

PyCRE course plan - 2022

| Level | Session | Duration | Date | Registration deadline | Instructor | Content | What you'll learn |
|---------------------|---------|----------|--------------|------------------------------|---------------------|---|--|
| - | 0 | 3 hrs. | Sep 19, 2022 | Sep 05, 2022 | Reza Monjezi | - How to install Python and required libraries | |
| Basic | 1 | 3 hrs. | Sep 26, 2022 | Sep 12, 2022 | Reza Monjezi | - Basics of Python, available packages for data science, ... - How to start coding in Python - Programming basics | |
| | 2 | 3 hrs. | Oct 10, 2022 | Sep 26, 2022 | Reza Monjezi | - Conditionals and loops - NumPy package: computation on NumPy arrays, simple calculations, indexing, slicing,... | - Conditionals, loops, and matrix calculations can be used in various applications |
| | 3 | 3 hrs. | Oct 24, 2022 | Oct 10, 2022 | Reza Monjezi | - Pandas package: data manipulation - Matplotlib package: plotting figures | - Importing raw experimental data - Checking criteria for intrinsic regime - Calculation of conversion, selectivity, ... - Plotting figures |
| | 4 | 3 hrs. | Nov 07, 2022 | Oct 24, 2022 | Reza Monjezi | - Plotting libraries (Matplotlib, Seaborn) | - Plot various types of figures |
| Intermediate | 5 | 3 hrs. | Nov 21, 2022 | Nov 07, 2022 | Ruben Van de Vijver | - Introduction to Cantera package - Building an input for Cantera - Cantera package: reactor simulation | - Reactor simulation (CSTR, PFR, batch reactor) - Rate of production analysis - Sensitivity analysis |
| | 6 | 3 hrs. | Dec 12, 2022 | Nov 21, 2022 | Reza Monjezi | - Introduction to SciPy package - SciPy package: differentiation, integration, ... - SciPy package: solving linear and non-linear systems | - Solving CSTR equations to find the concentrations |

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| | 7 | 3 hrs. | Jan 09, 2023 | <u>Dec 26, 2022</u> | Reza Monjezi | - SciPy package: linear and non-linear regression | <ul style="list-style-type: none"> - Optimize parameters for CSTR equations at various temperatures (isothermal regression) - Using the Arrhenius equation to calculate the apparent activation energy and pre-exponential factors (CSTR) - Non-isothermal regression to optimize parameters (CSTR) |
| | 8 | 3 hrs. | Jan 30, 2023 | <u>Jan 16, 2023</u> | Reza Monjezi | - SciPy package: solving ordinary differential equation (ODE) systems (+optimization problem) | <ul style="list-style-type: none"> - Solving batch/Plug flow reactor equations to find the concentrations - Parameter optimization (batch/Plug flow reactor) |
| | 9 | 3 hrs. | Feb 20, 2023 | <u>Feb 06, 2023</u> | Reza Monjezi | - Diffeqpy package: solving differential-algebraic equations (DAEs) system (+optimization problem) | <ul style="list-style-type: none"> - Solving fixed-bed reactor equations in a case that DAEs system appears - Parameter optimization |
| | 10 | 3 hrs. | Mar 13, 2023 | <u>Feb 28, 2023</u> | Reza Monjezi | - SciPy package: statistical tests | <ul style="list-style-type: none"> - F-test, t-test, parameters correlation, residual diagrams, ... |
| | 11 | 3 hrs. | Apr 03, 2023 | <u>Mar 20, 2023</u> | Maarten Dobbelaere | - RDKit package: reading molecules into a computer, visualizing them, calculating features of molecules, reactions, atoms, and bonds, generating 3D coordinates, ... | <ul style="list-style-type: none"> - Parse chemical data in an automatic fashion - Do transformations on data - Visualize the data |
| | 12 | 3 hrs. | Apr 24, 2023 | <u>Apr 10, 2023</u> | Maarten Dobbelaere | - TensorFlow: Machine learning | <ul style="list-style-type: none"> - Predicting properties of molecules - Classification of chemical data |