



# Dynamic optimisation

Dynamic optimisation is one of the most important technologies available to process modellers today.

Using rigorous dynamic optimisation techniques applied to an underlying dynamic model, it is possible to determine the best possible design or operational values for key process variables within the given process and equipment constraints.

Typical use of dynamic optimisation in gPROMS is in equipment design, design of operating procedures, and in quantifying other key capital and operating decisions. Optimisation can be used to give precise, optimal values for quantities such as equipment dimensions, control tuning values and setpoint trajectories – all determined simultaneously, in the same run if necessary – to answer questions such as those shown on the left.

All of these questions have one thing in common – they are aimed directly at improving plant profitability in an immediately quantifiable way.

## What is dynamic optimisation?

A much simpler concept than it sounds, dynamic optimisation is the process of optimising some aspects of process design and performance taking into account both steady-state and dynamic considerations. In contrast to steady-state optimisation, dynamic optimisation allows operability considerations to be taken into account at the design stage. Applicable to continuous, batch and semi-batch processes, it is the only meaningful way to optimise the latter two.

## Most simulation is really optimisation – the hard way

Arguably more than 75% of dynamic simulation models used today are used for dynamic optimisation – the hard way. With simulation you can only attempt to approach an optimum by repeated trial-and-error studies. Dynamic optimisation, in contrast with simulation, allows you to formulate the problem you are trying to solve directly, and then use the start-of-the-art numerical and optimisation solvers within gPROMS to determine the optimal values or time profiles of the optimisation variables.

## Disproportionate benefits

The best news about dynamic optimisation is that it comes with very little additional effort once you have made the investment in building a rigorous dynamic simulation model. The relatively simple process of formulating objective functions and constraints enables you to obtain far more value from the initial modelling investment.

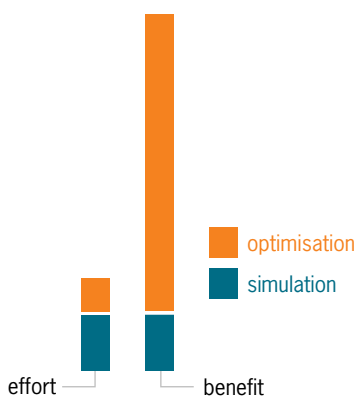
## Definition of a dynamic optimisation in gPROMS

Objective functions in gPROMS can be arbitrarily defined by combining any variables in the dynamic simulation model, such as feedstock, utility and product pricing notes and information. Constraints can likewise be constructed from any combination of model variables, and can be enforced at certain points in the simulation or over the entire time interval being considered. The optimisation variables are any time-varying controls or time-invariant equipment or other parameters that are normally specified during the simulation.

‘How do I start this unit up to full capacity in as short a time as possible?’

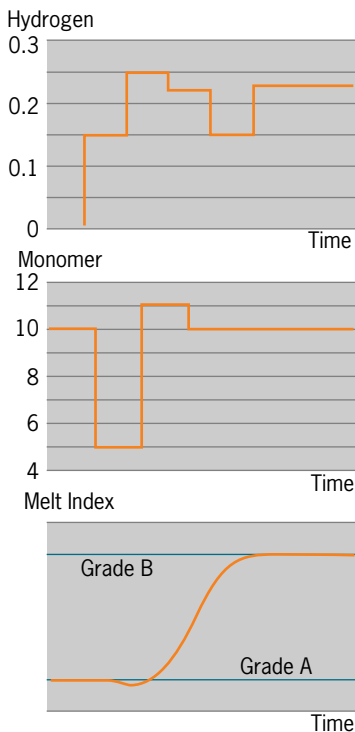
‘What setpoint values should I set and for how long in order to make the optimal changeover to the new feedstock?’

‘What are the optimum column diameter and control tunings to handle this range of anticipated disturbances in my distillation column?’



Dynamic optimisation is typically used for:

- the determination of optimal start-up and shut-down procedures
- optimal design and operation of multi-phase batch/semi-batch reactors
- optimal grade switching policies for continuous polymerisation reactors
- optimal operation of furnaces
- optimal tuning of PI and PID controllers
- the simultaneous optimisation of process and control design to deal with defined disturbances
- and optimal trajectory determination for Model Predictive Control applications.



### Technology overview

gPROMS deploys two powerful methods to optimise complex non-linear dynamic problems:

The **single-shooting method** is used for problems with many state variables, few control (optimisation) variables and few control intervals. The technique uses Control Vector Parameterisation, where time-varying controls are defined as simple functions of time over a number of control intervals.

The **multiple-shooting method** is used for problems with few state variables, many control (optimisation) variables and many control intervals. The technique optimises control intervals individually while then manipulating control variables to obtain a consistent solution at the interval boundaries.

### Applications

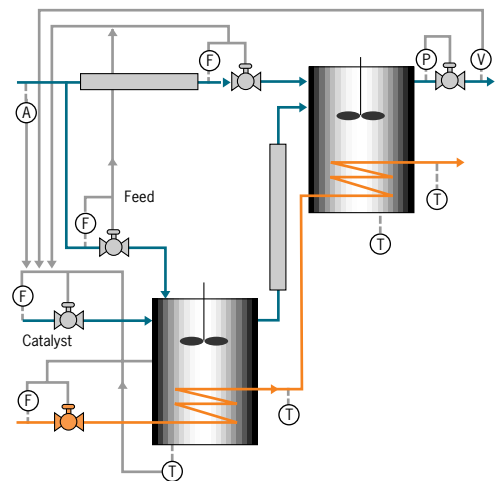
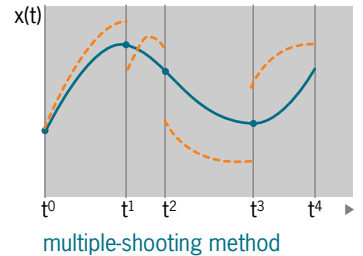
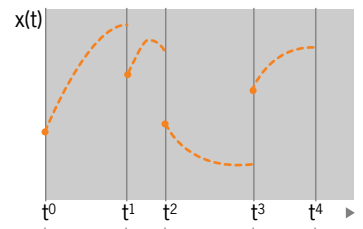
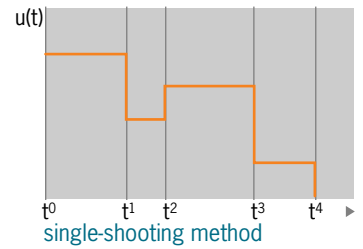
Dynamic optimisation is a technology that has been pioneered by PSE since the company's formation and there are now a large number of examples of successful application in industry. Here is one typical example from a major polymer manufacturer.

### Polymer grade change

**The requirement:** to change manufacture from grade A to grade B with the minimum off-spec production.

**The implementation:** a detailed model of the polymerisation reaction (using population balance models for accurate prediction of product properties, and with kinetics fitted from operating data using gPROMS' parameter estimation), models of the physical equipment, control system and operating procedures.

**The results:** (left) optimum setpoint trajectories for key process controllers during the changeover, resulting in minimum lost revenue.



Polymer grade change process flowsheet

