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How to Teach Programming to ChE's In the Age of AI

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ABSTRACT

At Rowan University we decided to address a perennial student complaint that the computer science programming class material was never used in later chemical engineering classes. In 2022, we replaced the required programming course with a required chemical engineering course called ChE Modeling. This course introduces students to the modeling of chemical processes using practical simulation tools; the same ones used in industry. Students learn how to build models of complex chemical processes, evaluate the accuracy of models, and use models for process optimization and design decisions. We start this course using the Begin Python with TCLAB [1] modules. This is a unique module in which they learn a programming language to control an Arduino that has 2 heaters and thermistors. This immediately addresses a common complaint that they never used the programming language taught by computer science in a chemical engineering class; they now use python immediately. John Hedengren, the developer of this program, estimates that students can complete the 12 modules in 2 – 3 hours.

In this course they learn how to control a system with 2 heaters and 2 thermistors. In this module they use on/off control, similar to a home heating/cooling system. The TCLAB can be used in several other courses in ChE. The material in the ChE modeling course then focuses on ChE computational tools solving problems introduced in the previous years (1st and 2nd). Based on the Felder, Rousseau and Bullard book they use python jupyter notebook templates, Excel Templates, and Aspen Plus Tutorials to perform rigorous multicomponent flash drum problems using the Rachford-Rice Equation [2], Adiabatic Flame Temperature, and Transient Material Balances. The energy balances are based on thermodynamic properties from DIPPR. We continue with fluid mechanics and use a solver to solve for the flowrate in pipes and complex pipe networks. Next are transport problems in momentum, mass, and heat transfer ODE's and finite difference approximations. Next are the linear and non-linear regressions with confidence intervals, root finding methods, and plug flow models. Finally of interest to this conference are the Machine Learning Basics that are introduced and the changes required to incorporate AI in teaching programming.

Table: Brief set of problems covered in this course.

Topic / Exercise	Software / Tools
TCLab Learn Python Modules	Python
Felder, Rousseau and Bullard: Flash Drum Calculations (multiple nonlinear equations)	Excel Solver, Aspen Plus, Python template
Felder, Rousseau and Bullard: Adiabatic Flame Temperature	Excel Solver, Python `fsolve`, Aspen Plus
Felder, Rousseau and Bullard: Transient Material Balance Example Problem	Python ODE solver
Example Adiabatic Flame Temperature	Excel Solver, Python `fsolve`, Aspen Plus
Flash Drum Interpolations	Excel and Python
Geankoplis: Binary Mass Transfer in a Stefan Tube	Python ODE solver
De Nevers: Calculation of Flow Rate	Excel Solver, Python `fsolve`

Geankoplis: Flow in Complex Pipe Networks	Excel Solver, Python `fsolve`
Geankoplis: Unsteady-State Diffusion Using Finite Difference Approximations in the Method of Lines	ODE solver, COMSOL
Process Flow Diagrams	MS Visio
Heat Conduction in a Wire with Electrical Heat Source	Python ODE solver, COMSOL
Linear Regressions with Confidence Intervals	Excel, Python `curve_fit`
Nonlinear Regressions with Confidence Intervals	Excel, Python `curve_fit`
Root Finding: Bisection, False Position, Newton-Raphson, Secant, and Modified Secant Methods	Excel and Python
Numerical Methods to Integrate ODEs: Euler and Runge-Kutta	Excel and Python
Data Acquisition Using Microcontrollers and Sensors	Python
Machine Learning Basics: Big Data	https://apmonitor.com/pds/index.php/Main/AutomotiveMonitoring
Case Study 1: Catalyst Light-Off	Python
Case Study 2: GIS Map Visualization	Python
Case Study 3: Fuel Efficiency Regression	Python
Geankoplis Plug Flow Mass Transfer Models for Gas Absorption	Python ODE solvers
Plug Flow Models: Double Pipe Heat Exchanger	Python ODE solver
Geankoplis Equilibrium Stage Models for Gas Absorption	Excel and Aspen Plus

REFERENCES

1. Hedengren J, Hedengren E. begin_python, https://github.com/APMonitor/begin_python
2. Deriving the Rachford-Rice Procedure for Isothermal Flash Distillation, LearnChemE, https://youtu.be/ACxOiXWq1SQ?si=v01KQtayp_89AGnj