Exploring Chemical Engineering Principles through Interactive Simulations

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In recent years popular scientific computational platforms such as *Mathematica*, MATLAB, and SAGE (an open-source mathematics software system based on Python) have incorporated sophisticated graphical user interface (GUI) functions for doing interactive computing. In principle, these features allow students *familiar* with the software, to enhance their understanding of complex phenomena by coding the underlying mathematics to explore how changes in multiple parameters affect outcomes. In *Mathematica,* for example, the key to doing interactive computing is the **Manipulate** function. This function enables one with a few lines of code to integrate into a simulation a wide range of controls (such as sliders, buttons, drop-down menus, animation,3-D viewing perspectives, etc.) that later can be used to change parameters in the simulation at will. What currently sets *Mathematica*'s implementation of interactive computing apart from say MATLAB or SAGE is that it is possible to run the interactive simulation *without having access to, or any knowledge of Mathematica*. In 2011 Wolfram, the makers of *Mathematica*, released a new document format called CDF- Computable Document Format. Unlike a static PDF, the CDF is interactive. To close the loop, there is a CDF Reader, which is a free download from the Wolfram site. Thus those faculty members or students familiar with *Mathematica* can create an interactive simulation in *Mathematica* and then save it as a CDF. Students or other faculty members without access to *Mathematica* can view the interactive simulation in a CDF Reader (in many cases via a web browser), and explore all the interactive features designed in the simulation.

The Wolfram Demonstration site (http://demonstrations.wolfram.com) has over 9000 interactive demonstrations that can be downloaded for free (including the source code for the demonstration). For the past 7 years the above authors have published several hundred demonstrations covering all aspect of chemical engineering on the Wolfram site. Listed below are some examples covering unit operations, thermodynamics, fluid mechanics, mass transfer and reaction engineering.

Examples

- Pressure Swing Distillation: http://demonstrations.wolfram.com/SeparatingBinaryAzeotropesUsingPressureSwingDistillation/
- Gas permeation: http://demonstrations.wolfram.com/ComputingGasPermeationUsingTheCompleteMixingModel/
- Rectification: http://demonstrations.wolfram.com/RectifyingAnAlcoholWaterMixtureWithVariableEnthalpies/
- Thermodynamics: http://demonstrations.wolfram.com/LocusOfBinaryAndTernaryAzeotropesInChloroformMethanolAcetone/
- Mass Transfer: http://demonstrations.wolfram.com/DiffusionControlledEvaporationOfAnAerosolDroplet/
- Fluid Mechanics: http://demonstrations.wolfram.com/2DStokesFlowInALidDrivenCavity/
- Reaction Engineering: http://demonstrations.wolfram.com/CascadeOfTwoContinuousStirredTankReactorsWithRecycle/