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Chemical Engineering Analysis through Systematic Optimization

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Building the Bridge in 21st Century Education: Chemical Engineering Industry + Academia

Outline

- Introduction
- Course design and organization rational
- Bridge the skills gap – distinguishing features
- Bridge the skills gap – assignments
- Conclusions
- Future work

Introduction

- With the rapid development of computing technology, computer-aided design skills are in high demand.
- CHE5031 Chemical Engineering Analysis, has been offered since 2015.
- Course aims to build a fundamental understanding of chemical engineering systems by developing mathematical and statistical models and simulations
  - ABET SLO1: Identify, formulate, and solve complex engineering problems by applying principles of engineering, science, and mathematics.
- It also aims to develop a systematic understanding and a critical awareness of process optimization and analysis of results.
  - ABET SLO6: Develop and conduct appropriate experimentation, analyze and interpret data, and use engineering judgment to draw conclusions.

Course design and organization rational

- MATLAB skill preparation
- Modeling in Chemical Engineering

Chemical Engineering Analysis

- Model fitting and spline functions
  - Optimization toolbox
    - Enhanced optimization
    - Global optimization
- Optimal experimental design
- Process integration and optimization
  - Complex equation systems
    - Data statistics and analytics

Bridge the skills gap – distinguishing features

- Most distinguishing feature is to apply systematic optimization for chemical engineering analysis to help students build their confidence for optimized data-driven decision-making.

?

=

But, 1=1

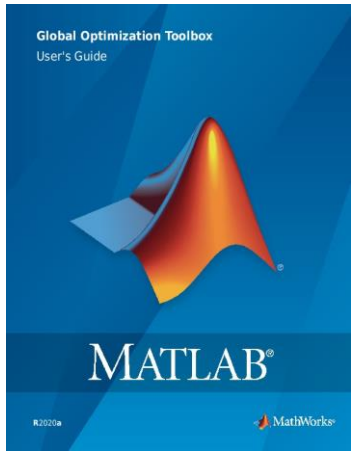
?

2 meters = 2 minutes

But, 2=2

Bridge the skills gap – distinguishing features

- Students do not just stop learning on the existing optimization toolbox and global optimization toolbox in MATLAB - they gain added knowledge of the limitations of MATLAB's optimization solvers.
- Advanced topics include enhanced optimization methods, such as
  - Lagrange's method of converting constrained optimization to non-constrained optimization,
  - Conversion of inequality constraints to equality constraints,
  - Penalty function method,
  - Enhanced constraints method to avoid the unwanted "zero" local optimal point.



$$F(x_1, x_2) = 10 * (x_2 - x_1^2)^2 + (1.5 - x_1)^2$$

$$\text{s.t.} \qquad g_1(\bar{x}) = -x_1 + x_2 \leq 0$$

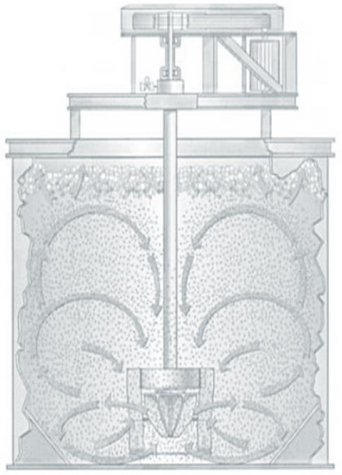
```
[x fval] = ga(@(x)(10*(x(2)-x(1)^2)^2+(1.5-x(1))^2), 2,[-1 1],0)
```

```
x =
   1.0484   1.0494
fval =
   0.2287
```

Wrong results! Genetic algorithm from MATLAB does not work.

Bridge the skills gap – distinguishing features

- The optimization techniques are demonstrated by case studies in model fitting, solving complex equations, and process optimization.
- Students also learn optimal experimental design to research influencing factors, their levels, the significance of each factor, and their combined effects.



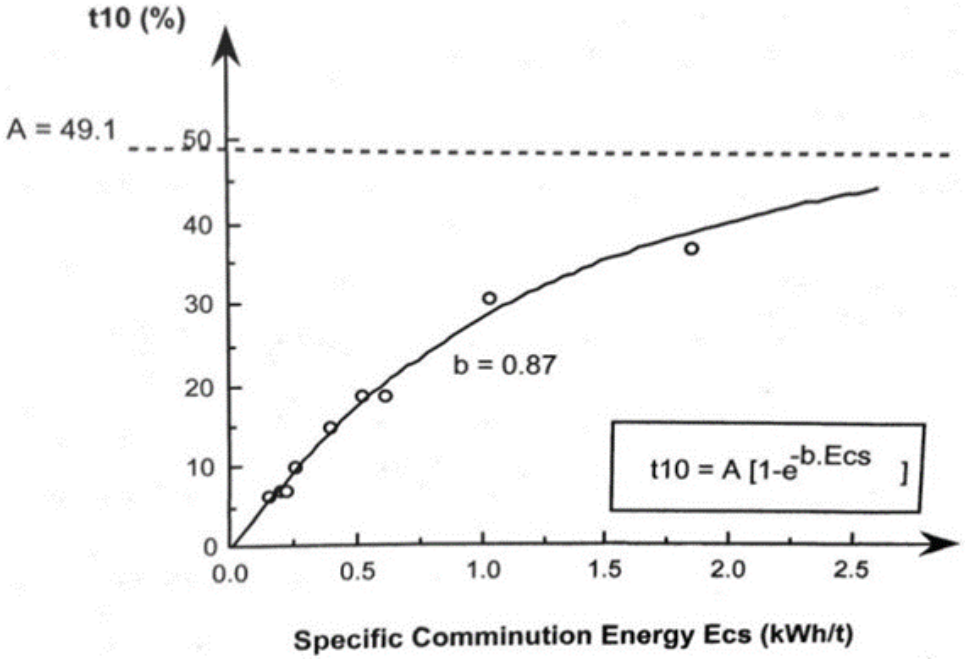
	Factor 1 (Impeller speed, rpm)	Factor 2 (Superficial gas velocity, cm/s)	Factor 3 (Water level, cm)	Factor 4 (Surfactant concentration, wt%)
Level 1	150	0.6	70	0
Level 2	190	0.8	85	2
Level 3	230	1.0	100	4
Level 4	270	1.2	106	6

Experimental round	factor 1	factor 2	factor 3	factor 4	factor 5
1	1	1	1	1	1
2	1	2	2	2	2
3	1	3	3	3	3
4	1	4	4	4	4
5	2	1	2	3	4
6	2	2	1	4	3
7	2	3	4	1	2
8	2	4	3	2	1
9	3	1	3	4	2
10	3	2	4	3	1
11	3	3	1	2	4
12	3	4	2	1	3
13	4	1	4	2	3
14	4	2	3	1	4
15	4	3	2	4	1
16	4	4	1	3	2

L16 (4^5) table

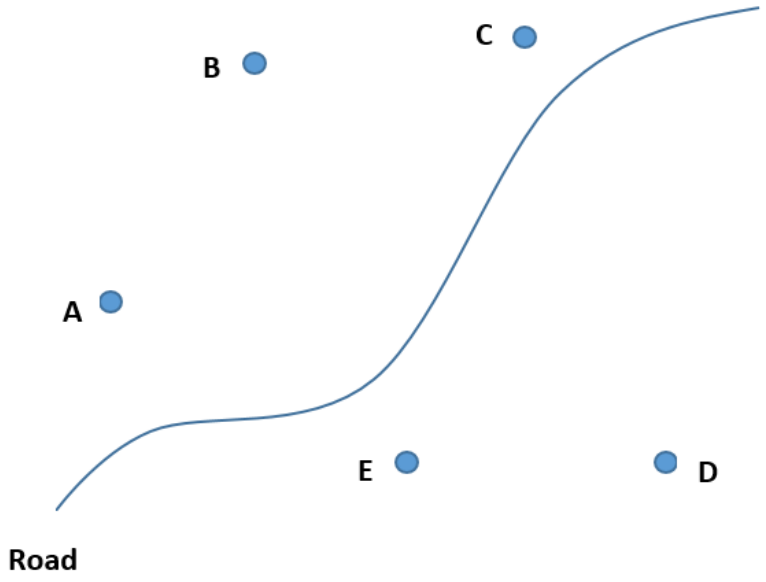
Bridge the skills gap – assignments

- Students have four main assignments:
  1) Model fitting of a particle size distribution via different ways by MATLAB apps and many optimization methods.



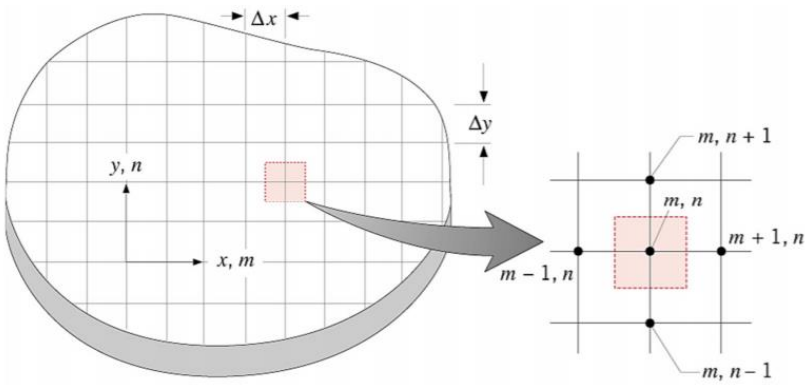
Bridge the skills gap – assignments

- Students have four main assignments:
  2) Optimization of the placement of a petrol station located on the road among 5 towns and further questions with weighted optimization, and with both equality and inequality constraints.



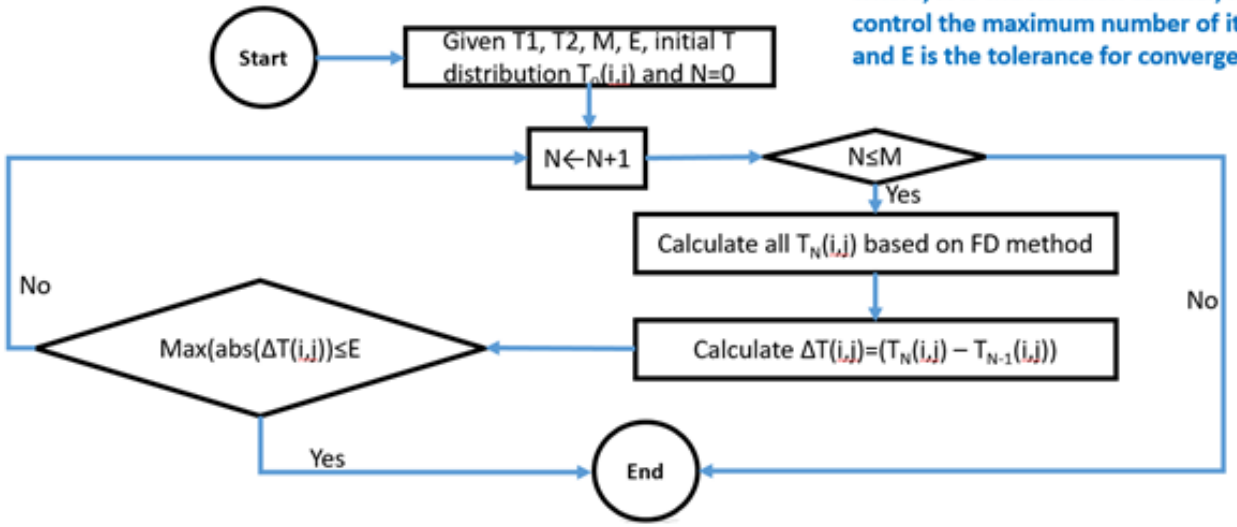
Bridge the skills gap – assignments

- Students have four main assignments:
  3) Optimization of a nodal network in a Cartesian grid to simulate steady-state 2D conduction heat transfer without internal heat resources.



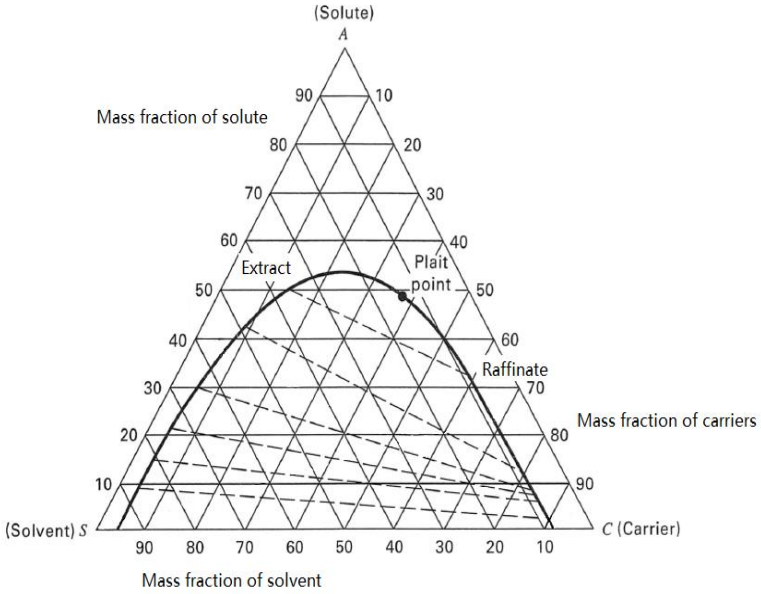
- A numerical algorithm flowchart for the above heat transfer problem:

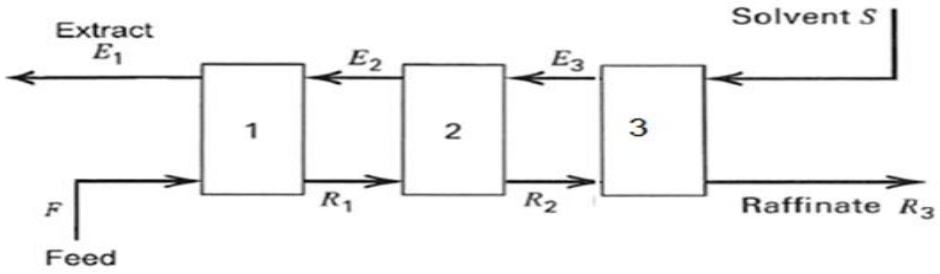
where, N is the iteration counter, M is to control the maximum number of iteration, and E is the tolerance for convergence.



Bridge the skills gap – assignments

- Students have four main assignments:
  4) Application of orthogonal experimental design for finding optimal parameters that minimize the operation costs in solvent extraction flowsheets using a ternary diagram.





Feed	Solvent
F = 300kg	S = 100kg
$X_{F,A}$= 0.40	$X_{S,A}$= 0.00
$X_{F,C}$= 0.60	$X_{S,C}$= 0.00
$X_{F,S}$= 0.00	$X_{S,S}$= 1.00

Conclusions

- Our Chemical Engineering Analysis course bridges the skills gap for our graduate students and some undergraduate students.
    1. To help them to realize the important of data analysis and learn some powerful optimization techniques.
    2. To enable them to use the "data science" techniques, skills, and modern engineering tools necessary for engineering practice.

Future work

- Publish a textbook on MATLAB for Advanced Users in Chemical Engineering
- Design online quizzes to train our students' coding skills faster and more efficiently

Thank you.