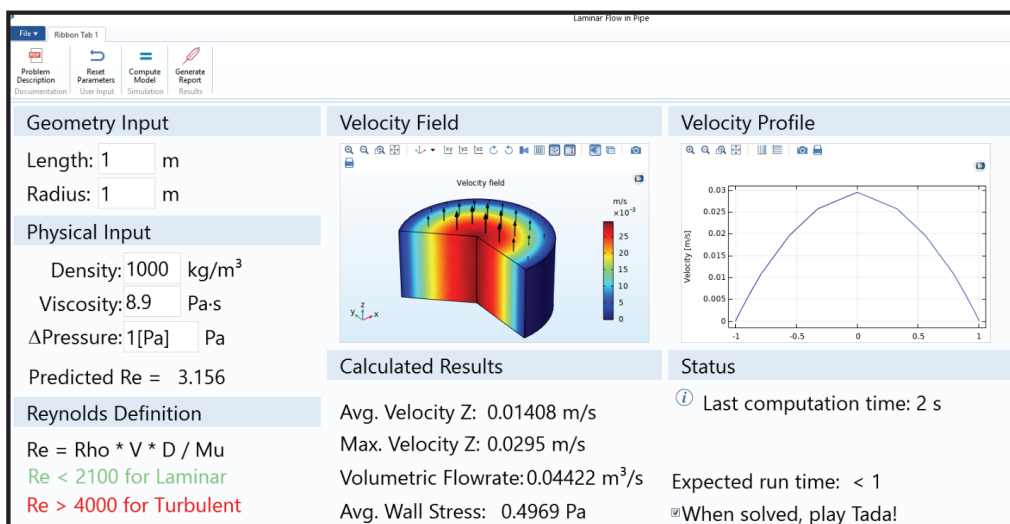

Figure 5. Screenshot of a COMSOL app created by Prof. Voronov for laminar flow in a pipe.

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