# Optimisation Guide

**Release v3.5**

**June 2012**

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Process Systems Enterprise Limited
6th Floor East
26-28 Hammersmith Grove
London W6 7HA
United Kingdom
Tel: +44 20 85630888
Fax: +44 20 85630999
WWW: http://www.psenterprise.com

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# Chapter 1. Overview

gPROMS can be used to optimise the steady-state and/or the dynamic behaviour of a continuous or batch process. Both plant design and operational optimisation can be carried out. The form of the objective function and the constraints can be quite general. Moreover, the optimisation decision variables can be either functions of time ("controls") or time-invariant quantities.

# Chapter 2. Dynamic Optimisation in gPROMS

## Introduction

This chapter describes how gPROMS can be used to perform (dynamic) optimisation calculations.

- A dynamic optimisation problem is described using a small example. We use this example throughout this guide to illustrate the dynamic optimisation facilities provided by gPROMS.
- A dynamic optimisation problem is described mathematically.
- A definition of what constitutes a solution to the dynamic optimisation problem is given.
- A description of how to specify dynamic optimisation problems in gPROMS is given.
- A description of how to specify point (including steady-state) optimisation problems in gPROMS is given.
- A description of how optimisation problems are executed in gPROMS is given.
- An explanation of the contents of the various output files that are generated is given.
- A discussion of various other features of the optimisation capabilities of gPROMS is made.

The optimisation capabilities in gPROMS have evolved significantly in recent versions of the software.

Some basic familiarity with the gPROMS language and concepts is assumed.

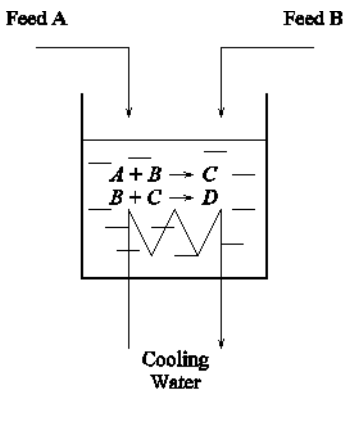
## What is dynamic optimisation?

In order to introduce the various elements of the definition of the problem of dynamic optimisation, we consider the semi-batch reactor shown in the figure below. Two exothermic reactions are taking place:

$$\begin{aligned} \mathrm{A} + \mathrm{B} &\rightarrow \mathrm{C} \\ \mathrm{B} + \mathrm{C} &\rightarrow \mathrm{D} \end{aligned}$$

where A and B are the raw materials, C the desirable product, and D the unwanted by-product.

**Figure 2.1. Batch Reactor**



The reactor receives two independent inputs of pure *A* and *B*, and is cooled with cooling water circulating through a coil. Starting with an empty reactor, we are free to vary the in-flows of *A* and *B*, as well as the cooling water flowrate.

For a given reactor design, our *operational* objective may be to determine the duration of the operation, and the time variation of the various material and energy flowrates over this duration, so as to maximise the final concentration of *C*. Of course, equipment design and resource availability usually impose certain limits within which our control manipulations must be maintained---for instance, there is an upper limit on the available flowrate of cooling water.

In general, the *design* of processes operating in the transient domain also leads to problems that are similar to operational optimisation problems, but may have additional degrees of freedom. For instance, we may wish to determine the optimal geometry of the reactor in addition to the optimal way of operating it over time.

Because of the transient nature of the underlying process, both the operational and design problems considered above are applications of *dynamic optimisation*[1]

and serve to introduce some of the important features of this problem in its most basic form. Some other complications that often arise in practical applications will be introduced later.

## What is the mathematical problem?

In this section we provide a mathematical statement of the class of dynamic optimisation problems solved by gPROMS.

### The process model

We consider processes described by mixed differential and algebraic equations of the form:

$$f(x(t), \dot{x}(t), y(t), u(t), v) = 0.$$

Here *x(t)* and *y(t)* are the *differential* and *algebraic* variables in the model while $\dot{x}(t)$ are the *time derivatives* of the *x(t)* (*i.e.*, $\dot{x} \equiv dx/dt$). *u(t)* are the *control variables* and *v* the time invariant parameters to be determined by the optimisation. In the context of the batch reactor example considered earlier, the differential variables will typically correspond to fundamental conserved quantities (such as molar component holdups and internal energy), while *y* will include various quantities related to them (e.g. component molar concentrations and temperature). The input flowrates of *A*, *B* and cooling water are the control variables *u* while, in the design case, the volume of the reactor acts as a time invariant parameter *v*.

#### Note

For simplicity, the mathematical description in this document assumes that the system behaviour is defined in terms of *ordinary*(with respect to time) differential and algebraic equations. However, the optimisation capabilities of gPROMS are equally applicable to mixed lumped and distributed systems described by general integral, partial differential and algebraic equations in time and one or more space dimensions.

### The initial conditions

In general, gPROMS assumes that the initial *t=0* condition of the system is described in terms of a set of general non-linear relations of the form:

$$I(x(0), \dot{x}(0), y(0), u(0), v) = 0.$$

It is important to note that, once we fix the time variation of the controls, *u(t)* and the values of any time invariant parameters, *v*, the modelling equations together with the initial conditions completely determine the transient response of the system. In practice, we could determine this response by performing a gPROMS dynamic simulation.

[1]Often, the term "optimal control" is also used, especially for problems that involve control variables but no time-invariant parameters (see also: What is the mathematical model?).

## The objective function

Dynamic optimisation in gPROMS seeks to determine

- the time horizon, $t_f$,
- the values of the time invariant parameters, $v$, and
- the time variation of the control variables, $u(t)$, over the entire time horizon $t \in [0, t_f]$,

so as to minimise (or maximise) the *final* value of a *single* variable $z$. This can be written mathematically as:

$$\min_{t_f, v, u(t),\, t \in [0, t_f]} z(t_f)$$

Here the *objective function* variable, $z$ is one of either the differential variables $x$ or the algebraic variables $y$. In the context of the batch reactor example, $t_f$ would be the duration of the batch reaction while $z$ would be the concentration of component C (either a differential or an algebraic variable, depending on the model used).

The above form of the objective function is not as restrictive as might appear at first. In particular, it is worth noting that:

- Maximisation can be carried out as well as minimisation.
- If we wish to optimise a function $\phi(x(t_f), \dot{x}(t_f), y(t_f), u(t_f), v)$ of several variables instead of a single variable, we can simply add an extra algebraic equation to the model:

  $$z = \phi(x, \dot{x}, y, u, v)$$

  The additional computational cost incurred because of this model extension is usually negligible.
- If we wish to minimise or maximise the *integral* of a function $\psi(x, \dot{x}, y, u, v)$ over the entire time horizon, we can simply add the differential equation:

  $$\dot{z} = \psi(x, \dot{x}, y, u, v)$$

  together with the initial condition:

  $$z(0) = 0$$

  We can easily verify that this is equivalent to:

  $$z(t_f) = \int_0^{t_f} \psi(x(t), \dot{x}(t), y(t), u(t), v)\, dt$$

  Again, very little additional computational cost is incurred in doing this.
- Minimising the time horizon itself can be achieved by adding the equation:

  $$\dot{z} = 1$$

  together with the initial condition above.

## Bounds on the optimisation decision variables

In practice, the time horizon $t_f$ will often be subject to certain lower and upper bounds:

$$t_f^{\min} \le t_f \le t_f^{\max}$$

In some cases, $t_f$ will, in fact, be fixed at a given value, $t^*_f$. This can be achieved simply by setting $t_f^{\min} = t_f^{\max} = t^*_f$.

As we have already seen in the batch reactor example, it is likely that the control variables and time invariant parameters will also be subject to lower and upper bounds:

$$^{\min} \leq u(t) \leq u^{\max}, \quad \forall t \in [0, t_f]$$

$$^{\min} \leq v \leq v^{\max}$$

## Other constraint types

### End-point constraints

In some applications, it is necessary to impose certain conditions that the system must satisfy at the *end* of the operation. These are called *end-point constraints*. For instance, in the batch reactor example, we may require:

- the final amount of material in the reactor to be at certain prescribed value;

and also

- the final temperature to lie within given limits.

In the first case, we have an *equality end-point constraint* of the type:

$$w(t_f) = w^*$$

where *w* is one of the system variables (*x* or *y*). In the second case, we have an *inequality end-point constraint:*

$$^{\min} \leq w(t_f) \leq w^{\max}$$

### Interior-point constraints

We can also have constraints that hold at one or more distinct times $t_I$ during the time horizon (e.g. at the middle of the horizon). These are called interior-point constraints. These may be represented mathematically as:

$$w_I^{\min} \leq w(t_I) \leq w_I^{\max}$$

where *w* is a system variable, and $t_I$ is a given time.

We note that both interior and end-point constraints are special cases of point constraints. However, for convenience, gPROMS treats them separately. It also treats any constraints that have to be satisfied at the initial time *t=0* as interior-point constraints

### Path constraints

We may also have certain constraints that must be satisfied at *all* times during the system operation. If these *path constraints* are equalities, then often they can simply be added to the system model effectively converting one of the control variables *u(t)* into an algebraic variable *y*. More often, they are inequalities of the form:

$$^{\min} \leq w(t) \leq w^{\max}, \qquad \forall t \in [0, t_f]$$

For instance, in our batch reactor example, we may require that the temperature never exceed a certain value so as to avoid some unwanted side-reactions that are not explicitly considered by our model.

Although we have assumed in equations representing end-point, interior-point and path constraints that the various constraints are imposed on a *single* variable *w*, this is not really restrictive. If we wanted to constrain a function $\phi$ of several variables, we could simply define a new variable *w* through an additional equation:

$$w = \phi(x, \dot{x}, y, u, v)$$

and then impose the required constraints on *w*.

# What is a "solution" of a dynamic optimisation problem?

Let us start by summarising the mathematical statement of the dynamic optimisation problem as defined in: What is the mathematical model?:

**Table 2.1. Mathematical statement of the dynamic optimisation problem**

| | |
|---|---|
| *Objective function* | $displaystyle\, \min_{t_f, v, u(t),\, t \in [0, t_f]} z(t_f)$ *subject to* |
| *Process model* | $f(x(t), \dot{x}(t), y(t), u(t), v) = 0\, t \in [0, t_f]$ |
| *Initial conditions* | $I(x(0), \dot{x}(0), y(0), u(0), v) = 0$ |
| *Time horizon bounds* | $t_f^{\min} \leq t_f \leq t_f^{\max}$ |
| *Control variable bounds* | ${}^{\min} \leq u(t) \leq u^{\max}\, t \in [0, t_f]$ |
| *Time invariant parameter bounds* | ${}^{\min} \leq v \leq v^{\max}$ |
| *End-point constraints* | $w(t_f) = w^*$<br><br>${}^{\min} \leq w(t_f) \leq w^{\max}$ |
| *Interior-point constraints* | $w_I^{\min} \leq w(t_I) \leq w_I^{\max}$ |
| *Path constraints* | ${}^{\min} \leq w(t) \leq w^{\max}\, t \in [0, t_f]$ |

Clearly, a "solution" to this problem comprises three key elements:

- The value of the time horizon, $t_f$.
- The values of the time invariant parameters, *v*.
- The variation of the control variables *u(t)* over the time horizon from *t = 0* to $t = t_f$.

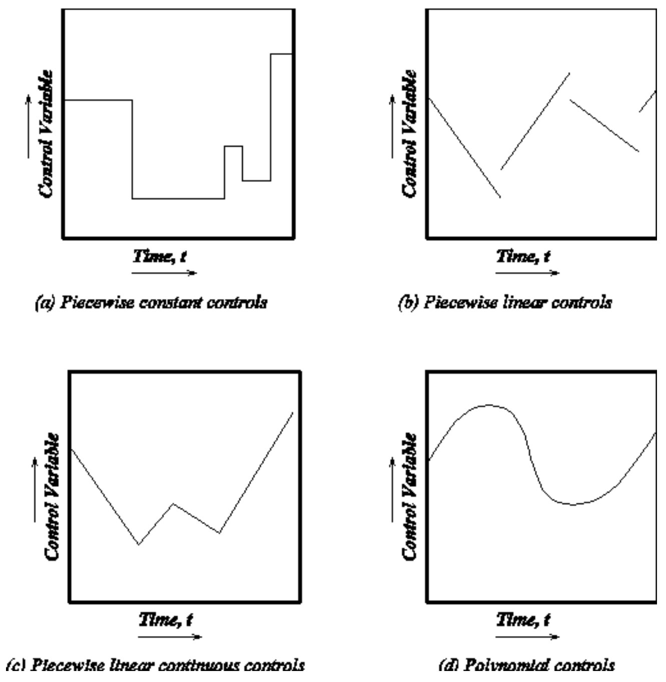
As has already been mentioned, if these are specified, we can solve the model equations to determine how the system behaves over the time horizon of interest, obtaining values of *x(t)* and *y(t)* for all $t \in [0, t_f]$. We can then evaluate the objective function, and also check whether the various end-point and path constraints are satisfied.

Normally, there will be more than one combination of $t_f$, *v* and *u(t)* that satisfies the bounds and the constraints---and this, of course, is what gives rise to the optimisation problem. The latter aims to find the combination that produces the *best* value of the objective function while satisfying all the constraints.

# Classes of control variable profile

For the above dynamic optimisation problem to be well defined, we need to be rather more specific regarding the *type* of the variation of the control variables over time that we are willing to consider. For instance, we could have:

**Figure 2.2. Different types of control variable profile**

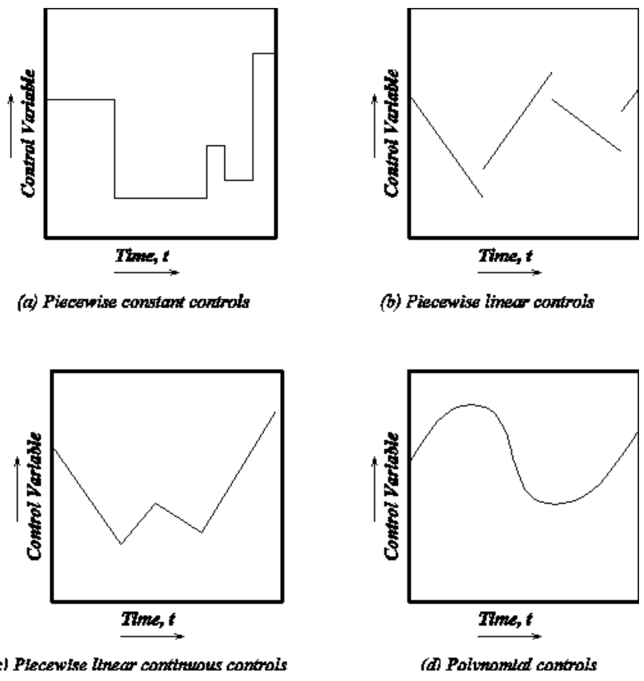


- Piecewise-constant controls---these remain constant at a certain value over a certain part of the time horizon before jumping discretely to a different value over the next interval: see subfigure (a) above.
- Piecewise-linear controls---these take a certain linear time variation over a certain part of the time horizon before jumping discretely to a different linear variation over the next interval: see subfigure (b) above.
- Piecewise-linear continuous controls---these are similar to the piecewise-linear controls described above, with the additional requirement that their values be continuous at the interval boundaries: see subfigure (c) above.
- Controls that vary smoothly over time---perhaps as polynomials of a given degree: see subfigure (d) above.

It is important to appreciate that, in most cases, the choice of the form of the control variables is an *engineering* rather than a mathematical issue: it very much depends on the capabilities of the actual control system (automatic or manual!) that we will eventually use to implement these controls on the real plant. For instance, piecewise-constant controls may often be preferable to other types as they are much easier to implement.

## Control variable profiles in gPROMS

**Figure 2.3. Different types of control variable profile**



The dynamic optimisation facilities in gPROMS support piecewise-constant and piecewise-linear controls of the types shown in subfigures (a) and (b) respectively. These are by far the most commonly encountered in practical applications. However, if necessary, it is relatively straightforward to introduce several other types of control. For instance, a piecewise-linear continuous control of the type shown in subfigure (c) can be defined by adding the equations:

$$\begin{aligned} \dot{z} &= U \qquad (1) \\ u &= z + \alpha \end{aligned}$$

where:

- *z* is a new differential variable with initial condition *z(0)=0*;
- *U* is a new piecewise-constant control variable (*cf.* subfigure (a)) to be determined by the optimisation;
- $\alpha$ is a new time invariant parameter representing the initial value of *u* (*i.e.* $(0) = \alpha$), to be determined by the optimisation.

We note that this is equivalent to:

$$(t) = \alpha + \int_0^t U(\tau)\,d\tau$$

which expresses the fact that the time gradient of a piecewise-linear continuous control is a piecewise-constant function of time.

Also a cubic polynomial control variation of the form:

$$(t) = \alpha + \beta t + \gamma t^2 + \delta t^3$$

can be introduced by adding the following to the model equations:

$$\dot{z} = 1$$

Together with the initial condition *z(0)=0*, this equation effectively defines *z* as time.

$$u = \alpha + \beta z + \gamma z^2 + \delta z^3$$

By virtue of this equation, the variable *u* becomes one of the algebraic variables *y* to be determined by solving the model equations.

The actual control variation is determined by the values of $\alpha$, $\beta$, $\gamma$ and $\delta$ which should now be treated as time invariant parameters *v*.

# Specifying dynamic optimisation problems in gPROMS

Most of the information needed for specifying dynamic optimisation problems in gPROMS will be present in the various entities used for dynamic simulation of the process. Some additional information will have to be specified in separate entities.

We consider each of these sources of information in turn.

## Process entities for optimisation

Just like a dynamic simulation experiment, a dynamic optimisation problem in gPROMS is defined in a Process entity. In fact, there is no difference in syntax between a simulation and an optimisation Process. Thus, the latter specifies most of the information required for defining mathematically the optimisation problem to be solved:

- The Unit specification, together with parameter Setting, effectively determine the set of model equations *f(.)=0*.
- The Assign specifications mark certain system variables as fixed for the purposes of dynamic simulation. As far as optimisation is concerned, some of these variables will be either controls or time invariant parameters (see also: Optimisation Entity).
- The Initial specifications provide the initial conditions *I(.)=0*.
- An optional Preset specification may be used to override the default initial guesses and bounds for any system variable. In particular, the bounds on the controls and time invariant parameters to be used for the purposes of the dynamic optimisation are either those specified here or the default values specified in the Variable Type entities.
- There are two standard mathematical solvers available in gPROMS for solving dynamic optimisation problems. The first (default) implements a control vector parameterisation algorithm based via single-shooting. This can be specified in the Solutionparameters section of a Process entity through the syntax:

  ```
  SOLUTIONPARAMETERS
    DOSolver := "CVP_SS" ;
  ```

  The second solver is an implementation of control vector parameterisation via multiple-shooting. This is specified in the Solutionparameters using:

  ```
  SOLUTIONPARAMETERS
    DOSolver := "CVP_MS" ;
  ```

  In general, CVP_MS is more suited than CVP_SS for solving dynamic optimisation problems with relatively few differential variables but a large number of control variables and/or control intervals. A detailed description of the two solvers and the various parameters that can be used for configuring their precise behaviour is given in: standard solvers for optimisation.
- Any Schedule specification in the Process is ignored for the purposes of dynamic optimisation. This also means that any Intrinsic Tasks[2] used by your Models will not be executed.

[2]See the section "Defining Tasks" in the Model Developer Guide

Experience indicates that most of the effort in defining a dynamic optimisation problem is, in fact, incurred in the construction of a robust model of your process. This will probably be exactly the same model as that used for dynamic simulations within gPROMS. However, it is worth investing some effort in ensuring that it behaves properly for the *entire* range of possible values of the control variables and time invariant parameters. In particular, you should check that the differential and algebraic variables *x* and *y* remain within any specified bounds even for extreme values of *u* and *v*.

The various Variable Type, Model and Process entities for the batch reactor example in this chapter are shown within a project called "ReactorOpt.gPJ" (see the dynamic optimisation example).

## The Optimisation entity

The complete specification of a dynamic optimisation problem requires some additional information which is not provided in the gPROMS Process entity. This includes information on the time horizon and the objective function, the form of the control variable profiles, and any end-point and path constraints that have to be imposed on the process.

All of the above information has to be specified in a separate entity which appears under the Optimisations entry in the gPROMS project tree. In order to create such an entity:

1. Pull-down the Entity menu from the top pane in gPROMS ModelBuilder.
2. Click on New Entity. A dialog box will appear.
3. Choose Optimisation for the Entity type and fill in the Name field. The name of the Optimisation entity must be the name of the relevant Process entity in the gPROMS project.

The structure of the Optimisation entity is shown in the table below, with keywords having their first letter capitalised. Most of the information presented is adequately explained by the comments in the second column. However, it is worth clarifying some points regarding the selection of control variables and time invariant parameters, and also the specification of interior-point constraints and path constraints.

An example of such an entity is shown in the dynamic optimisation example for the batch reactor.

### Note

- To omit any *lower* bound from the optimisation, specify it as -1E30.
- To omit any *upper* bound from the optimisation, specify it as 1E30.

**Table 2.2. Syntax of a gPROMS Optimisation entity**

| Specification | Comments |
|---|---|
| # | Lines starting with hash (#) symbols are treated as comments |
| PROCESS {name of Process} | name of Process must correspond to the name of one of the Processes in the Project. This specification allows one to have more several Optimisation entities in a gPROMS Project all referring to the same Process: e.g. to perform different optimisation experiments on the same system. |
| OPTIMISATION_TYPE<br><br>{optimisation type} | The optimisation type can be one of the following values: POINT, STEADY_STATE and DYNAMIC<br><br>Optional—If omitted, dynamic or point optimisation will be used, depending on whether or not a horizon is specified. |
| HORIZON<br><br>{IV} : {LB} : {UB} | Time horizon specification |

| Specification | Comments |
|---|---|
| | Initial guess for $t_f$ followed by $t_f^{\min}$ and $t_f^{\max}$ (*cf.* constraint in: Bounds on the optimisation decision variables). |
| INTERVALS<br><br>{number of intervals}<br><br>{IV} : {LB} : {UB}<br><br>...<br><br>{IV} : {LB} : {UB} | Intervals in control variable profiles.<br><br>There follows one line per interval.<br><br>Initial guess, lower bound and upper bound for the length of each interval. |
| PIECEWISE_CONSTANT<br><br>{variable name}<br><br>{initial profile specification} | Specification of a piecewise-constant control variable.<br><br>Its full gPROMS path name.<br><br>Optional—see also: control variables and time invariant parameters. |
| PIECEWISE_LINEAR<br><br>{variable name}<br><br>{initial profile specification} | Specification of a piecewise-linear control variable.<br><br>Its full gPROMS path name.<br><br>Optional—see also: control variables and time invariant parameters. |
| TIME_INVARIANT<br><br>{variable name}<br><br>{initial value specification} | Specification of a time-invariant parameter.<br><br>Its full gPROMS path name.<br><br>Optional—see also: control variables and time invariant parameters. |
| ENDPOINT_EQUALITY<br><br>{variable name}<br><br>{value} | Specification of a variable on which an equality end-point constraint is to be imposed.<br><br>Its full gPROMS path name.<br><br>The value $*$ in the constraint in: end-point constraints. |
| ENDPOINT_INEQUALITY<br><br>{variable name}<br><br>{LB} : {UB} | Specification of a variable on which an inequality end-point constraint is to be imposed.<br><br>Its full gPROMS path name.<br><br>The values $\min$ and $\max$ in the constraint in: end-point constraints. |
| INTERIORPOINT<br><br>{variable name}<br><br>{LB} : {UB} | Specification of a variable on which an interior-point constraint is to be imposed.<br><br>Its full gPROMS path name.<br><br>The values $\min$ and $\max$ in the constraint in: interior-point constraints.<br><br>Note: an alternate syntax for specifying varying interior-point constraints will be presented later. |
| MAXIMISE | or MINIMISE |

| Specification | Comments |
|---|---|
| {variable name) | The objective function variable *z* (see objective function equation) |

## Specifications of control variables and time-invariant parameters

All of the variables specified as PIECEWISE_CONSTANT, PIECEWISE_LINEAR and TIME_INVARIANT must be Assigned in the gPROMS Process entity. Any variables that are Assigned in the Process entity but are *not* included here will retain the value(s) which are assigned to them: these may be constants or functions of TIME. Effectively, these variables are removed from the optimisation problem.

By default, the initial control-variable profiles are taken to be constant (at the Assigned value) throughout the time horizon. Similarly, the initial guesses for time-invariant parameters are also taken to be the corresponding Assigned values. In both cases, if the Assigned value is a function of TIME, then the initial value of this will be used. Also the upper and lower bounds are taken, by default, to be the values specified in Variable Type entities or in the Preset section of the Process entity (see also: Process entities for optimisation).

The defaults for initial control-variable profiles may be overridden by an INITIAL_PROFILE specification of the following type:

```
INITIAL_PROFILE
{InitialValue} : {LowerBound} : {UpperBound}
...
{InitialValue} : {LowerBound} : {UpperBound}
```

where *InitialValue*, *LowerBound* and *UpperBound* are real constants. For piecewise-constant controls, one such line must be included for each of the time intervals specified in Intervals earlier in the file, with each specification referring to the value of the control over the corresponding interval. For piecewise-linear controls, there must be *two* such lines for each interval, corresponding to the value of the control at the beginning and at the end of the interval respectively.

The default initial guesses for time-invariant parameters may be overridden by an INITIAL_VALUE specification of the type:

```
INITIAL_VALUE
{InitialValue} : {LowerBound} : {UpperBound}
```

where *InitialValue*, *LowerBound* and *UpperBound* are real constants.

## Interior-point constraints

The INTERIORPOINT specifications force the named variable to lie within the specified lower and upper bounds at a set of discrete times, namely the time-interval boundaries[3]The most frequent use of such specifications is as an approximate way of enforcing path constraints—the latter are not handled directly by gPROMS.

In some applications, it can be useful to specify different bounds at each of the time-interval boundaries—for example, a batch reaction procedure might require the temperature to lie in a narrower range in the final stages of reaction than in the earlier stages. This can be achieved in gPROMS through the use of an alternative syntax for the INTERIORPOINT segment of the input file as shown in the table below.

**Table 2.3. Alternative syntax for Interiorpoint constraints**

| Specification | Comments |
|---|---|
| INTERIORPOINT | Specification of a variable on which an interior-point constraint is to be imposed. |

[3]This includes the initial point but *not* the final one. An ENDPOINT_INEQUALITY specification should be used to enforce a final-time constraint, if necessary.

| Specification | Comments |
|---|---|
| {variable name} | Its full gPROMS path name. |
| VARYING<br><br>{lower bound} : {upper bound}<br><br>...<br><br>{lower bound} : {upper bound} | Keyword to indicate distinct bounds at each interval boundary<br><br>Bounds at start of first interval.<br><br>Bounds at start of last interval. |

## Inequality path constraints

It is worth noting that enforcing a path constraint at the interval boundaries does *not* automatically guarantee that the constraints are not violated *within* the intervals. For many applications, this is not a major problem as path constraints tend to be "soft" and minor violations can be tolerated. However, if this is not the case, a more stringent way of enforcing the constraint is to define a *violation variable z* within the relevant Model entity in the gPROMS project through the equation:

$$\dot{z} = \Big(\max(0, w^{\min} - w, w - w^{\max})\Big)^2$$

with initial condition,

$$z(0) = 0$$

and then impose the additional end-point equality constraint:

$$z(t_f) = 0$$

It can be verified that this end-point equality constraint can be satisfied if and only if the original path constraint is satisfied. In many cases, it is still worthwhile retaining the Interiorpoint constraints on *w* as this often leads to improved numerical performance. It may also be better to relax the end-point equality constraint to an inequality constraint:

$$(t_f) \leq \epsilon$$

where $\epsilon$ is a small positive tolerance. An implementation of path constraints is shown for the batch reactor example in the Reactor Model entity, the Initial section of the OPTIMISE_REACTOR Process entity, and the OPTIMISE_REACTOR Optimisation entity.

# Point Optimisation

By default, gPROMS treats optimisation problems as dynamic ones, optimising the behaviour of a system over a finite non-negative time horizon. However, in some cases, it is desired to optimise a system at a single time point—performing a so-called "point" optimisation. From the mathematical point of view, this is equivalent to solving a purely algebraic problem in which a generally nonlinear objective function is maximised or minimised subject to generally nonlinear constraints by manipulating a set of optimisation decision variables that may be either continuous or discrete.

## Specification of point Optimisation Entities

The specification of a point optimisation problem in gPROMS is achieved simply by omitting the `HORIZON` part of the corresponding Optimisation Entity. One can also use the following language to specify a point optimisation:

```
OPTIMISATION_TYPE
  POINT
```

It is worth noting that point Optimisation Entities:

- may contain TIME_INVARIANT controls as well as ENDPOINT_INEQUALITY and ENDPOINT_EQUALITY constraints; such constraints are interpreted as simple algebraic constraints to be satisfied by the optimal solution;
- must not contain time-varying controls PIECEWISE_CONSTANT or PIECEWISE_LINEAR ones or constraints, or specifications of control Intervals, all of which are meaningless in this context.

Moreover,

- the value of the global TIME variable used in any Assignments in the corresponding Process Entity is taken to be zero;
- any Initial conditions specified in corresponding Process Entity are taken as additional equality constraints to be satisfied by the optimisation.

Note that, for the purposes of point optimisation, any time derivative terms of the form $x, that may occur in gPROMS Model Entities, are treated as distinct to the variables x.

## Specification of steady-state optimisation problems

A steady-state optimisation problem is a special case of a point optimisation one. As such, its specification must obey all the rules outlined in: point optimisation entities.

If the underlying model is a dynamic one (i.e. its Model Entities contain one or more time derivative terms of the form $x) , then the initial-condition of the system must be specified as `STEADY_STATE` in the Initial section of the Process Entity.

It may be considerably easier to initialise complex models from a given set of initial conditions and to integrate until steady state is obtained (rather than initialising using the `STEADY_STATE` initial condition). In these cases, a special type of optimisation can be performed by using the SSOptTR solver and specifying:

```
OPTIMISATION_TYPE
  STEADY_STATE
```

in the Optimisation entity (and omitting the `HORIZON` and `INTERVALS` sections).

The SSOptTR solver is selected in one of two ways, depending on the type of problem being solved:

- Continuous variables only
  - use the Solution Parameters tab to specify the value of the MINLPSolver Parameter to be SSOptTR; or
  - specify the following in the `SOLUTIONPARAMETERS` section of the Process

    ```
    DOSolver := "CVP_SS" [
      "MINLPSolver" := "SSOptTR"
    ]
    ```
- Mixed integer optimisation
  - use the Solution Parameters tab to specify the value of the MINLPSolver Parameter to be OAERAP and the value of its NLPSolver Parameter to be SSOptTR; or
  - specify the following in the `SOLUTIONPARAMETERS` section of the Process

    ```
    DOSolver := "CVP_SS" [
      "MINLPSolver" := "OAERAP" [
        "NLPSolver" := "SSOptTR"
      ]
    ]
    ```

Finally, the time horizon needs to be specified. A simulation experiment can be performed to identify how long is required for steady state to be established. This value is then specified using the TimeRelaxationHorizon Solution Parameter for SSOptTR. This can be done using the Solution Parameters tab or by specifying the following in gPROMS language (for a continuous problem):

```
SOLUTIONPARAMETERS
  DOSolver := "CVP_SS" [
    "MINLPSolver" := "SSOptTR" [
      "TimeRelaxationHorizon" := 20000.0
    ]
  ]
```

The default value is 20000, but can be anything from $10^{-20}$ to $10^{20}$ depending on the problem.

The SSOptTR solver takes advantage of nature of the steady-state optimisation problem to increase the performance of the optimisation relative to a full dynamic optimisation. One of the largest computation overheads associated with dynamic optimisation is the integration of the sensitivity equations, which provide the optimiser with the gradients of the constraints and objective function with respect to the decision variables. For steady-state optimisations, SSOptTR need not perform these expensive sensitivity integrations until the steady-state solution has been found, thus significantly reducing the computational effort.

Another feature of the steady-state optimisation problem that can be exploited relates to reinitialisation. In a dynamic optimisation problem, the system needs to be reinitialised for every minor optimisation iteration (where the decision variables are optimised along a fixed search direction) and this means reinitialising using the initial conditions and performing a full sensitivity integration each time. The SSOptTR solver can simply use the steady-state solution from the last minor iteration to reinitialise the problem and then perform the sensitivity evaluation, thus avoiding the more complex initialisation and sensitivity integration. This behaviour can be controlled using the following Solution Parameter:

```
"MINLPSolver" := "SSOptTR" [
      "TimeRelaxationInitialConditions" := "MAJOR"
    ]
```

The three possible values are

- `INITIAL`: all reinitialisations are performed using the initial conditions and initial values (`PRESET`) specified in the Process;
- `MAJOR` (default): reinitialisations are performed using the solution of the last successful major iteration as the initial guess (each major iteration determines a new search direction for the decision variables);
- `MINOR`: reinitialisations are performed using the solution of the last successful minor iteration as the initial guess.

Although the reinitialisation strategies outlined above can significantly reduce the solution time of steady-state optimisation problems, there may be cases where the integration to obtain steady-state during the initial iteration is difficult and time consuming. This behaviour can occur if there are Selector Variables in the Model and these switch many times during the integration from the initial condition to the steady state. In such cases, the expensive initial integration can be bypassed by using Saved Variable Sets to specify the steady-state solution, thus further reducing the solution time. A Saved Variables Set can be specified for use in the optimisation by including the following command:

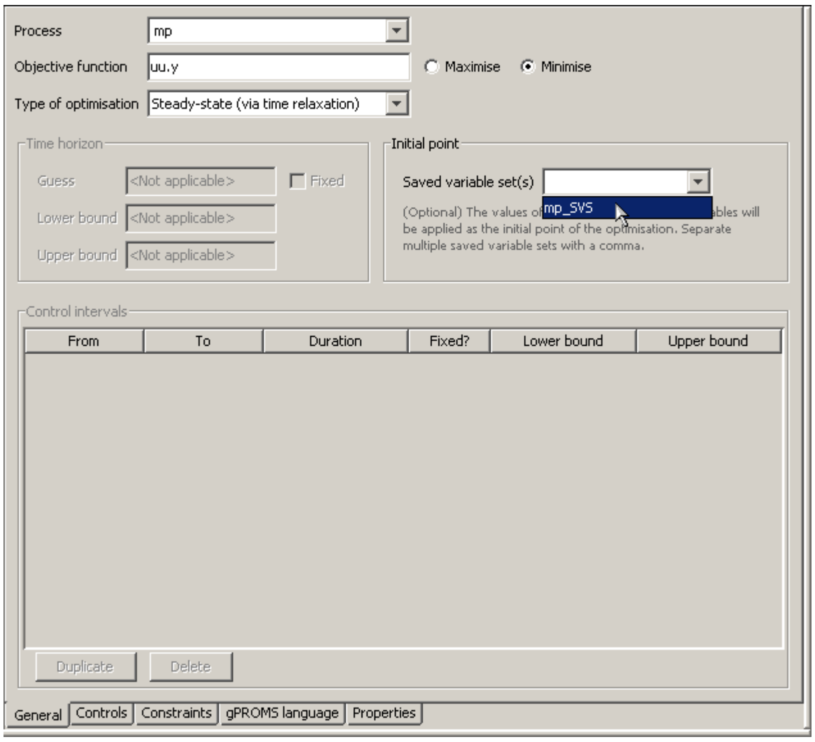
```
RESTORE "Filename"
```

where *`Filename`* is the name of a Saved Variable Set. It is also possible to specify more than one Saved Variable Set: this can be done by including several `RESTORE` commands and/or by providing a list of Saved Variable Sets to a single `RESTORE` command. For example:

```
RESTORE "Filename1", "Filename2", "Filename3"
```

The Saved Variable Sets may also be specified using a ComboBox in the Optimisation entity. This will contain all of the Saved Variable Sets in the Project and one can select one of them for use in the steady-state optimisation.

**Figure 2.4. Selecting a Saved Variable Set for use in a steady-state optimisation**


Process: mp
Objective function: uu.y
Maximise [✓ Minimise]
Type of optimisation: Steady-state (via time relaxation)

Time horizon
Guess: <Not applicable>
Fixed
Lower bound: <Not applicable>
Upper bound: <Not applicable>

Initial point
Saved variable set(s): mp_SVS
(Optional) The values of ...bles will be applied as the initial point of the optimisation. Separate multiple saved variable sets with a comma.

Control intervals

| From | To | Duration | Fixed? | Lower bound | Upper bound |
|---|---|---|---|---|---|

The Saved Variable Set can be selected by using the mouse or by typing in the name in the ComboBox (where **CTRL+space** may be used to autocomplete the selection).

During initial iteration, the SSOptTR solver will first initialise the system using the initial conditions specified in the Process. Once complete, the `RESTORE` will be performed: all differential and Selector Variables in the system that are present in the SavedVariableSet will be restored and the system reinitialised. This will be used as the initial point of the time trajectory used for the steady-state optimisation. When performing mixed integer optimisation, this procedure is applied only to the initial relaxed NLP problem.

To summarise, there are two ways to perform a steady-state optimisation:

- If the model solves quickly and is robust using the `STEADY_STATE` initial condition, then
  - perform a Point optimisation by specifying

    ```
    OPTIMISATION_TYPE
      POINT
    ```

    in the Optimisation entity, omitting the `HORIZON` and `INTERVALS` sections and do not use the SSOptTR solver;
- otherwise,
  - perform a Steady-State optimisation by specifying

    ```
    OPTIMISATION_TYPE
      STEADY_STATE
    ```

    in the Optimisation entity, omitting the `HORIZON` and `INTERVALS` sections and using the SSOptTR solver. Specify the horizon required for steady state to be reached using the `TimeRelaxationHorizon` Solution Parameter of the SSOptTR solver.

# Running optimisation problems in gPROMS

As explained in: specifying dynamic optimisation problems, before an optimisation problem can be executed, it must be specified completely in a gPROMS project that contains:

- one or more Model entities;
- a Process entity named, for example, *ppp*; and
- an Optimisation entity named *ppp*.

In order to run the optimisation problem:

1. Select the Optimisation entity in the gPROMS project tree.
2. Either:
    a. pull down the Activities menu from the top toolbar and select Optimise;
    b. left click on the optimise button on the toolbar below.
3. If there are any syntactical, cross-referencing mistakes etc. these will be detected. Otherwise, the gRMS and execution windows are opened by gPROMS, the optimisation run starts and output is directed to the screen of the execution window.

**Figure 2.5. Executing an optimisation run via the Activities menu.**

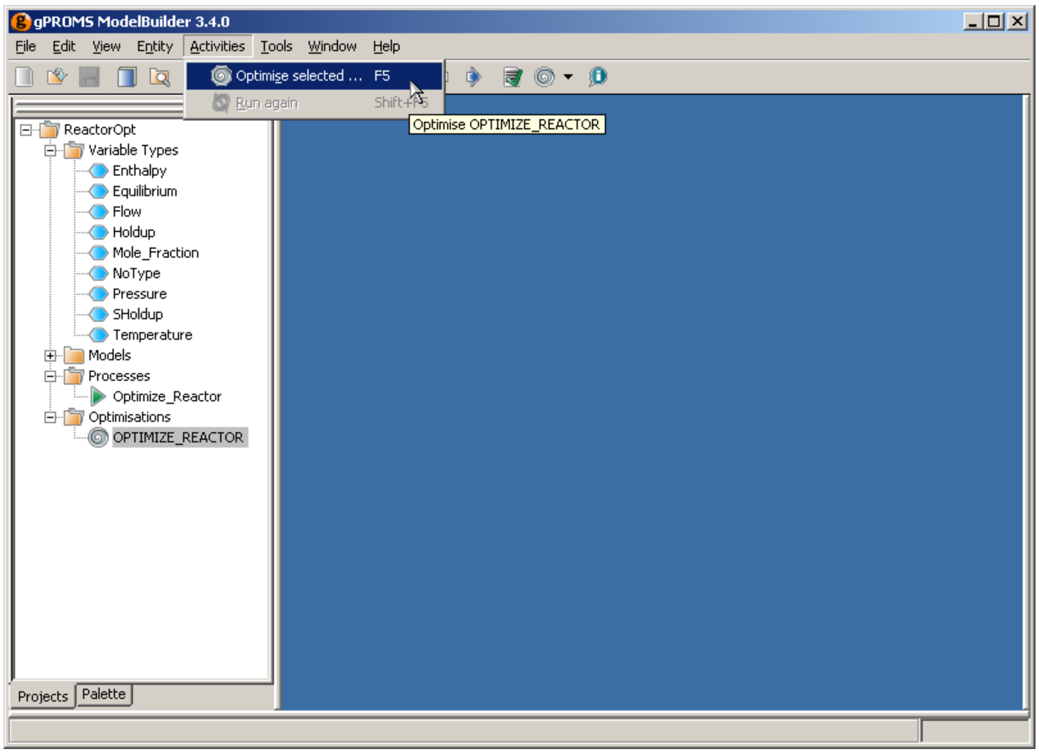
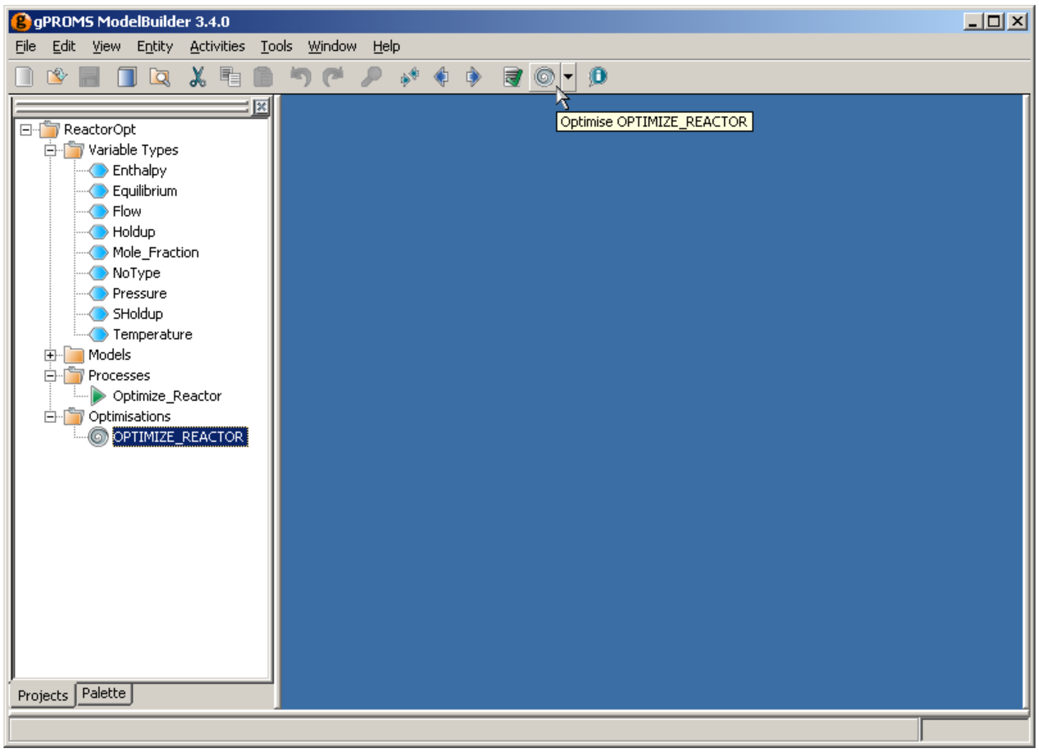


**Figure 2.6. Executing an optimisation run via the Optimisation button.**



## Results of the optimisation run

The execution of an optimisation run will generate five files in the Results folder of the Case:

- *PPP*
- *PPP*.out
- *PPP*.SCHEDULE
- *PPP*_SVS
- *PPP*.point

where *PPP* is the name (in capitals) of the optimisation entity that has been executed to produce these results (*cf.* running optimisation problems).

## The comprehensive optimisation report file

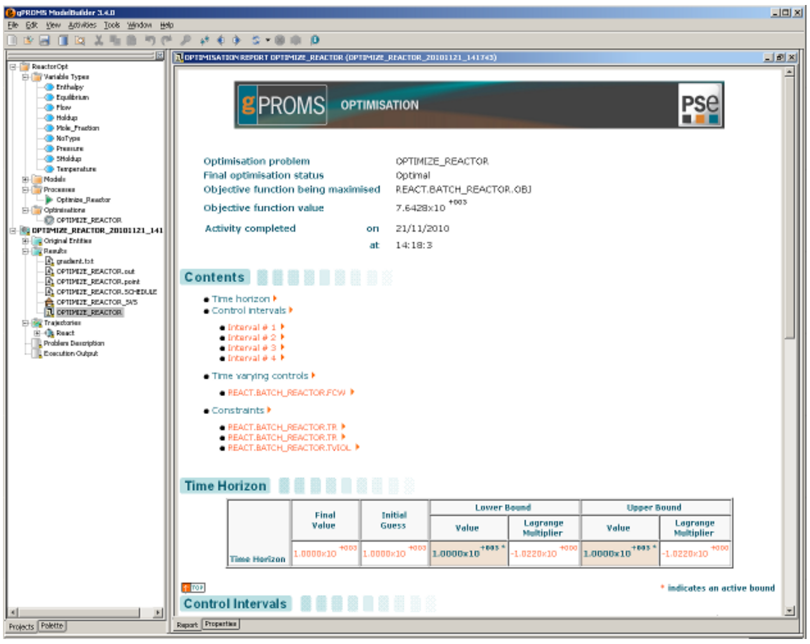
Double-clicking on the report entry, *PPP*, in the Case tree causes a report window to appear in the main window, see the figure below. The report, presented in HTML format, includes:

- a table of contents that allows quick access to the information listed below via "hyperlinks";
- general information such as the date and time of the execution of the activity, its final status and the value of the objective function;
- information on the various optimisation decision variables (time horizon, control interval durations, and time-invariant and time-varying controls), including the values of:
  - the initial guess used,
  - the final value obtained,

- the lower and upper bounds,
- the Lagrange multipliers corresponding to the above bounds.

All active bounds are automatically highlighted.

**Figure 2.7. Comprehensive optimisation report.**



OPTIMISATION REPORT OPTIMIZE_REACTOR (OPTIMIZE_REACTOR_20101121_141743)

| | |
|---|---|
| Optimisation problem | OPTIMIZE_REACTOR |
| Final optimisation status | Optimal |
| Objective function being maximised | REACT.BATCH_REACTOR.OBJ |
| Objective function value | $7.6428\times10^{+003}$ |
| Activity completed on | 21/11/2010 |
| at | 14:18:3 |

Contents

- Time horizon
- Control intervals
  - Interval # 1
  - Interval # 2
  - Interval # 3
  - Interval # 4
- Time varying controls
  - REACT.BATCH_REACTOR.FCW
- Constraints
  - REACT.BATCH_REACTOR.TR
  - REACT.BATCH_REACTOR.TR
  - REACT.BATCH_REACTOR.TVIOL

Time Horizon

| | Final Value | Initial Guess | Lower Bound | | Upper Bound | |
|---|---|---|---|---|---|---|
| | | | Value | Lagrange Multiplier | Value | Lagrange Multiplier |
| Time Horizon | $1.0000\times10^{+003}$ | $1.0000\times10^{+003}$ | $1.0000\times10^{+003}$ * | $-1.0220\times10^{+000}$ | $1.0000\times10^{+003}$ * | $-1.0220\times10^{+000}$ |

* indicates an active bound

Control Intervals

# The optimisation report file

The *PPP*.out file contains a summary report on the optimisation run in a simple text format, including:

- the outcome of the optimisation run;
- the final value of the objective function;
- the final value of the time horizon and the lengths of the time intervals;
- the final values of the time-invariant parameters, and the control-variable profiles; the latter are specified in terms of a single value per interval for piecewise-constant controls, and a pair of values for piecewise-linear controls (as usual, corresponding to the value of the control at the start and end of each interval); and
- the values of variables on which end-point and/or interior-point constraints where specified, at the corresponding final and/or interior-points.

The file also contains computational statistics on the performance of the numerical method.

A sample *PPP*.out file is listed in the dynamic optimisation example at the end of this guide.

# The SCHEDULE file and the Saved Variable Set

The *PPP*.Schedule presents the *most recent* optimisation solution point in the form of a gPROMS Schedule. A sample *PPP*.SCHEDULE file is listed in the dynamic optimisation example at the end of this guide.

The Schedule file can be used to reproduce the detailed results of the optimisation by carrying out a simulation activity within gPROMS. This provides you access to the full facilities of the gPROMS Results Management.

Once the final solution of an optimisation problem is obtained, gPROMS creates a Saved Variable Set from the initialisation of this point. The Saved Variable Set is called *PPP*_SVS and is used in the SCHEDULE to restore the exact conditions at the final point.

In order to do this:

1. Paste the contents of the Schedule file into the relevant Process entity of your gPROMS project.
2. Copy the generated Saved Variable Set from the result Case into the gPROMS project.

A optimal Process entity that contains these changes is shown for the batch reactor example. It is useful for you to compare it with the original Process entity and the Schedule results file.

### Note

The contents of the Schedule file does not always represent an optimal or even a feasible solution to the problem: if the optimisation run is interrupted by the user, or ends without finding a satisfactory solution, the file will simply show the point last considered by gPROMS. Only if a comment at the top of the file states the following:

```
# Final Optimisation Status         :     Optimal Solution Found
```

should the results be relied upon as a (locally) optimal solution.

## The point file

The *PPP*.point file is generated at every iteration of the optimisation calculation. It contains the same information as the Schedule file, but in the format of an Optimisation entity (except that constraints are not reproduced). This is useful if there is a need to restart an optimisation after a system crash or other catastrophic event, or, following a successful solution, to provide a good 'initial guess' for a slightly altered optimisation problem.

A sample *PPP*.point file is listed in the dynamic optimisation example at the end of this guide.

# Other features

The following apply to the current version of gPROMS:

- The initial conditions specified in the Process entity must be:
  - equations of the form:

    *VariableName* = *Value* ;

    where *VariableName* is the full gPROMS pathname of a differential or algebraic variable, and *Value* is a numerical value;
  - or equations of the form:

    $*VariableName* = *Value* ;
  - or the steady-state specification:

    ```
    INITIAL
      STEADY_STATE
    ```
- Many applications involve the optimisation of the initial values of some of the system variables. For instance, it may be that you want to determine the optimal initial amount of catalyst to be charged to a batch reactor. This kind of requirement can easily be accommodated as follows:
  - In the Model entity containing the variable, $z$, whose initial value is to be optimised, introduce:
    - an additional variable,$z_0$, of the same type as $z$;
    - an additional variable, $\delta z$, of type NoType;

- the additional equation:

  $\delta z = z - z_0$

- In the Process entity,
  - assign $z_0$ to a default value:

    ```
    ASSIGN
      Z0 := 1.0 ;
    ```

  - set the initial value of $\delta z$ to zero:

    ```
    INITIAL
      \DeltaZ = 0.0 ;
    ```

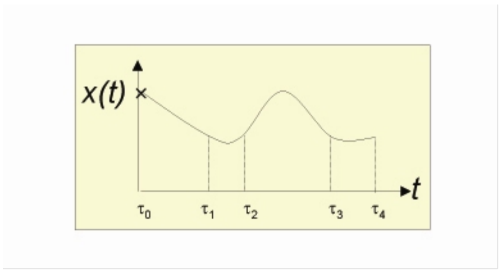
- In the Optimisation entity, declare $z_0$ as a time-invariant parameter, specifying an initial guess and lower and upper bounds for it.

## Standard solvers for optimisation

There are two standard mathematical solvers for optimisation in gPROMS, namely CVP_SS and CVP_MS. CVP_SS can solve optimisation problems with both discrete and continuous decision variables ("mixed integer optimisation"). Both steady-state and dynamic problems are supported. CVP_MS can solve dynamic optimisation problems with continuous decision variables.

For dynamic optimisation problems, both CVP_SS and CVP_MS are based on a control vector parameterisation (CVP) approach which assumes that the time-varying control variables are piecewise-constant (or piecewise-linear) functions of time over a specified number of control intervals. The precise values of the controls over each interval, as well as the duration of the latter, are generally determined by the optimisation algorithm[4]. As the number of control variables is usually a small fraction of the total number of variables in the problem, the optimisation algorithm has to deal only with a relatively small number of decisions, which makes the CVP approach applicable to large problems.

**Figure 2.8. Single-shooting algorithm**



The CVP_SS solver implements a "single-shooting" dynamic optimisation algorithm. This involves the following steps (see the figure above):

1. the optimiser chooses the duration of each control interval, and the values of the control variables over it;
2. starting from the initial point at time *t=0* (shown as a cross on the vertical axis in the figure, the dynamic system model is solved over the entire time horizon to determine the time-variation of all variables *x(t)* in the system;
3. the above information is used to determine the values of[5]:

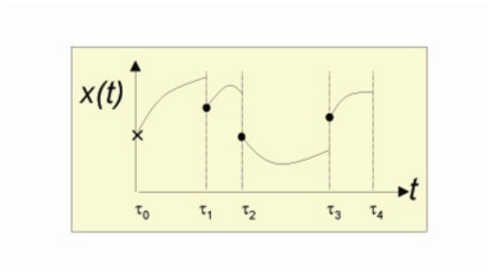
[4]In addition, as explained earlier in this guide, many dynamic optimisation problems involve time-invariant parameters that also have to be chosen by the optimiser.
[5]In practice, the solution of the model also needs to determine the values of the partial derivatives (sensitivities) of the objective function and constraints with respect to all the quantities specified by the optimiser.

   - the objective function to be optimised;
   - any constraints that have to be satisfied by the optimisation;

4. based on the above, the optimiser revises the choices it made at the first step, and the procedure is repeated until convergence to the optimum is achieved.

The term "single-shooting" arises from the second step in the above algorithm which involves a single integration of the dynamic model over the entire horizon.

**Figure 2.9. Multiple-shooting algorithm**



The CVP_MS solver implements a "multiple-shooting" dynamic optimisation algorithm with the following steps (see the figure above):

1. the optimiser chooses the duration of each control interval, the values of the control variables over it, and, additionally, the values of the differential variables *x(t)* at the start of each control interval other than the first one (shown as solid circles in the figure);
2. for each control interval, starting from the initial point that is either known (for the first interval) or is chosen by the optimiser (for all subsequent intervals), the dynamic system model is solved over this control interval to determine the time-variation of all variables *x(t)* in the system;
3. the above information is used to determine the values of:
   - the objective function to be optimised;
   - any constraints that have to be satisfied by the optimisation;
   - the discrepancies between the computed values of the variables *x(t)* at the end of each interval and the corresponding values chosen by the optimiser at the start of the next interval;
4. based on the above, the optimiser revises the choices it made at the first step, and repeats the above procedure until it obtains a point that:
   - optimises the objective function;
   - satisfies all constraints;
   - ensures that all differential variables *x(t)* are continuous at the control interval boundaries.

The "multiple-shooting" term reflects the fact that each control interval is treated independently at the second step above.

Both solvers, by default, employ the DASOLV code (details in the Model Developer Guide) for the solution of the underlying DAE problem and the computation of its sensitivities. In principle, this can be replaced by a third-party solver with similar capabilities.

The choice between the CVP_SS and CVP_MS solvers for any dynamic optimisation problem depends primarily on the number of optimisation decision parameters that the algorithm has to deal with in computing the sensitivities of the model variables. In principle:

- CVP_MS should normally be preferred for problems with many time-varying control variables and/or many control intervals, but with relatively few differential ("state") variables;
- CVP_SS should normally be preferred for large problems (potentially involving several hundreds or thousands of differential ("state") variables) but with relatively few time-varying control variables and control intervals.

In practice, some experimentation may be required to determine the better algorithm for any particular application.

The DOsolver solution parameter may be used to change and/or configure the solver used for optimisation activities. If this parameter is not specified, then the CVP_SS solver is used, with the default configuration. See also: CVP_SS solver.

## The CVP_SS solver

CVP_SS can solve steady-state and dynamic optimisation problems with both continuous and discrete optimisation decision variables. The algorithmic parameters used by CVP_SS along with their default values are shown below. This is followed by a detailed description of each parameter.

```
"CVP_SS"  [ "DASolver"    := "DASOLV";
            "MINLPSolver" := "OAERAP"];
```

DASolver - A quoted string specifying a differential-algebraic equation solver.

- The solver to be used for integrations of the model equations and their sensitivity equations at each iteration of the optimisation. This can be either the standard DASOLV solver or a third-party differential-algebraic equation solver (see the gPROMS System Programmer Guide). The default is DASOLV.

  This parameter can be followed by further specifications aimed at configuring the particular solver by setting values to its own algorithmic parameters (see also: specifying solver-type algorithmic parameters in the Model Developer Guide).

MINLPSolver - A quoted string specifying a mixed integer optimisation solver.

- The solver to be used for mixed integer optimisation problems. This can be either the standard OAERAP solver or a third-party mixed integer optimisation solver (see the gPROMS System Programmer Guide). For optimisation problems that do not involve any discrete decision variables, this can be any CAPE-OPEN compliant solver that is capable of solving NLPs but not MINLPs, e.g. the standard NLP solver SRQPD. The default is OAERAP.

This parameter can be followed by further specifications aimed at configuring the particular solver by setting values to its own algorithmic parameters (see also: specifying solver-type algorithmic parameters in the Model Developer Guide).

## The OAERAP solver

The OAERAP solver employs an outer approximation (OA) algorithm for the solution of the MINLP. As outlined in the algorithm below, this involves solving a sequence of simpler optimisation problems, including nonlinear programs (NLPs) at steps 1 and 3 and mixed integer linear programs (MILPs) at step 2. The OAERAP code has been designed so that it can make direct use of any CAPE-OPEN compliant NLP and MILP solvers (see the gPROMS System Programmer Guide) without the need for any additional interfacing or modification.

*Outline of the OAERAP algorithm for the solution of a MINLP problem (minimisation case)*

**Given** initial guesses for all optimisation decision variables, both discrete (*y*) and continuous (*x*):

**Step 0: Initialisation**

- Set the objective function of the best solution that is currently available, $\phi^{best} := +\infty$.
- Set the objective function of the best solution that may be obtained, $\phi^{LB} := +\infty$.

**Step 1: Solve fully relaxed problem**

- Solve a continuous optimisation problem (NLP) treating all discrete variables as continuous (i.e. allow them to take any value between their lower and upper bounds) to determine optimal values $x^{FR}$, $y^{FR}$ of the optimisation decision variables and of the objective function, $\phi^{FR}$.
- If above problem is infeasible, terminate: original problem is infeasible as posed.
- If all discrete optimisation decision variables have discrete values at the solution of the above problem, then terminate: optimal solution of original problem is $x^{FR}$, $y^{FR})$ with an objective function value of $\phi^{FR}$.

**Step 2: Solve master problem**

- Construct a mixed integer linear programming (MILP) problem which:
  - involves appropriate linearisations of the objective function and the constraints carried out at the solutions of all continuous optimisation problems solved so far,
  - excludes all combinations of discrete variable values that have been considered at step 2 so far.
- Solve the above MILP problem to determine optimal values of both the continuous and discrete variables $x^{MP}$, $y^{MP}$, and the corresponding value of the objective function $\phi^{MP}$.
- If the above problem is infeasible or if $\phi^{best} - \phi^{MP} \leq \varepsilon \max(1, |\phi^{best}|)$, then terminate: there are no more combinations of discrete variables that can be usefully considered.
  - If $\phi^{best} = +\infty$, then original problem was infeasible.
  - Otherwise, the optimal solution is $x^{best}$, $y^{best})$ with a corresponding objective function value of $\phi^{best}$.
- The MILP provides an improved bound on the best solution that may be obtained; therefore, update $\phi^{LB} := \phi^{MP}$.

**Step 3: Solve primal optimisation problem**

- Fix all discrete optimisation decision variables to their current values.
- Solve continuous optimisation problem (NLP) to determine:
  - optimal value of objective function, $\phi^{PR}$;
  - optimal values of continuous optimisation decision variables, $x^{PR}$.
- If the above NLP is feasible and $\phi^{PR} < \phi^{best}$, then an improved solution to the original problem has been found; record its details by setting $\phi^{best} := \phi^{PR}$; $x^{best} := x^{PR}$; $y^{best} := y^{PR}$.

**Step 4: Iterate**

- Set the next set of values of the discrete optimisation decision variables to be considered $y^{PR} := y^{MP}$.
- Repeat from step 2.

The OAERAP solver also includes an equality relaxation (ER) scheme for handling equality constraints. It should be emphasised that, in the case of optimisation problems defined in gPROMS, this relaxation is applied only to any ENDPOINT_EQUALITY constraints that may appear in the Optimisation Entity.

The algorithm described above is guaranteed to obtain the globally optimal solution to the optimisation problem posed only if the latter is convex. This is unlikely to be the case in many problems of engineering interest.

An augmented penalty (AP) strategy is employed in order to increase the probability of a global solution being obtained.

The algorithmic parameters used by OAERAP along with their default values are shown below. This is followed by a detailed description of each parameter.

```
"OAERAP" ["MILPSolver"                    := "LPSOLVE",
          "NLPSolver"                     := "SRQPD",
          "MaxIterations"                 := 10000,
          "NLPSubProblemInitialGuesses"   := "MILPMasterProblem",
          "OptimisationTolerance"         := 1.0E-4,
          "OutputLevel"                   := 0]
```

MILPSolver - A quoted string specifying a mixed integer linear programming solver.

- Specifies a CAPE-OPEN compliant solver to be used for the solution of the mixed integer linear programming (MILP) problems at step 2 of the algorithm described above.

NLPSolver - A quoted string specifying a nonlinear programming solver.

- Specifies a CAPE-OPEN compliant solver to be used for the solution of the nonlinear programming (NLP) problems at steps 1 and 3 of the algorithm described above.

MaxIterations - An integer in the range [1, 100000].

- The maximum number of iterations involving step 2-4 of the algorithm described above. This is essentially the maximum number of distinct alternatives to be considered by the algorithm

NLPSubProblemInitialGuesses - either "MILPMasterProblem" or "FullyRelaxedNLP"

- Determines the source of initial guesses for the NLP Primal Optimisation.

  The OAERAP algorithm employs two methods of obtaining initial guesses for the NLP Primal Problems (step 3 above).

  The first is to use the solution of the fully-relaxed problem (step 1) as initial guesses for the solution of the primal problem (step 3) at each iteration. To use this method, specify "NLPSubProblemInitialGuesses" := "FullyRelaxedNLP".

  An alternative approach is to use the solution of the MILP master problem, at the current iteration, to provide the initial guesses for the NLP primal problem. This is the default method, specified by setting "NLPSubProblemInitialGuesses" := "MILPMasterProblem".

  The method that will be most effective will depend on the problem being solved. One advantage of obtaining initial guesses from the MILP master problem is that because the discrete variables in the NLP problem will be set to the values in the solution of the MILP, the values of the continuous variables will be consistent with the discrete ones and so should provide a good initial guess for the NLP problem. A common example of this behaviour is process synthesis problems, where binary variables can be used to represent the existance of a process in a flowsheet. If the solution of an MILP implies that a unit does not exist, then the MILP of step 2 will force some related continuous variables (e.g. the flows through these units) to be zero and these are, of course, excellent initial guesses for the NLP problem (by contrast, these might not be zero in the solution of the fully-relaxed NLP). However, if the problem is highly non-linear, then the solution of the linearised equations in the MILP may not be such a good initial guess for the NLP. In these cases, it may be better to use the solution of the relaxed NLP as the initial guess for each NLP primal problem.

OptimisationTolerance - A real number in the range [0.0, 1.0].

- The optimisation tolerance $\varepsilon$ used in the termination criterion at step 2 of the algorithm described above.

OutputLevel - An integer in the range [-1, 0].

- The amount of information generated by the solver. The following table indicates the lowest level at which different types of information are produced:

| | |
|---|---|
| -1 | (None) |
| 0 | Solution of fully relaxed point,<br><br>solution of master problem,<br><br>solution of primal optimisation problem,<br><br>final solution |

## The SRQPD solver

The SRQPD solver employs a sequential quadratic programming (SQP) method for the solution of the nonlinear programming (NLP) problem. The algorithmic parameters used by SRQPD along with their default values are shown below. This is followed by a detailed description of each parameter.

```
"SRQPD" [
            "ConvergenceCriterion"        := "ImprovedEstimateBased",
            "HandleDiscreteVariables"     := FALSE,
            "InitialHessian"              := 0,
            "InitialLineSearchStepLength" := 1.0,
            "MaxFun"                      := 10000,
            "MaximumLineSearchSteps"      := 20,
            "MaxLineSearchStepLength"     := 1.0,
            "MinimumLineSearchStepLength" := 1.0E-5,
            "NoImprovementTolerance"      := 1.0E-12,
            "OptimisationTolerance"       := 0.0010,
            "OutputLevel"                 := 0,
            "Scaling"                     := 0
        ]
```

ConvergenceCriterion - Either "ImprovedEstimateBased" or "OptimalityBased"; default "ImprovedEstimateBased".

- The "ImprovedEstimateBased" convergence criterion is:

  $$a + \frac{b}{|f| + 1} \le \varepsilon_o$$

  where:

  $$a = \sum_{i=1}^{meq} |c_i| + \sum_{i=meq+1}^{m} \max(0, -c_i) + \sum_{j=1}^{n} \max\left(0, (x_j^L - x_j)(x_j - x_j^U)\right);$$

  $$b = |\nabla_x f^{\mathrm{T}} d| + \sum_{i=1}^{m} |\lambda_i c_i| + \sum_{i=1}^{n} |\mu_i| \max\left(0, (x_j^L - x_j)(x_j - x_j^U)\right);$$

  #$_o$ is the optimisation tolerance given by the Solution Parameter OptimisationTolerance;

  *f* is the objective function;

  *c* is the constraint vector (right-hand side);

  *meq* is the number of equality constraints;

  *m* is the total number of constraints;

  *n* is the size of the variable vector *x* (i.e. the number of variables);

$x_j^L$ and $x_j^U$ are the lower and upper bounds of variable $x_j$;

$d$ is the vector of corrections to $x$ (i.e. the change in $x$ during the current step);

$\lambda_j$ is the Lagrange multiplier that corresponds to the equality constraint imposed on variable $x_j$;

$\mu_j$ is the Lagrange multiplier that corresponds to the bound constraints imposed on variable $x_j$.

- The "OptimalityBased" convergence criterion uses two tolerances: $\#_o$, specified by the OptimisationTolerance Solution Parameter and $\#_i$, specified by NoImprovement Tolerance. Given the following definitions:

$$\tau_1 = \sum_{i=1}^{meq} |c_i| + \sum_{i=meq+1}^{m} \max(0, -c_i) + \sum_{j=1}^{n} \max\left(0, (x_j^L - x_j)(x_j - x_j^U)\right);$$

$\tau_{2a} = |f^k - f^{k-1}|$, where $k$ is the current iteration number;

$\tau_{2b} = \max_j(dx_j)$, where $dx_j$ is the step calculated for $x_j$ in the latest line-search step;

$$\tau_3 = \max_j \left( |\frac{\partial L}{\partial x_j}| \right);$$

$$\tau_4 = \sum_{i=1}^{m} |\lambda_i c_i| + \sum_{i=1}^{n} |\mu_i| \max\left(0, (x_j^L - x_j)(x_j - x_j^U)\right);$$

$L(x) = f(x) + \sum_{i=1}^{m} \lambda_i h_i(x) + \sum_{j=1}^{n} \mu_j^U (x_j - x_j^U) + \mu_j^L (x_j^L - x_j)$ is the Lagrange function,

$\lambda_i$ the Lagrange multipliers for the equality and inequality constraints

$h_i(x)$ and and the Lagrange multipliers for the upper and lower bound constraints;

the following tests are applied:

| | |
|---|---|
| At the end of each major iteration: | `If` $\tau_1 + \tau_3 + \tau_4 \le \varepsilon_o$, `then` terminate due to optimality; |
| | `Else if` $\tau_{2a} \le \varepsilon_i$ and $\tau_1 \le \varepsilon_o$, `then` terminate due to no-improvement in the objective function. |
| At the end of each line-search step: | `If` $\#_{2b} \le \#_i$ and $\#_1 \le \#_o$, `then` terminate due to no-improvement in the optimisation variables; |
| | `Else if` $\#_{2b} \le \#_i$, `then` terminate due to failure to find a feasible point within the non-improvement tolerance. |

HandleDiscreteVariables - TRUE or FALSE; default FALSE.

- This parameter determines whether the solver handles mixed-integer non-linear optimisation problems by transforming discrete controls into continuous ones.

InitialHessian - An integer in the range [0, 2]; default 0.

- By default, the initial hessian matrix is assumed to be the identity matrix (InitialHessian := 0).
- At present no other options are available but may be introduced in the future.

InitialLineSearchStepLength - A real number in the range [$10^{-10}$, 1.0]; default 1.0.

- The length of the line search step for the first optimisation iteration. An initial line search step length less than 1 is recommended when the initial approximation of the Hessian (i.e. identity matrix) is very different to the actual values in the Hessian. This could result in a very large initial step and therefore several line search trials before the optimiser finds a better point.

MaxFun - An integer in the range [0, 100000]; default 10000.

- The maximum number of *optimiser* function evaluations (i.e. solutions of the underlying steady-state or dynamic model) to perform before halting the solution process (if no optimum has been found by that point).

MaximumLineSearchSteps - An integer in the range [1, 100]; default 20.

- The maximum number of line search steps in one optimisation iteration.

MaxLineSearchStepLength - A real number in the range [$10^{-10}$, 1.0]; default 1.

- The maximum length of a line search step.

MinimumLineSearchStepLength - A real number in the range [$10^{-10}$, 1.0]; default $10^{-5}$.

- The minimum length of a line search step.

NoImprovementTolerance - A real number in the range [$10^{-20}$, 1.0]; default $10^{-12}$.

- The solution tolerance for non-improving objective function or optimisation variables. Only used when ConvergenceCriterion := "OptimalityBased" (see above).

OptimisationTolerance - A real number in the range [$10^{-20}$, 1.0]; default 0.001.

- The solution tolerance for the optimisation. Convergence is deemed to occur when a linear combination of the gradients of the Lagrangian function on one hand, and the violation of the constraints on the other, drops below this tolerance. The convergence criterion used is specified by the ConvergenceCriterion parameter described above.

OutputLevel - An integer in the range [-1, 4]; default 0.

- The amount of information generated by the solver. The following table indicates the lowest level at which different types of information are produced:

| | |
|---|---|
| -1 | (None) |
| 0 | Failed integrations and initialisations, optimisation failure,<br><br>summary information from the SRQPD nonlinear programming code,<br><br>final solution point and constraint values,<br><br>best available point after failure |
| 1 | Values of optimisation decision variables, objective function and constraints in each major optimisation iteration |
| 2 | Start and end times of each interval of integration,<br><br>optimisation decision variables and objective function at each line search trial |
| 3 | Derivatives of objective function and constraints |

Scaling - An integer in the range [0, 3]; default 0.

- The form of scaling to be applied to the optimisation decision variables, including control variables, time-invariant parameters, the length of the time horizon and the lengths of individual control intervals. These decision variables may vary significantly in magnitude, which may adversely affect the performance of the optimisation algorithms. Consequently, appropriate scaling of the optimisation decision variables is strongly recommended[6]

  The scaling performed is of the general mathematical form:

  $$\tilde{q}_j \equiv \frac{q_j - c_j}{d_j}$$

  where $q_j$ is the *j*th original optimisation decision variable and $\tilde{q}_j$ is the corresponding scaled decision variable. The constants $c_j$ and $d_j$ are determined automatically depending on the value of Scaling, as described below:

  - **Scaling = 0**: No scaling (default).

    $$\begin{aligned} d_j &= 1, \\ c_j &= 0. \end{aligned}$$

  - **Scaling = 1:** Scaling according to the ranges of the optimisation decision variables so that the scaled variables vary between -1 and 1.

    $$\begin{aligned} d_j &= \frac{1}{2}\left(q_j^{\max} - q_j^{\min}\right), \\ c_j &= \frac{1}{2}\left(q_j^{\max} + q_j^{\min}\right) \end{aligned}$$

  - **Scaling = 2:** Scaling according to the initial guesses of the optimisation variables.

    $$\begin{aligned} d_j &= \begin{cases} q_j^0 & \text{if } |q_j^0| > \varepsilon, \\ \frac{1}{2}\left(q_j^{\max} - q_j^{\min}\right) & \text{otherwise} \end{cases} \\ c_j &= 0 \end{aligned}$$

    where $q_j^0$ is the initial guess for the *j*th optimisation variable and $\varepsilon$ is a small constant (currently set at $10^{-8}$).

  - **Scaling = 3:** Scaling according to the value and the gradients of the objective function $\Phi$ at the initial guess.

    $$\begin{aligned} d_j &= \begin{cases} \frac{1+|\Phi(q^0)|}{2\left|\frac{\partial \Phi}{\partial q_j}\right|_{q^0}} & \text{if } \left|\frac{\partial \Phi}{\partial q_j}\right|_{q^0} > \varepsilon, \\ \frac{1}{2}\left(q_j^{\max} - q_j^{\min}\right) & \text{otherwise} \end{cases} \\ c_j &= 0 \end{aligned}$$

    where 0 is the vector of initial guesses of the optimisation decision variables and $\varepsilon$ is a small constant (currently set at $10^{-8}$).

## The CVP_MS solver

The algorithmic parameters used by CVP_MS along with their default values are shown below. This is followed by a detailed description of each parameter[7]

[6]A useful indication as to whether scaling is necessary is the condition number estimate that is printed out at each iteration of the optimisation calculation. It is recommended that scaling be undertaken for problems with condition numbers exceeding $10^{10}$.

[7]For full details, please consult the information at http://www.systemtechnik.tu-ilmenau.de/fg_opt/omuses/omuses.html

```
"CVP_MS"                [ "OutputLevel"              := 0;
                          "MaxFun"                   := 10000;
                          "SQPMinAlpha"              := 1E-10;
                          "SQPHeLa"                  := "BFGS";
                          "SQPHeLaEps"               := 1E-10;
                          "SQPHeLaScale"             := TRUE;
                          "SQPHeLaEigenCtrl"         := TRUE;
                          "SQPMaxIters"              := 500;
                          "SQPMaxInfIters"           := 10;
                          "SQPWatchdogStart"         := 10;
                          "SQPWatchdogCredit"        := 0;
                          "SQPWatchdogLogging"       := FALSE;
                          "SQPSolver"                := "Powell";
                          "SQPQPSolver"              := "Franke";
                          "QPEps"                    := 1E-10;
                          "QPMatSolver"              := "RedSpBKP";
                          "QPMaxIters"               := 250;
                          "OptTol"                   := 1E-3;
                          "InfDefault"               := 1E10;
                          "NumSen"                   := FALSE;
                          "SetBounds"                := FALSE;
                          "NeedLagrangeMultipliers"  := FALSE;
                          "DASolver"                 := "DASOLV"];
```

OutputLevel - An integer in the range [0, 4].

- The amount of information generated by the solver. The following table indicates the lowest level at which different types of information are produced:

| | |
|---|---|
| 0 | Failed integrations and initialisations, optimisation failure,<br><br>summary information from the HQP nonlinear programming code,<br><br>final solution point and constraint values,<br><br>best available point after failure |
| 1 | Values of optimisation decision variables, objective function and constraints in each major optimisation iteration |
| 2 | For each multiple-shooting interval in each major optimisation iteration:<br><br>the values of the optimisation decision variables,<br><br>the values and derivatives of the matching conditions, the constraints and the objective function. |

MaxFun - An integer in the range [0, 100000].

- The maximum number of *optimiser* function evaluations (i.e. solutions of the underlying dynamic model) to perform before halting the solution process (if no optimum has been found by that point).

SQPMinAlpha - A real number in the range [0, $10^5$].

- Lower limit for the step length in the line search of the sequential quadratic programming (SQP) sub-solver.

SQPHeLa - A quoted string.

- The method to be used for constructing the approximation of the Hessian matrix of the Lagrangian. Permitted values are:
  - "BFGS": partitioned BFGS update with Powell's damping
  - "DScale": numerical approximation with a diagonal matrix

SQPHeLaEps - A real number in the range [0, $10^5$].

- $\epsilon$ parameter used in SQP algorithm, see the Omuses document.

SQPHeLaScale - A boolean value.

- Use "DScale" approach to initialise Hessian rather than setting it to the identity matrix.

SQPHeLaEigenCtrl - A boolean value.

- Control of positive definite Hessian blocks based on eigenvalues (only used with the BFGS method).

SQPMaxIters - An integer in the range [0, 100000].

- Total number of SQP iterations allowed.

SQPMaxInfIters - An integer in the range [0, 100000].

- Number of infeasible SQP iterations (i.e. points where the integration fails) allowed before failure.

SQPWatchdogStart - An integer in the range [0, 100000].

- Iteration at which to start watchdog algorithm if using "Powell" algorithm (see SQPSolver parameter below).

SQPWatchdogCredit - An integer in the range [0, 100000].

- Number of "bad" iterations until backtracking and regular step are performed (0 means disable watchdog).

SQPWatchdogLogging - A boolean value.

- Specifies whether watchdog log output should be produced.

SQPSolver - A quoted string.

- The type of sequential quadratic programming (SQP) algorithm to be used for the optimisation. Permitted values:
  - "Powell"
  - "Schittkowski"

SQPQPSolver - A quoted string.

- The type of quadratic programming (QP) solver to be used at each iteration of the optimisation. Permitted values are:
  - "Franke"
  - "Mehrotra"

QPEps - A real number in the range [0, $10^5$].

- The tolerance to which the quadratic programming sub-problems are to be solved.

QPMatSolver - A quoted string.

- The matrix solver to use for the solution of the quadratic programming sub-problems in the optimisation. Permitted values are (refer to Omuses document for details):
  - "SpBKP"
  - "RedSpBKP"
  - "SpSC"
  - "LQDOCP"

QPMaxIters - An integer in the range [0, 100000].

- Maximum number of QP iterations to attempt.

OptTol - A real number in the range [0.0, 1.0].

- The solution tolerance for the optimisation.

InfDefault - A real number in the range [0, $10^{35}$].

- Upper and lower bounds greater than this value in magnitude are treated as $pm\infty$ (as appropriate).

NumSen - A boolean value.

- Specifies whether sensitivities should be calculated numerically -- i.e. by repeated "normal" integrations with perturbed values -- rather than 'analytically', i.e. with a special sensitivity integration. **Not recommended** except perhaps for large problems with very few parameters per interval.

DASolver - A quoted string specifying a differential-algebraic equation solver.

- The solver to be used for integrations of the model equations and their sensitivity equations at each stage and each iteration of the optimisation. This can be either the standard DASOLV solver or a third-party differential-algebraic equation solver (see the gPROMS System Programmer Guide). The default is DASOLV.

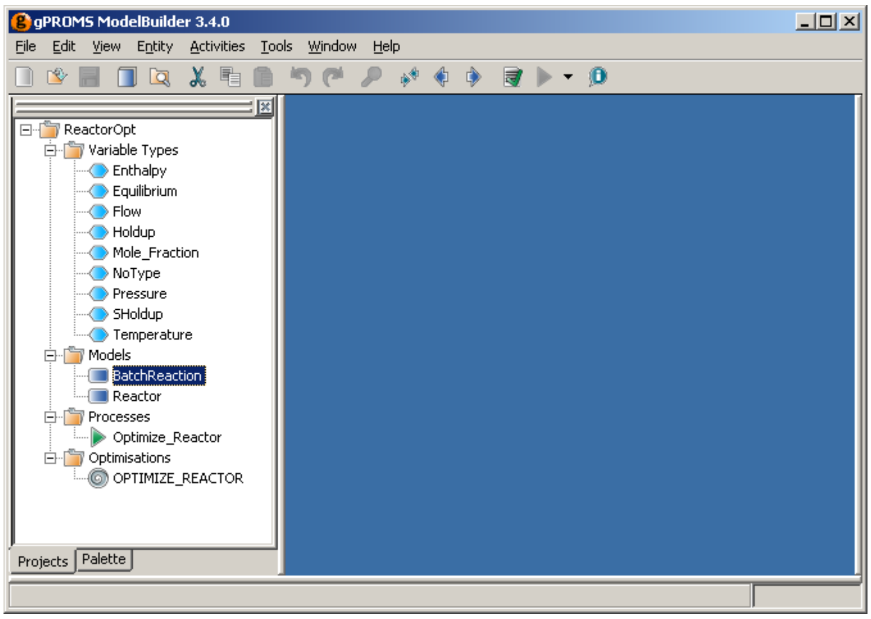
  This parameter can be followed by further specifications aimed at configuring the particular solver by setting values to its own algorithmic parameters (see also: specifying solver-type algorithmic parameters in the Model Developer Guide).

## Dynamic Optimisation Example

Here, an example of a dynamic optimisation is given using a batch-reactor Model.

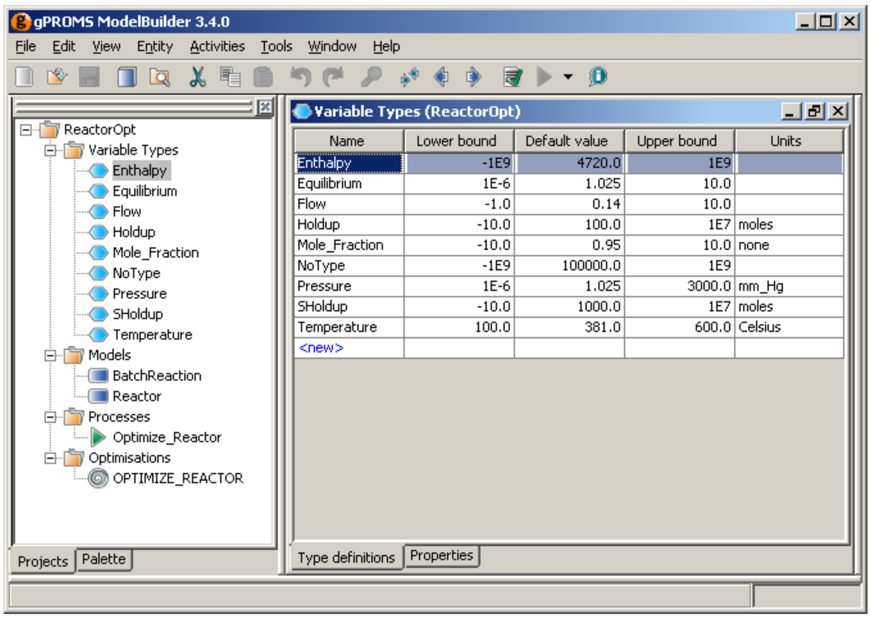
## Project tree ReactorOpt.gPJ

Figure 2.10. Project tree for the dynamic optimisation example.



## Variable Type entities in ReactorOpt.gPJ

Figure 2.11. Variable Type entities in the ReactorOpt project.



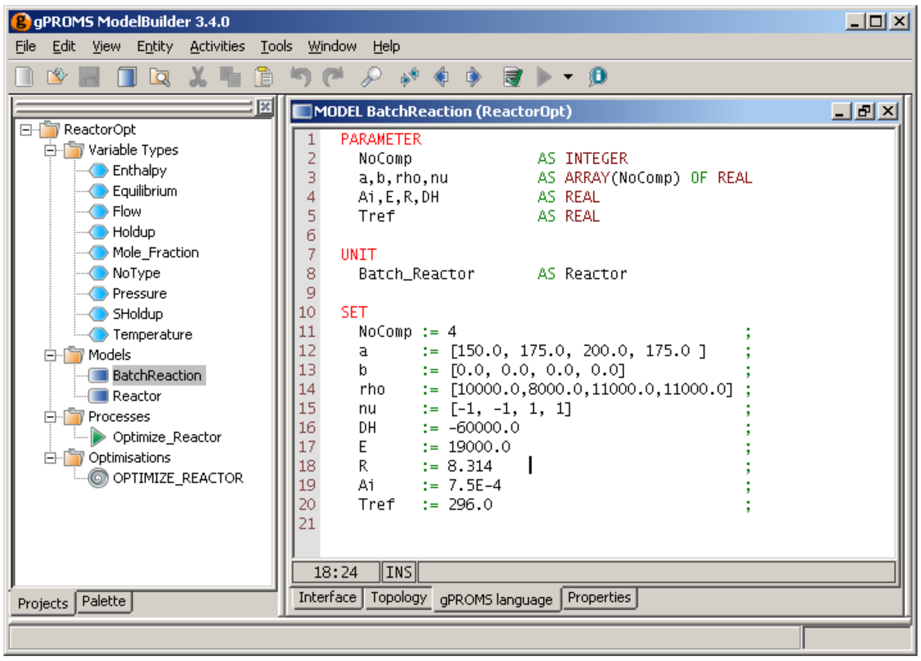
| Name | Lower bound | Default value | Upper bound | Units |
|---|---|---|---|---|
| Enthalpy | -1E9 | 4720.0 | 1E9 | |
| Equilibrium | 1E-6 | 1.025 | 10.0 | |
| Flow | -1.0 | 0.14 | 10.0 | |
| Holdup | -10.0 | 100.0 | 1E7 | moles |
| Mole_Fraction | -10.0 | 0.95 | 10.0 | none |
| NoType | -1E9 | 100000.0 | 1E9 | |
| Pressure | 1E-6 | 1.025 | 3000.0 | mm_Hg |
| SHoldup | -10.0 | 1000.0 | 1E7 | moles |
| Temperature | 100.0 | 381.0 | 600.0 | Celsius |
| <new> | | | | |

## Text contained within the Reactor Model entity

```
#----------------------------------------------------------------
# Model of an externally cooled batch reactor: A + B -> C + D
#
# The reactor model takes into account mass and energy balances.
#----------------------------------------------------------------
PARAMETER
  NoComp              AS     INTEGER
  a,b,rho         AS    ARRAY (NoComp) OF REAL
  nu              AS    ARRAY (NoComp) OF REAL
  Ai,E,R,DH       AS    REAL
  Tref            AS    REAL

VARIABLE
  N,C,h           AS    ARRAY (NoComp) OF NoType
  HR,Rate,V       AS    NoType
  QcR,TR,K,Fcw    AS    NoType
  Uacc,Tviol      AS    NoType
  Obj             AS    NoType

EQUATION

  # Component material balance
  $N = V * Rate * nu ;

  # Definition of reaction rate
  Rate = K * C(1)* C(2) ;

  # Rate constant
  K = Ai * exp( - E / (R *TR) ) ;

  # Energy balance
  $HR = ( V * Rate * ( -DH ) ) - QcR ;

  # Cooling load as a function of cooling water flowrate
  QcR = 4200* 40 *Fcw ;

  # Cumulative cooling water consumption
  $Uacc= Fcw ;

  # Definition of total enthalpy content of reactor
  HR = sigma(N * h ) ;

  # Pure component specific enthalpies
  h = ( a * (TR -  Tref ) + ( b * ( TR^2  - Tref^2 ) / 2 ) ) ;

  # Relate molar concentrations C to component holdups N
  V * C = N ;

  # Volumetric holdup in reactor
  V = sigma( N / rho ) ;

  # Path constraint
    $Tviol = MAX(TR - 450,0)^2 ;

  # Objective to be maximised: value of product (3) - cooling water
  Obj = 2*N(3) - Uacc ;
```

## BatchReaction Model entity

**Figure 2.12. BatchReaction Model entity for the dynamic optimisation example.**



```
PARAMETER
  NoComp            AS INTEGER
  a,b,rho,nu        AS ARRAY(NoComp) OF REAL
  Ai,E,R,DH         AS REAL
  Tref              AS REAL

UNIT
  Batch_Reactor     AS Reactor

SET
  NoComp := 4                                    ;
  a      := [150.0, 175.0, 200.0, 175.0 ]        ;
  b      := [0.0, 0.0, 0.0, 0.0]                 ;
  rho    := [10000.0,8000.0,11000.0,11000.0]     ;
  nu     := [-1, -1, 1, 1]                       ;
  DH     := -60000.0                             ;
  E      := 19000.0                              ;
  R      := 8.314                                ;
  Ai     := 7.5E-4                               ;
  Tref   := 296.0                                ;
```

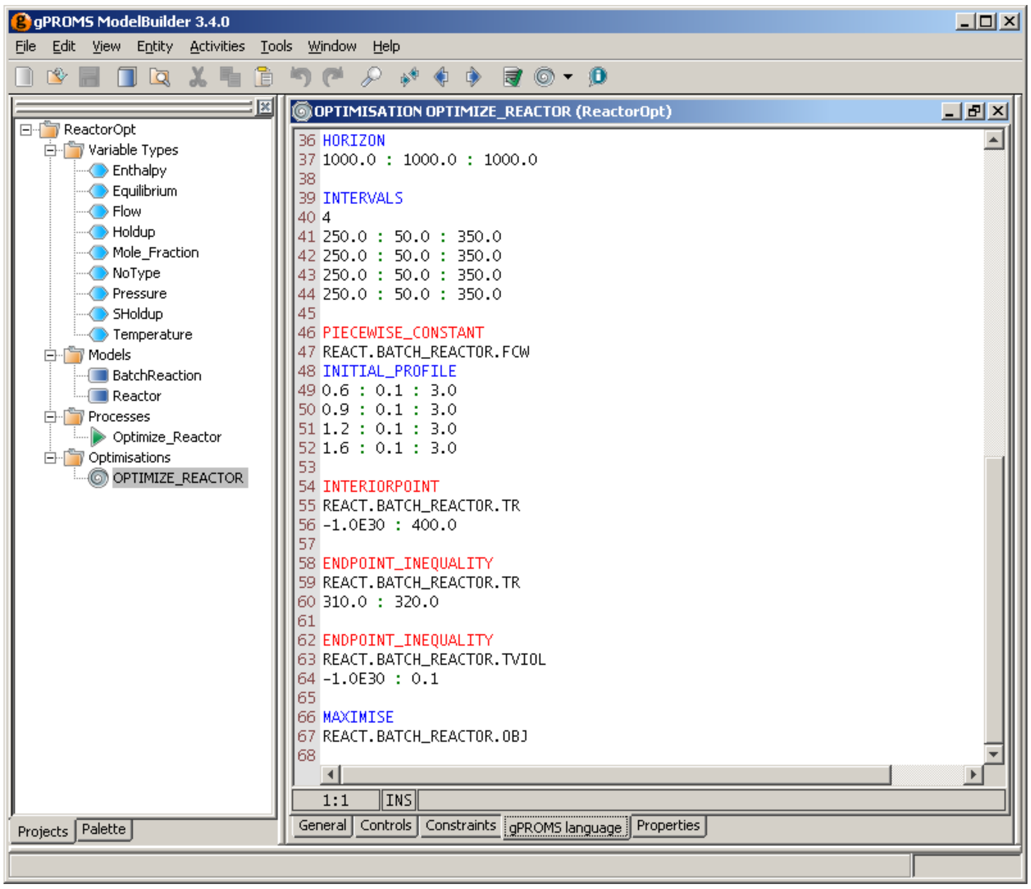
## Text contained within the OPTIMISE_REACTOR Process entity

```
UNIT
  React      AS   BatchReaction

ASSIGN
  # This will be overridden in the Optimisation entity
  WITHIN React.Batch_Reactor DO
    FcW := 0.0 ;
  END

PRESET
  REACT.BATCH_REACTOR.RATE  := 7.28422E+00 ;
  REACT.BATCH_REACTOR.HR    := 6.50000E+06 ;
  REACT.BATCH_REACTOR.C(1)  := 4.44444E+03 ;
  REACT.BATCH_REACTOR.C(2)  := 4.44444E+03 ;
  REACT.BATCH_REACTOR.C(3)  := 0.00000E+00 ;
  REACT.BATCH_REACTOR.C(4)  := 0.00000E+00 ;
  REACT.BATCH_REACTOR.OBJ   := 0.00000E+00 ;
  REACT.BATCH_REACTOR.H(1)  := 6.00000E+02 ;
  REACT.BATCH_REACTOR.H(2)  := 7.00000E+02 ;
  REACT.BATCH_REACTOR.H(3)  := 8.00000E+02 ;
  REACT.BATCH_REACTOR.H(4)  := 7.00000E+02 ;
  REACT.BATCH_REACTOR.FCW   := 0.00000E+00 ;
  REACT.BATCH_REACTOR.K     := 3.68763E-07 ;
  REACT.BATCH_REACTOR.QCR   := 0.00000E+00 ;
  REACT.BATCH_REACTOR.V     := 1.12500E+00 ;

INITIAL
  WITHIN React.Batch_Reactor DO
```

```
    N(1)   = 5000.0    ;
    N(2)   = 5000.0    ;
    N(3)   =    0.0    ;
    N(4)   =    0.0    ;
    TR     =  300.0    ;
    Uacc   =    0.0    ;
    Tviol  =    0.0    ;
  END

SOLUTIONPARAMETERS
  ABSOLUTEACCURACY  := 1.0E-6 ;
  REPORTINGINTERVAL := 100 ;

SCHEDULE
  # This will be ignored by the dynamic optimisation
  SEQUENCE
    CONTINUE FOR 2000
  END
```

## Optimisation entity (OPTIMISE_REACTOR)

**Figure 2.13. Optimisation entity for the dynamic optimisation example.**



```
HORIZON
1000.0 : 1000.0 : 1000.0

INTERVALS
4
250.0 : 50.0 : 350.0
250.0 : 50.0 : 350.0
250.0 : 50.0 : 350.0
250.0 : 50.0 : 350.0

PIECEWISE_CONSTANT
REACT.BATCH_REACTOR.FCW
INITIAL_PROFILE
0.6 : 0.1 : 3.0
0.9 : 0.1 : 3.0
1.2 : 0.1 : 3.0
1.6 : 0.1 : 3.0

INTERIORPOINT
REACT.BATCH_REACTOR.TR
-1.0E30 : 400.0

ENDPOINT_INEQUALITY
REACT.BATCH_REACTOR.TR
310.0 : 320.0

ENDPOINT_INEQUALITY
REACT.BATCH_REACTOR.TVIOL
-1.0E30 : 0.1

MAXIMISE
REACT.BATCH_REACTOR.OBJ
```

## Sample optimisation report file (OPTIMISE_REACTOR.out)

```
gPROMS Dynamic Optimisation

gPROMS Process                    :  OPTIMIZE_REACTOR
Final Optimisation Status         :  Optimal Solution Found
Objective Function Being Maximised:  7642.78

Current Values of Optimisation Decision Variables
([*] denotes an active bound)

Decision Variable     Type  Value    Lower Bound  Upper Bound

Time horizon                1000     1000[*]      1000[*]

Control Interval # 1        249.718  50           350
Control Interval # 2        159.781  50           350
Control Interval # 3        288.055  50           350
Control Interval # 4        302.446  50           350



1. REACT.BATCH_REACTOR.FCW (piecewise constant)
Control
Interval  Type        Value     Lower Bound  Upper Bound
# 1       Continuous  0.1       0.1[*]       3
# 2       Continuous  1.84372   0.1          3
# 3       Continuous  0.554775  0.1          3
# 4       Continuous  3         0.1          3[*]


Current Values of Constrained Variables
([*] denotes violation of constraint)

Constrained Variable       Type      Time     Value     Lower Bound  Upper Bound

REACT.BATCH_REACTOR.TR     Interior  0        300       -1E+030      400
REACT.BATCH_REACTOR.TR     Interior  249.718  394.578   -1E+030      400
REACT.BATCH_REACTOR.TR     Interior  409.499  397.018   -1E+030      400
REACT.BATCH_REACTOR.TR     Interior  697.554  398.378   -1E+030      400
REACT.BATCH_REACTOR.TR     Endpoint  1000     320       310          320[*]
REACT.BATCH_REACTOR.TVIOL  Endpoint  1000     0.100812  -1E+030      0.1[*]
Computational Statistics


Total CPU Time                                      : 6.84375  seconds

  CVP_SS Optimiser Statistics

    CPU Time                                        : 0.015625 seconds (0.228311 % of t
    Number of MINLP Iterations                      : 0
    Number of NLP Iterations                        : 61
    Number of NLP Line Search Steps                 : 72

  DASOLV Integrator Statistics

    CPU Time                                        : 5.23438  seconds (76.484018 % of 
    CPU Time Spent on State Integration Only        : 1.9375   seconds (37.014925 % of 
      16292 steps, 30038 residuals                  : 0.546875 seconds
      4140 Jacobians                                : 0.109375 seconds
    CPU Time Spent on Sensitivity Integration Only  : 3.29688  seconds (62.985075 % of 
      13674 steps, 37422 residuals                  : 0.328125 seconds
      17198 Jacobians                               : 0.5      seconds
    Mean (Sensitivity+State)/(State) CPU Ratio      : 2.70161
```

## Sample gPROMS schedule file (OPTIMISE_REACTOR.SCHEDULE)

```
#
#           Schedule generated by gOPT for process OPTIMIZE_REACTOR
#
#           Final Optimisation Status         :  Optimal Solution Found
#           Objective Function Being Maximised:  7642.78
#
SCHEDULE

   SEQUENCE

      PARALLEL

         RESTORE "OPTIMIZE_REACTOR_SVS" ;

         RESET

            REACT.BATCH_REACTOR.FCW := 0.1;

         END

      END

      CONTINUE FOR 249.718

      RESET

         REACT.BATCH_REACTOR.FCW := 1.84372;

      END

      CONTINUE FOR 159.781

      RESET

         REACT.BATCH_REACTOR.FCW := 0.554775;

      END

      CONTINUE FOR 288.055

      RESET

         REACT.BATCH_REACTOR.FCW := 3;

      END

      CONTINUE FOR 302.446
   END
```

## Sample point file (OPTIMISE_REACTOR.point)

```
# .gOPT segment generated by gOPT for process OPTIMIZE_REACTOR
# at final solution.

HORIZON
1000      :  1000   :  1000

INTERVALS
4
249.718   :  50     :  350
159.781   :  50     :  350
288.055   :  50     :  350
302.446   :  50     :  350



PIECEWISE_CONSTANT
REACT.BATCH_REACTOR.FCW
INITIAL_PROFILE
0.1         :    0.1    :    3
1.84372     :    0.1    :    3
0.554775    :    0.1    :    3
3           :    0.1    :    3
```

## Simulating the optimal solution within a Process

```
UNIT
  React      AS   BatchReaction

ASSIGN
{ This was the previous ASSIGN section
  # This will be overridden in the Optimisation entity
  WITHIN React.Batch_Reactor DO
    FcW := 0.0 ;
  END
}

# This is the new one using the first RESET statement
# from the SCHEDULE file
         REACT.BATCH_REACTOR.FCW:=     1.00000E-01;


PRESET
  REACT.BATCH_REACTOR.RATE  := 7.28422E+00 ;
  REACT.BATCH_REACTOR.HR    := 6.50000E+06 ;
  REACT.BATCH_REACTOR.C(1)  := 4.44444E+03 ;
  REACT.BATCH_REACTOR.C(2)  := 4.44444E+03 ;
  REACT.BATCH_REACTOR.C(3)  := 0.00000E+00 ;
  REACT.BATCH_REACTOR.C(4)  := 0.00000E+00 ;
  REACT.BATCH_REACTOR.OBJ   := 0.00000E+00 ;
  REACT.BATCH_REACTOR.H(1)  := 6.00000E+02 ;
  REACT.BATCH_REACTOR.H(2)  := 7.00000E+02 ;
  REACT.BATCH_REACTOR.H(3)  := 8.00000E+02 ;
  REACT.BATCH_REACTOR.H(4)  := 7.00000E+02 ;
  REACT.BATCH_REACTOR.FCW   := 0.00000E+00 ;
  REACT.BATCH_REACTOR.K     := 3.68763E-07 ;
  REACT.BATCH_REACTOR.QCR   := 0.00000E+00 ;
  REACT.BATCH_REACTOR.V     := 1.12500E+00 ;

INITIAL
  WITHIN React.Batch_Reactor DO
    N(1)   = 5000.0    ;
    N(2)   = 5000.0    ;
    N(3)   =    0.0    ;
    N(4)   =    0.0    ;
    TR     =  300.0    ;
    Uacc   =    0.0    ;
    Tviol  =    0.0    ;
  END

SOLUTIONPARAMETERS
  ABSOLUTEACCURACY  := 1.0E-6 ;
  REPORTINGINTERVAL := 100 ;

{ This is the previous SCHEDULE
SCHEDULE
  # This will be ignored by the dynamic optimisation
  SEQUENCE
    CONTINUE FOR 2000
  END
}

# This is the new one taken from the SCHEDULE results file

#           Final Optimisation Status         :  Optimal Solution Found
#           Objective Function Being Maximised:  7642.78
#
SCHEDULE

   SEQUENCE

      PARALLEL

         RESTORE "OPTIMIZE_REACTOR_SVS" ;

         RESET

            REACT.BATCH_REACTOR.FCW := 0.1;

         END

      END

      CONTINUE FOR 249.718

      RESET

         REACT.BATCH_REACTOR.FCW := 1.84372;

      END

      CONTINUE FOR 159.781
      RESET

         REACT.BATCH_REACTOR.FCW := 0.554775;

      END

      CONTINUE FOR 288.055

      RESET

         REACT.BATCH_REACTOR.FCW := 3;

      END

      CONTINUE FOR 302.446

   END
```

## Interpretation of screen output

The purpose here is to explain the detailed meaning of the screen output produced by gPROMS during optimisation, which can be of value in determining whether the problem is unsatisfactorily posed, for example.

This output is essentially of four kinds. We will review these together with a brief explanation of each. The examples below refer to when the single-shooting algorithm CVP_SS is chosen. This output is very similar to that when the multiple-shooting algorithm CVP_MS is invoked.

1. **Display of the solution point**

   This is indicated by a line of the type:

   ```
   After   73 cycles,  the solution point is:
   ```

   A report is then given of values of:

   - the time invariant parameters,
   - the time interval lengths and control values,

   for the current solution point.

   Note that the SCHEDULE and point files are updated at the same time that these values are written to the screen.

2. **Output from the integration**

   During optimisation, gPROMS repeatedly carries out integrations for a different choices of time invariant parameters and controls. This computation, similar to the execution of a conventional gPROMS simulation, will produce some output if the method parameter IPRINT is not set to zero. This may be of use if there are problems with these integrations.

3. **Report on constraint residuals**

   Following a successful simulation, gPROMS outputs both the objective function value and a report on the status of the constraints. The latter are marked with [*] if they are violated (for equality constraints, a violation is indicated if the actual value differs from the desired one by more than one millionth of its magnitude).

4. **Optimiser reports**

   Following a gradient evaluation, the optimiser will produce a report of this type:

```
  No. of       No. of     Step    Objective    Current    Constraint
       Iterations   Functions   Length   Function     Accuracy   Violations

           18           63      1.587E-03  -7.473E+03   8.493E-02   5.684E-14
```

These values have the following meanings:

- No. of Iterations: this refers to the number of *full* optimiser iterations, *i.e.* the number of gradient evaluations used to determine new search directions.
- No. of Functions: the total number of simulations carried out so far. Since the optimiser works by selecting a search direction and then carrying out a *line search* along that direction, it generally evaluates the objective function considerably more often than it evaluates its gradient.
- Step Length: this provides a measure of how much the optimiser is altering the optimisation decision variables between simulations.
- Objective Function: the present objective function value, negated if a maximisation is in progress.
- Current Accuracy: this shows how close the optimiser considers the current point is to optimality. When this value falls below $10^{-4}$ (or the value supplied with the ACC keyword in the PARAMETERS entity), the optimisation will report that the solution has been found, and terminate (after its output integration).
- Constraint Violations a measure of the total constraint violation of the current point --- zero (or very small) if the point is feasible.

Finally, here is an example of one iteration's output for the problem OPTIMISE_REACTOR. Again, a wide screen format is needed.

```
 Optimisation Iteration   10
 ---------------------------
Values and gradients of objective function and constraints to be evaluated
at the following point:

Time Horizon:     1.00000E+03

Current Control Profiles

                     Duration       Control 1
  Interval 1        3.50000E+02    3.83448E-01
  Interval 2        3.26555E+02    1.48681E+00
  Interval 3        1.23949E+02    1.99611E+00
  Interval 4        1.99496E+02    3.00000E+00

  Control  1 = REACT.BATCH_REACTOR.FCW

 Objective function and constraint residuals:

Objective Function to be Maximised:     7.48409E+03

Constraint Residuals:  ([*] denotes violation)

  Variable                          Type        Lower Bound         Upper Bound        Cu
  --------                        --------      -----------         -----------         -
  REACT.BATCH_REACTOR.TR          Endpoint      3.10000E+02         3.20000E+02         3
  REACT.BATCH_REACTOR.TVIOL       Endpoint        N/A               1.00000E-01         0


       No. of       No. of     Step    Objective    Current    Constraint
```

```
     Iterations   Functions   Length   Function     Accuracy   Violations

          9           27      3.490E-03  -7.484E+03   8.236E-02   5.684E-14

 Searching Along Optimisation Step.....  (  28)
 After   37 cycles,  the solution point is:

Time Horizon:     1.00000E+03

Current Control Profiles

                      Duration       Control 1
  Interval 1         3.50000E+02    1.00000E-01
  Interval 2         5.00000E+01    1.35623E+00
  Interval 3         2.50000E+02    3.00000E+00
  Interval 4         3.50000E+02    3.00000E+00

  Control  1 = REACT.BATCH_REACTOR.FCW

 About to perform a function evaluation.
```