



# gPROMS Process: Developing custom unit operation models

Day one – Monday 11<sup>th</sup> September 2023

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

## Day two – Tuesday 12<sup>th</sup> September 2023

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