

IQ182 – Topics in Chemical Engineering I

*First term of 2025, Tuesdays, 18h00–21h00
Room SIFEQ-3 (Av. Albert Einstein, 500, Block B)*

Syllabus

Process modeling and systems of equations. Sparse systems and incidence matrix. Equation-oriented and sequential-modular approaches. Partitioning and tearing algorithms and convergence methods. Process simulation and analysis in Aspen Plus®. Process optimization.

Weekly workload: T: 01, P: 02

Total workload: 45 h (3 credits)

Instructor

Prof. Dr. Jean Felipe Leal Silva
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Program

- Process modeling and system of equations (9 h)
 - Design, optimization and operation problems
 - Linear and non-linear systems of equations
 - Sparse systems and incidence matrix
 - Equation-oriented and sequential-modular approaches
 - Partitioning, tearing algorithms, and convergence methods
- Fundamentals of process models (6 h)
 - Components and databanks
 - Thermodynamic models
 - User defined components and properties
 - Data regression
- Process simulation tools (30 h)
 - Block models
 - Recycle, purge and makeup streams
 - Automatization
 - Process specification
 - Sensitivity analysis
 - Optimization

Methodology

The course will consist of lectures on concepts necessary to understand the operation of process simulation software, followed by practical activities to establish these concepts. In practical classes, students will be required to submit a file resulting from the simulated case study in that class and a short report related to the simulated case study. During the last stage of the course, students will simulate a process whose final report must be delivered as part of the evaluation activities.

Assessment methods

- Assignments (*ASSI*) will consist of the grade given to the assignments delivered at the end of the practical classes. It will be a simple average of all assignments given throughout the semester, graded from 0 (zero) to 10 (ten).
- Exam (*EXAM*): individual test covering concepts related to process analysis and simulation. The test will be graded from 0 (zero) to 10 (ten) depending on the adequacy of the answers to the questions.
- Project Design (*PROJ*): a report related to the simulation of a case study proposed at the end of the term. The simulation and the quality of the report will be evaluated. Group activity. The report and simulation will be graded from 0 (zero) to 10 (ten).

Grading policy

At the end of the term, the final grade (*FG*) of the student will be calculated as follows:

$$FG = 0.2 \times ASSI + 0.4 \times EXAM + 0.4 \times PROJ$$

The final grade (*FG*) of the student will be converted to the letter grade (*LG*) system used at the University of Campinas according to the following rule:

$$LG = \begin{cases} 8.5 \leq FG \leq 10, & \text{grade A} \\ 7.0 \leq FG < 8.5, & \text{grade B} \\ 5.0 \leq FG < 7.0, & \text{grade C} \\ 0.0 \leq FG < 5.0, & \text{grade D} \end{cases}$$

The student is approved if *FG* is greater than 5.0 and frequency is greater than 75%.

Suggested bibliography

- Sandler, S.I.: Using Aspen Plus in Thermodynamics Instruction: A Step-by-Step Guide. Wiley, 2015
- Biegler, L.T., Grossmann, I.E., Westerberg, A.W.: Systematic methods for chemical process design. Pearson, 1997.
- Edgar, T.F., Himmelblau, D.M., Lasdon, L.: Optimization of Chemical Processes. McGraw-Hill, 2001.