



gPROMS Process: Developing custom unit operation models

Day one – Monday 11th September 2023

Time	Topic
09:00	Model prerequisites
09:15	Implementing a simple lumped model in gPROMS: <ul style="list-style-type: none">• Creating a model• Defining and running a simulation Hands-on session: <ul style="list-style-type: none">• Develop a simple gas-phase valve model
11:30	Implementing more complex lumped models in gPROMS: <ul style="list-style-type: none">• Using arrays and intrinsic functions• Defining simulations with operating procedures Hands-on session: <ul style="list-style-type: none">• Develop a gas-phase CSTR model for the synthesis of methanol and simulate in steady-state and dynamic modes
12:30	Lunch
13:30	Modeling support tools
13:40	Handling discontinuities Hands-on session: <ul style="list-style-type: none">• Handling discontinuities in the gas-phase CSTR model for the synthesis of methanol
15:00	Physical properties Hands-on session: <ul style="list-style-type: none">• Including thermodynamics within the gas-phase CSTR model for the synthesis of methanol
15:50	Basic troubleshooting Hands-on session: <ul style="list-style-type: none">• Handling common errors
16:30	Developing your own distributed model
17:00	End of day

Day two – Tuesday 12th September 2023

Time	Topic
09:00	Hands-on session: <ul style="list-style-type: none">• Developing and simulating a 2D gas-phase PFR
10:10	Combining models in a hierarchy <ul style="list-style-type: none">• How to construct abstract composite models Hands-on session: <ul style="list-style-type: none">• Interacting a cooling jacket and valve model with a gas-phase CSTR for synthesis of methanol
11:20	Making models robust: <ul style="list-style-type: none">• Initialisation procedures Hands-on session: <ul style="list-style-type: none">• Making models robust
12:20	Troubleshooting
12:40	Lunch
13:40	Estimating model parameters from experimental data: <ul style="list-style-type: none">• What is required prior to a model validation exercise• Setting up an already performed experiment• Simulate a performed experiment Hands-on session: <ul style="list-style-type: none">• Creating and simulating an already performed experiment
14:50	Setting up and executing a parameter estimation Hands-on session: <ul style="list-style-type: none">• Creating a parameter estimation entity and estimating reaction parameters for synthesis of methanol in a gas-phase CSTR
16:00	Analysing the results from parameter estimation Hands-on session: <ul style="list-style-type: none">• Re-parameterisation of the model of kinetic reaction scheme
17:00	End of day