CACHE News
Summer 2019

Jupyter Notebooks for Chemical Engineering Education

Jeffrey C. Kantor
University of Notre Dame

Five years ago I was looking for an open-source alternative to proprietary software for distributing problem-solving notes to students in chemical engineering. Python was emerging as a credible open-source programming language. A spin-off of the IPython project was underway at Berkeley with a goal of creating a notebook style user interface. Intrigued, I began using these tools to create handouts for various topics that I was teaching.

Since then the IPython project evolved into the open-source Jupyter notebook web application that enables the use of narrative text, equations, visualizations, and live code in an integrated document. The use of Jupyter notebooks has undergone explosive growth. There are now close to 5 million notebooks publically available on github.com covering every field of technology and science.

The notebooks that I created evolved into a set of notebook repositories available on github covering a range of topics in chemical engineering. In addition, I've also created a python toolset called nbpages to automate the routine tasks involved in creating and maintaining large collections of notebooks.

The main purpose of these notebooks is to summarize computational methods for solving problems encountered in the textbooks and when doing homework. In many cases, I will ask students to bring their laptops to classes in which we will work, collaboratively, to develop the main elements of a notebook addressing a specific topic which the students will then complete and submit as a homework assignment.

My colleague, Alex Dowling, is in the process of developing a similar collection of notebooks for CBE 20228 Numerical and Statistical Analysis, a required Sophomore course at Notre Dame.

Here is a brief synopsis of the notebook repositories available on github that may of interest to the CACHE audience:

- CBE20255 Introduction to Chemical Engineering Analysis is a collection of over 40 Jupyter notebooks illustrating topics covered in a traditional first course in Chemical Engineering. It is organized in a Chapter/Section format that follows the sequence of

topics in “Elementary Principles of Chemical Processes, 4th Edition” by Felder, Rousseau, and Bullard.

For this first course, the notebooks make minimal assumptions about a student’s knowledge of Python. Using only a web browser and cloud services, notebooks can be directly accessed with nbviewer, and live notebooks can be executed on Google Colaboratory. The net result is that no complicated software installations are required by students, and the instructor can concentrate on the chemical engineering content rather than computer support.

Topics covered in the notebooks include units and basic calculations, stoichiometry, process modeling, material balances, reaction equilibrium, vapor/liquid equilibrium, steam calculations, and energy balances. Students learn to use Python plotting libraries, numerical and symbolic solutions of algebraic equations, and basic physical property data.

- CBE 30338 Chemical Process Control comprises over 70 Jupyter notebooks covering a range of topics in the traditional process control course taught in most chemical engineering departments. These notebooks are in a period of rapid development as we continue to reorganize the course at Notre Dame around a hands-on learning experience using the Arduino-based Temperature Control Laboratory developed by John Hendegren and colleagues at Brigham Young University.

  The notebooks in this repository are written at a level that assumes students have prior computing experience. Student should be able to find help with routine Python questions on their own, and should be able to code simple Python functions that return a value. Students should understand simple data structures including lists, and control structures such as for loops and iterators.

  The notebooks work best if students download and install an interactive development environment for Python, such as the widely used Anaconda distribution. Installation of TCLab is required to provide a python interface to the hardware of the Temperature Control Laboratory.

  The covered topics include process modeling, identification, degree of freedom analysis, simulation, linearization, PID control, frequency domain control design, optimization, optimal control, and predictive control. Several appendices of notebooks are devoted to real-time control implementation using the Temperature Control Laboratory.

- CBE 40455 Process Operations is a repository of over 40 notebooks supporting a senior elective course on topics in process operations. The course makes extensive use of optimization modeling languages such as MathProg (an open-source alternative to AMPL) and Pyomo.

An important element of this course is learning the principles of simulating discrete-event systems as a tool for the analysis of chemical operations. The notebooks demonstrate the use of the open-source SimPy library for the generic modeling of discrete event systems with application to warehouse, retail, and batch process operations. Additionally, Pyomo is used to create a generic modeling tool for state-task networks (STN) that are more specific to chemical process operations.

Topics include discrete-event modeling, linear optimization, scheduling, logistics, optimization under uncertainty, financial risk and diversification.

A selection of the notebooks from this and the other repositories have been adapted for the ND Pyomo Cookbook, a public repository intended for a web audience interested in the use of Pyomo for modeling and optimization.

The nontrivial amount of work required to create and maintain a collection of several hundred notebooks is reduced by adopting certain conventions and practices, and by employing a python toolset to automate the menial work. For example, I have found it useful to use the github pages feature to publish notebooks in a book-like chapter/section organizational scheme. The notebooks have a common header, navigation bars, table of contents, and keyword index. These are inserted and maintained using a system of templates and nbpages, a python utility that I've created for this purpose.

The CACHE corporation has steadfastly "promoted the development and distribution of technology based materials and software in chemical engineering education" for over five decades benefitting multiple generations of faculty and students. While the mission has stayed steady, the underlying technology has changed dramatically from the early days of Fortran and punched cards. Juptyer notebooks have much promise for the current and next generation students.