Model predictive control of the melt index during grade changes at poly-ethylene production

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Award date:
1996

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Final report of the graduate study
Applied Physics

Abstract

Model Predictive Control (MPC) can be described as a method in which a model of the process that must be controlled is used to predict the future effect of possible changes to the process. A practical performance criterion is minimized in order to calculate the optimal inputs, bringing the process behaviour very near to the preferred behaviour. This procedure of finding the optimal control steps is repeated every time step of the process. Contrary to most other control strategies, MPC can very easily deal with constraints put on the inputs and outputs of the process. This report is the result of a study to the possible application of MPC in controlling the melt index (or equally the melt flow rate) during grade changes at polyethylene production.

Before starting out on MPC, a model describing the quantity to be controlled (the melt index) as a function of the manipulated variables (modifier concentration in the tube reactor, the total reactor mass flow, and the temperature profile in the reactor) had to be developed. A statistical model was developed describing the melt index directly after the tube reactor as a function of the modifier concentration, the peak temperatures in the tube reactor, the temperature after the preheater and the pressure and temperature in the suction section of the compressor unit. The last two variables uniquely determine the total reactor mass flow.

For the MPC controller design, step responses were estimated for all the temperatures. This was done by step experiments on the plant. The step responses for the modifier concentration were calculated from a second order model, describing the modifier concentration as a function of the modifier flow into the system ,the flow of the purge and the ethylene conversion in the tube reactor. The step responses of the pressure and temperature in the suction section of the compressor were found to be of the same order as those of the temperatures.

In Matlab an MPC simulation was built and simulations were performed for investigating the optimal setting for the MPC controller in controlling the melt index during grade changes. The plant was taken the same as the model found by identification. The performance of the MPC controller with the optimal settings was then compared with the present, manual operator control of the plant. From the simulations performed in Matlab it can be concluded that an MPC controller will decrease the time needed for grade changes with 20%. Furthermore the simulations showed that the MPC controller is also applicable to steady state control of the plant.

It should be noted that in the simulations the melt index directly behind the tube reactor is calculated, and not the melt index at the extrusion die-plate of the extruder (the actual location of the melt index measurement). This implies that the dynamic behaviour (residence time and partial mixing) of the separator and extruder was not taken into account. And an optimal control strategy would be to lower the level in the separator before and during a grade change, resulting in minimum off-spec production during grade changes.

Contents

Chapter 1 Introduction

This report is the result of the author's final degree project as a graduate student in Applied Physics at Eindhoven University of Technology. The project was carried out at a real-life polyethylene plant from September 1995 to July 1996. The goal of the project is to investigate the application of MPC in Melt Index control during grade changes and normal control during the production of polyethylene.

The aim of this project is to study the applicability of MPC on chemical plants. By applying MPC to a real life plant one can learn from all the practical advantages and difficulties of MPC. First of all a model of the polyethylene plant was made by means of dynamic black box modelling tools PRIMAL and Matlab. Although a lot of experiments had been performed, it didn't seem possible to identify proper dynamic black box models from these experiments, due to unpredictable reactor pollutions. Furthermore the insight was gained that the production of polyethylene is a very fast process with regard to the sampling time at which the plant is operated. Thus so satisfactory statistical models could be used, and were made with SPSS. In Matlab an MPC controller was designed for simulating the polyethylene plant and controlling it by means of MPC. The results of the simulations are shown in this report, and also some general conclusions about the applicability of MPC in chemical plants are drawn.

In Chapter 2 of this report a general description of the polyethylene production process and the Melt Index are given. A short outline of MPC is given in Chapter 3, and the application of MPC on the Melt Index control is shown in Chapter 4. The results of the simulations are shown in Chapter 5 and the conclusions are drawn in Chapter 6 of this report.

Chapter 2 polyethylene production

2.1 History of polyethylene production

In 1933, chemists of the Imperial Chemical Industries laboratories were elaborating on the reaction between benzaldehyde and ethylene at a pressure of 1500 bar and temperatures between 100°C and 160°C. Without their knowledge, traces of oxygen had been enclosed in the reaction unit, enough to start polymerisation of ethylene. The chemists discovered a wax-like powder: polyethylene. Soon they also discovered that the () polyethylene had very useful mechanical properties (e.g. thermal and electrical insulation).

ICI managed to develop a reaction based on the compression of ethylene at high temperatures into a tank reactor together with peroxydes and oxygen. During the Second World War, the German company BASF applied tube reactors to manufacture polyethylene in a continuous process. In 1954, Ziegler discovered high density polyethylene through production at low pressures and temperatures, using special catalysts.

As different production processes for polyethylene were developed several types of poly-ethylene were discovered. The different types of polyethylene can be classified as shown in Table 2.1.

Table 2.1: Overview of the different types of polyethylene, their densities and the total year production in 1989 [RAY85].

type of polyethylene	density range	total worldwide production 1989
lldpe (linear low density polyethylene)	0.880 g/cm^3 - 0.950 g/cm^3	4.700.000.000 kg
ldpe (low density polyethylene)	0.910 g/cm^3 - 0.940 g/cm^3	10.000.000.000 kg
hdpe (high density polyethylene)	0.940 g/cm^3 - 0.980 g/cm^3	8.300.000.000 kg

In Figure 2.1 a schematical overview of the molecular chain structures of the different types of polyethylene is given.

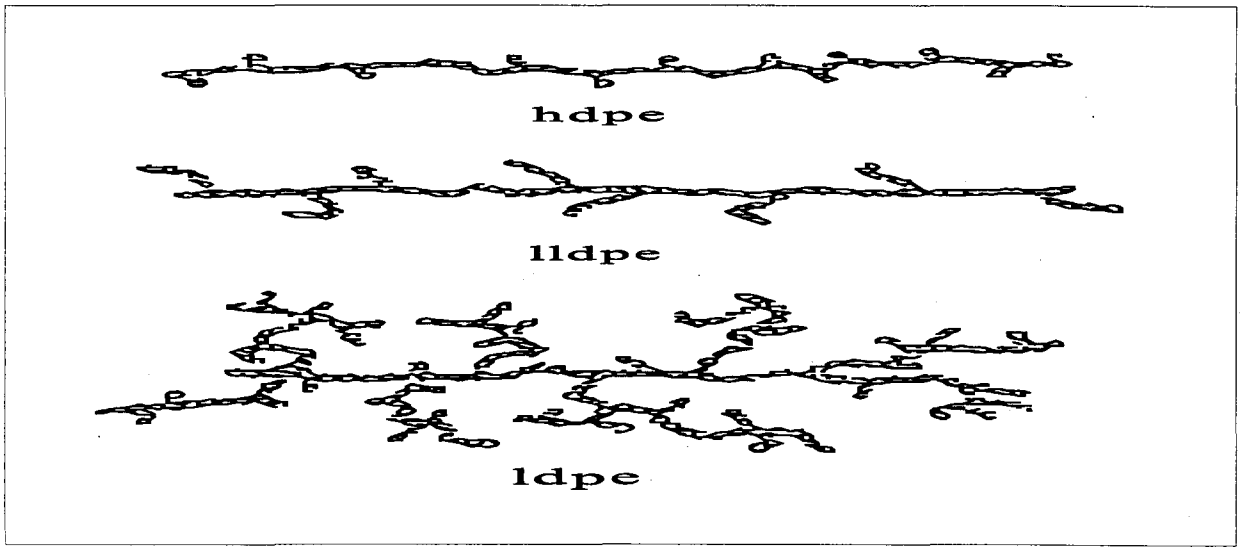

Figure 2.1: schematic overview of the molecular chain structure of polyethylene [ART93].

2.2 General description of the plant

In the following a, schematic overview of the plant and a description of the different parts of the plant will be given by means of Figure 2.2.

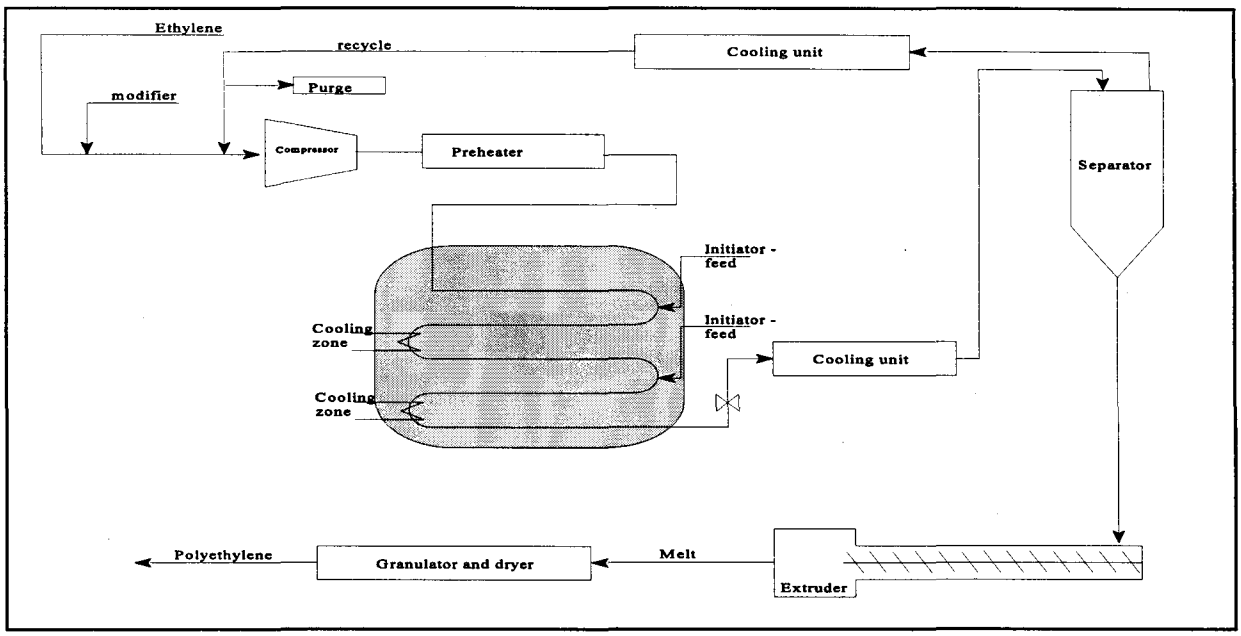

Figure 2.2: schematic overview of the polyethylene plant.

2.2.1 The ethylene inlet

Before the fresh ethylene is fed to the compressor, a modifier is added to the process gas. Since there are inert pollutions in the ethylene inlet such as methane, ethane and carbon dioxide, a purge is installed at the recycle coming from the separator unit in order to reduce the impurities and modifier concentration when necessary.

2.2.2 The compression unit

In the compression unit the process gas is compressed to a very high pressure. This is the pressure in which the polyethylene is formed in the tube reactor.

2.2.3 The preheating units

Before the process gas is led into the tube reactor, the temperature of the gas is increased to the desired inlet temperature of the tube reactor by the preheating unit. After gas has passed the preheater, the inlet temperature of the reactor is measured. Thus the temperature of the preheater can be taken as the first bottom temperature of the reactor, and is a controllable quantity.

2.2.4 The tube reactor

The tube reactor is embedded in a cooling jacket. The cooling jacket is divided in several regions. The total flow of chilled water flowing through each region of the cooling jacket can be controlled. This way only the parts of the reactor are cooled where the strong exothermic polymerization reactions are taking place. Furthermore, the process runs at very high pressures and thus the tube jacket has to be rather thick, which has a dampening effect on the heat transfer through the tube jacket.

In the tube reactor there are two reaction zones in which initiator is fed to the process by plunger pumps. The added initiator will stimulate the polymerization reaction and thus raise the temperature. Since the polymerization reaction is exothermic, the peak temperatures occurring after the initiator feed, directly depend on the amount of initiator added to the process. The peak temperatures are controlled variables: the amount of initiator is PID-controlled with the setpoint of the peak temperatures. When all the radicals introduced by the initiator are used up, the polymerization reaction will stop. At this point the process gas is fed

through a cooling zone (i.e. the cooling jacket around the tube reactor). Since cooling of the process gas is required after each initiation, there are also two cooling zones. This results in the temperature profile in the reactor as shown in Figure 2.3. Summarizing the temperature profile is controlled by the initiator feed, the temperature of the cooling water and flow of the cooling water through the cooling zones.

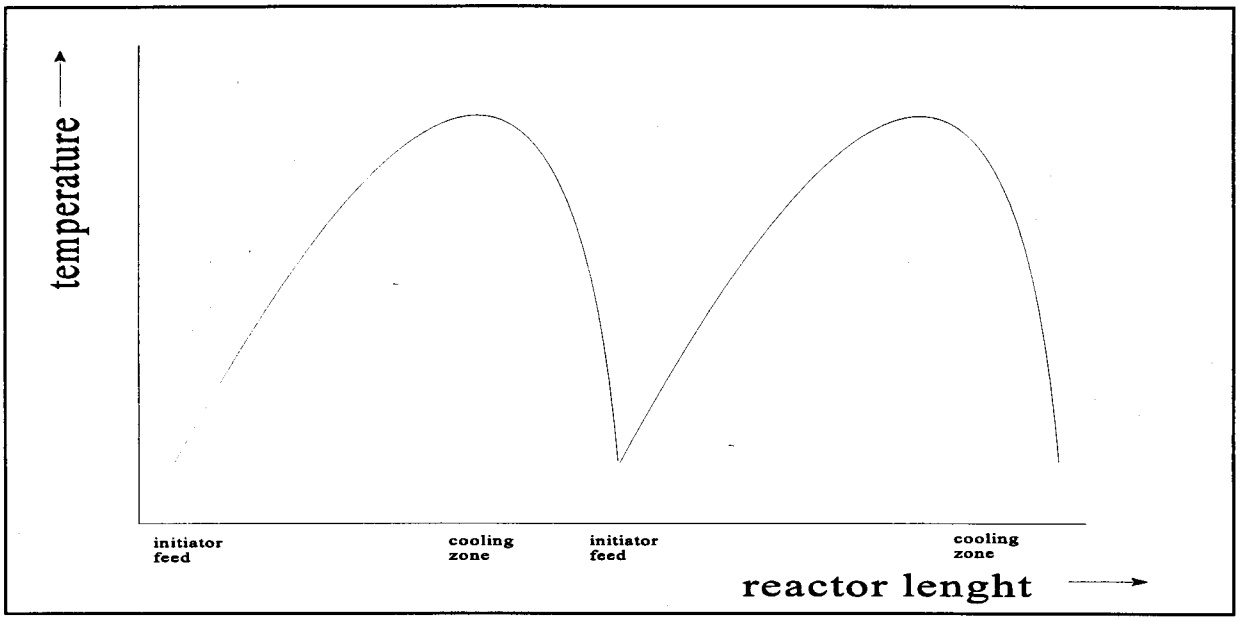

Figure 2.3: the temperature profile inside the tube reactor.

The total reactor mass flow is defined as (see Figure 2.2):

$$\phi_{m,R} = \phi_{m,ethylene} + \phi_{m,modifier} + \phi_{m,recycle} - \phi_{m,purge} \qquad \textbf{(2.1)}$$

with:
- $\phi_{m,R}$ the total reactor mass flow,
- $\phi_{m,ethylene}$ the ethylene mass flow into the system,
- $\phi_{m,modifier}$ the modifier mass flow into the system,
- $\phi_{m,recycle}$ the total recycle flow from the separator,
- $\phi_{m,purge}$ the purge mass flow.

In Figure 2.4 a schematic overview is given of the reactor pressure control structure. At the beginning of the tube reactor the pressure is measure (PI in Figure 2.4). This pressure is held constant by PID-control of the valve at the end of the tube reactor. An increase in the total reactor mass flow $\phi_{m,R}$ will thus result in a higher pressure drop over the tube reactor (Δp_R). Since the pressure before the tube reactor is held constant, the average pressure in the tube reactor will decrease (see Figure 2.4).

The total reactor flow can be described as a function of the pressure and the temperature of the

suction section of the compressor. Since the volume of the suction section of the compressor and the speed of revolutions of the engine which moves the suction remain constant, the volume flow is uniquely determined by the temperature and pressure in the suction section of the compressor. Since the density of the ethylene / modifier mix going into the tube reactor is almost constant, and the inlet temperature is too, the volume flow can transformed to a mass flow.

The total reactor mass flow can then be calculated from the following equation:

$$\dot{\phi}_{m,R} = a * p_{comp} - b * T_{comp} + c \qquad \textbf{(2.2)}$$

with:
- $\dot{\phi}_{m,R}$ the total reactor mass flow,
- p_{comp} the pressure in the compressor,
- T_{comp} the temperature in the compressor.

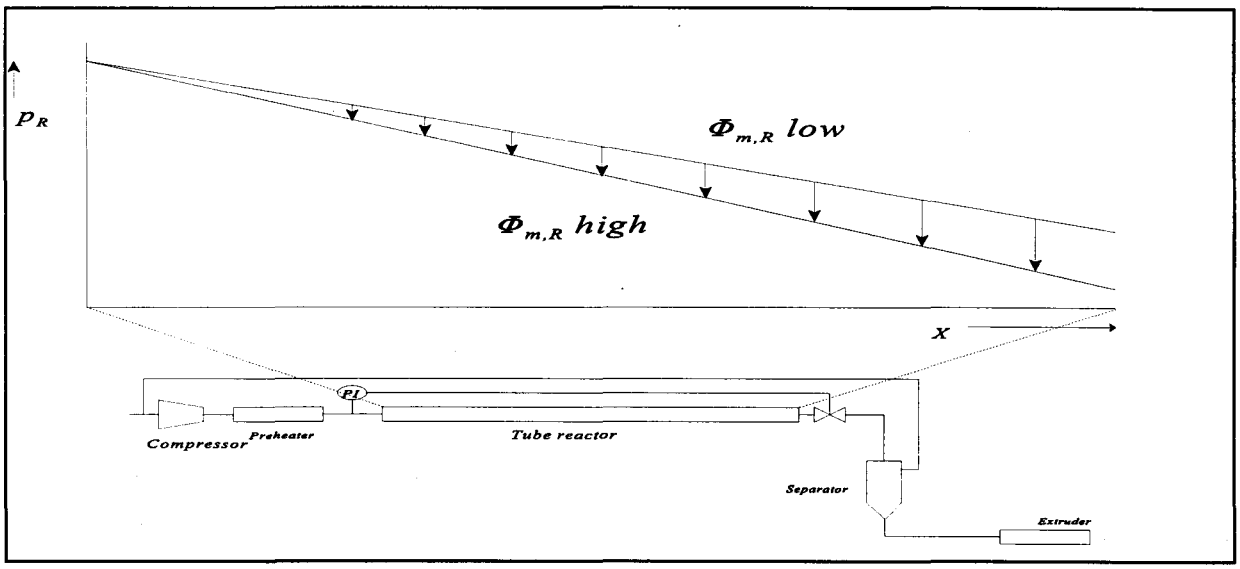

Figure 2.4: the increase in the pressure drop in the reactor, as a result from a higher total reactor mass flow, with p_R the reactor pressure, x the place, and PI the pressure indicator at the beginning of the tube reactor.

2.2.5 The cooling unit

At the end of the tube reactor, there is an extrusion valve for controlling the pressure in the tube reactor. When the ethylene-polyethylene mixture leaves the reactor, an expansion takes place. Since the temperature might still be to high after the expansion, a cooling unit is installed to lower the temperature.

2.2.6 The separator

In the separator, the ethylene is separated from the polyethylene. This is possible because at the lower pressure the ethylene-polyethylene mixture starts to separate into two phases. The polyethylene is fed to the extruder and the ethylene is fed back to the compressor unit via the recycle. In this recycle circuit the purge is situated, because at this stage the concentration of inert pollutions is at its maximum. This can be seen in Figure 2.2: in the separator the separation between the polyethylene and the ethylene reaction mix is reached. Since the inert pollutions are separated from the polyethylene here, the concentration of the pollutions in the remaining ethylene mix will be at it's maximum.

2.2.7 The extruder

In the extruder, the polyethylene melt is homogenized and degassed. In Figure 2.5 a schematic overview of the extruder is shown.

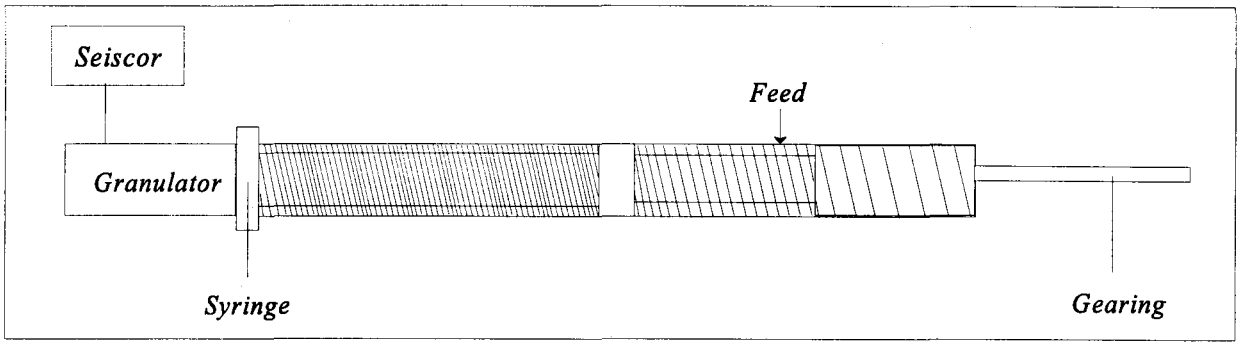

Figure 2.5: schematic overview of the extruder.

The polymer melt is pressurized by the syringe at the beginning of the extruder and eventually fed to a syringe and then to the granulator. It is here, at the end of the extruder that the melt index is measured by measuring the flow coming through a tube of a specified diameter at a standardized pressure and standardized temperature. The melt index is reciprocal to the viscosity of the polyethylene.

2.2.8 The granulator and dryer

In the granulator the melt flow is converted to pellets by cutting the melt flow from the syringe to appropriate pieces and cooling these in water. The pellets are then transported to the dryer. Finally the polyethylene is filtered and packed for transportation.

2.3 Reaction types

The polymerization of ethylene to polyethylene is a chain reaction. In the production of polyethylene so called radical initiators are used to start the polymerization. Several steps in the process can be identified: initiation, propagation and termination. Furthermore, some side reactions also take place, some of these are treated in this report. The reactions taking place as a result of the added radical initiators are described in Appendix A.

Furthermore a modifier is added to control the average molecular length of the polymer. The reactions which involve the modifier are described below. For further reading the reader is referred to [KIP93].

2.3.1 Modifier reactions

To the polymerization reaction the modifier mainly acts as an inert pollution, slowing down the rate of polymerization, which results in shorter chain lengths and therefore a lower viscosity.
Actually, the modifier is not totally inert with respect to the polymerization reactor. Some of the modifier is built into the polyethylene. This can be written as follows:

$$M_x + modifier \xrightarrow{k_{modifier}} M_{x\,+\,modifier} \qquad (2.3)$$

with:
- M_x the polyethylene,
- $M_{x+modifier}$ the polyethylene with the modifier,
- modifier the modifier,
- $k_{modifier}$ the reaction rate coefficient for the modifier reaction.

The reaction rate coefficient is found to be related to the ethylene conversion as follows:

$$k_{modifier} = a * \eta + b \qquad (2.4)$$

with:
- $k_{modifier}$ the reaction rate coefficient,
- η the ethylene conversion.

2.4 The melt index

For commercial polyethylenes product properties are usually specified by melt index and density. As already described in the previous, the melt index is an important product quality which is measured online at the end of the extruder, before the granulator. The melt index is measured by a device in which the polymer melt is led through a tube of a certain diameter under standardized pressure and temperature. The melt index is now defined as the mass flow of polymer melt through the tube. The tube diameter to be used for melt index measurements is dependent on the operating range of the actual melt index.

The melt index has a reciprocal relation to the average length of the molecules in the polyethylene, since a long average chain length will result in a high viscosity of the polyethylene, which in its turn results in a low melt index (i.e. the melt flow through the melt index measurer per unit of time).

The melt index depends on three key quantities: the pressure and the temperature in the reactor and the modifier concentration. This can be expressed as:

$$mi = f(p_R, T_R, [modifier]) \tag{2.5}$$

with:
- mi — the melt index,
- p_R — the average pressure in the tube reactor,
- T_R — the temperature profile in the tube reactor,
- [modifier] — the modifier concentration in the reactor.

It is widely accepted that the melt index and the density of the produced polyethylene respond instantaneously to changes in the gas composition and reactor temperature and pressure (see [AUL93]). Since that radical polymerization reactions have stopped when the peak in the temperature profile is reached, it can be stated that the partial melt index is produced in the up going part of the temperature profile. The tube reactor can be divided into four parts: two up going parts and two down going parts according to the temperature profile.

In the following, a qualitative description of the dependency of the melt index of the key quantities in the plant will be given. For a clear understanding of the processes in the tube reactor, the melt index will be described as being dependent on the average pressure in the reactor, the temperature profile in the reactor and the modifier concentration in the reactor.

2.4.1 The pressure in the reactor

As stated before, the inlet pressure in the tube reactor is held constant by means of a PID-control loop which operates a valve at the end of the tube reactor (see Figure 2.4). Because the pressure at the beginning of the tube reactor remains constant, the pressure drop over the

reactor is determined by the total reactor mass flow, $\phi_{m,R}$. An increase in the total reactor mass flow will result in an increase of the pressure drop over the reactor and thus in a decrease of the average pressure in the tube reactor. An decrease in the average pressure in the tube reactor will generally lead to an decrease in the average molecular chain length, resulting in a higher melt index. Because of the properties of the gas mixture the effect often will reverse. This is the reason why an increase in the total reactor mass flow mostly lead to an increase in the melt index, and not a decrease.

Since the total reactor mass flow is not a measured quantity, the relation between the total reactor mass flow and the temperature and pressure in the suction section of the compressor unit has to be used in predicting the influence of the average reactor pressure on the melt index. From equation 2.2 we see that the temperature of the suction section of the compressor has a negative influence on the total reactor mass flow, whereas the pressure in the suction section has a positive influence on the total reactor mass flow. Combining this with the knowledge that an increase in the total reactor mass flow will result in an increase in the melt index, because of the harmonica effect on the peak temperatures, it can be stated that the temperature in the suction section of the compressor has a negative influence on the melt index, and the pressure in the suction section of the compressor has a positive influence on the melt index.

2.4.2 The temperature profile

The temperature profile (see Figure 2.3) in the reactor is determined by the amount of initiator added to the process at the two inlet points, the temperature of the chilled water, the flows of the cooling water into the cooling zones of the reactor jacket and the total reactor mass flow. The peak temperatures are PID-controlled by the amount of initiator, and the bottom temperatures are a result of the previous peak temperatures, the temperature and total flow of the chilled water in the cooling jacket around the tube reactor and the total reactor mass flow. The temperature after the preheater (i.e. the inlet temperature of the reactor) also is a controllable quantity.

The temperature profile in the reactor actually determines the conversion rate of ethylene to polyethylene by means of its absolute height and gradient in the up going parts. In general it can be stated that a larger temperature range in the up going part of the temperature profile will result in a higher conversion rate, and thus in more polymerization reactions, resulting in a lower average molecular chain length and a higher melt index. So it follows that an increase in the peak temperatures and a decrease in the bottom temperatures (or equally a decrease in the temperature after the preheater, which can be seen as the first bottom temperature) both will result in an increase of the melt index.

2.4.3 The chain transfer agents

In the third place, the concentrations of the modifier affects the melt index. An increase of the modifier concentration will result in shorter chains in the polymer and thus in a higher melt index. The concentration of the modifier can be calculated from the total reactor mass flow, the ethylene conversion, the fresh modifier flow and the flow of the purge. A model was deduced describing the modifier concentration as a function of the given quantities.

2.4.4 The melt index model

From the previous paragraphs it can be concluded that a model describing the melt index as a function of the properties of the gas mixture in the tube reactor is should contain the following quantities: the temperature and pressure in the suction section of the compressor, the peak temperatures and the bottom temperatures in the tube reactor, the temperature after the preheater and the modifier concentration. This results in a model for the melt index of the following form:

$$mi = f(p_{comp}, T_{comp}, T_{preh}, T_{peak1,2}, T_{bottom}, [modifier]) \qquad \textbf{(2.6)}$$

with:
- mi — the melt index,
- p_{comp} — the pressure in the suction section of the compressor unit,
- T_{comp} — the temperature in the suction section of the compressor unit,
- T_{preh} — the temperature after the preheater,
- T_{peakx} — the x-th peak temperature,
- T_{bottom} — the bottom temperatures,
- [modifier] — the modifier concentration.

Later on we will see that implementing the bottom temperatures in the model for the melt index is very difficult, since the bottom temperatures are not controlled variable (see above). Furthermore the modifier concentration is controlled by the fresh modifier flow and the flow of the purge, thus these quantities are taken as controlled variables, rather than the modifier concentration.

Chapter 3 Model Predictive Control

3.1 Introduction

During the last decade Model Based Predictive Control (MBPC, or generally MPC) has emerged as a powerful control technique, especially in (petro-) chemical industry. The strength of MPC is that it can deal with processes which are multi-variable and have constraints in a very clear way. The first ideas about MPC emerged in the early 1960's, when Zadeh, Whalen and Propoi [ZAD62] and [PRO63] started out on linear programming and moving horizons in time for optimal control purposes. Further work was done in the 1970's and at the end of that decade MPC was stimulated even further by the application of MPC in the petrochemical industry by Richalet et al. [RIC78] and Cutler and Ramaker [CUT79].

In short MPC can be described as a method in which a model of the process that must be controlled is used to predict the future effect of possible changes to that process. A practical performance criterion is minimized in order to calculate the optimal inputs, bringing the process behaviour very near to the preferred behaviour. This procedure of finding the optimal control steps for the process by minimizing a performance criterion is repeated every time a new control move is implemented to the process (e.g. each sampling time of the process).

3.2 Outlines of MPC

In general MPC can handle constrained multi-input-multi-output (MIMO) processes. The inputs of the process usually are called manipulated variables (MV's) and in the case of disturbances which can be measured from the process: measured disturbances (MD's). The outputs of the process usually are the quantities to be controlled, or the controlled variables (CV's). Furthermore there are the preferred reference trajectories for the CV's, or just the reference trajectories.
As an example we will now consider a SISO process (see Figure 3.1).
In an MPC controller a discrete time model is used to predict the future outputs (CV's) of the process p steps ahead (the crosses and circles in Figure 3.1). At each time step ($k \rightarrow k+1$) a sequence of m control actions on the inputs (MV's) is calculated which satisfies the performance criterion best (the solid lines in Figure 3.1), taking into account the measured disturbances (MD's) and the desired reference trajectories (PV's, the upper solid line in Figure 3.1). In this example the performance criterion is taken to be the squared deviation of the output from the desired reference trajectory.

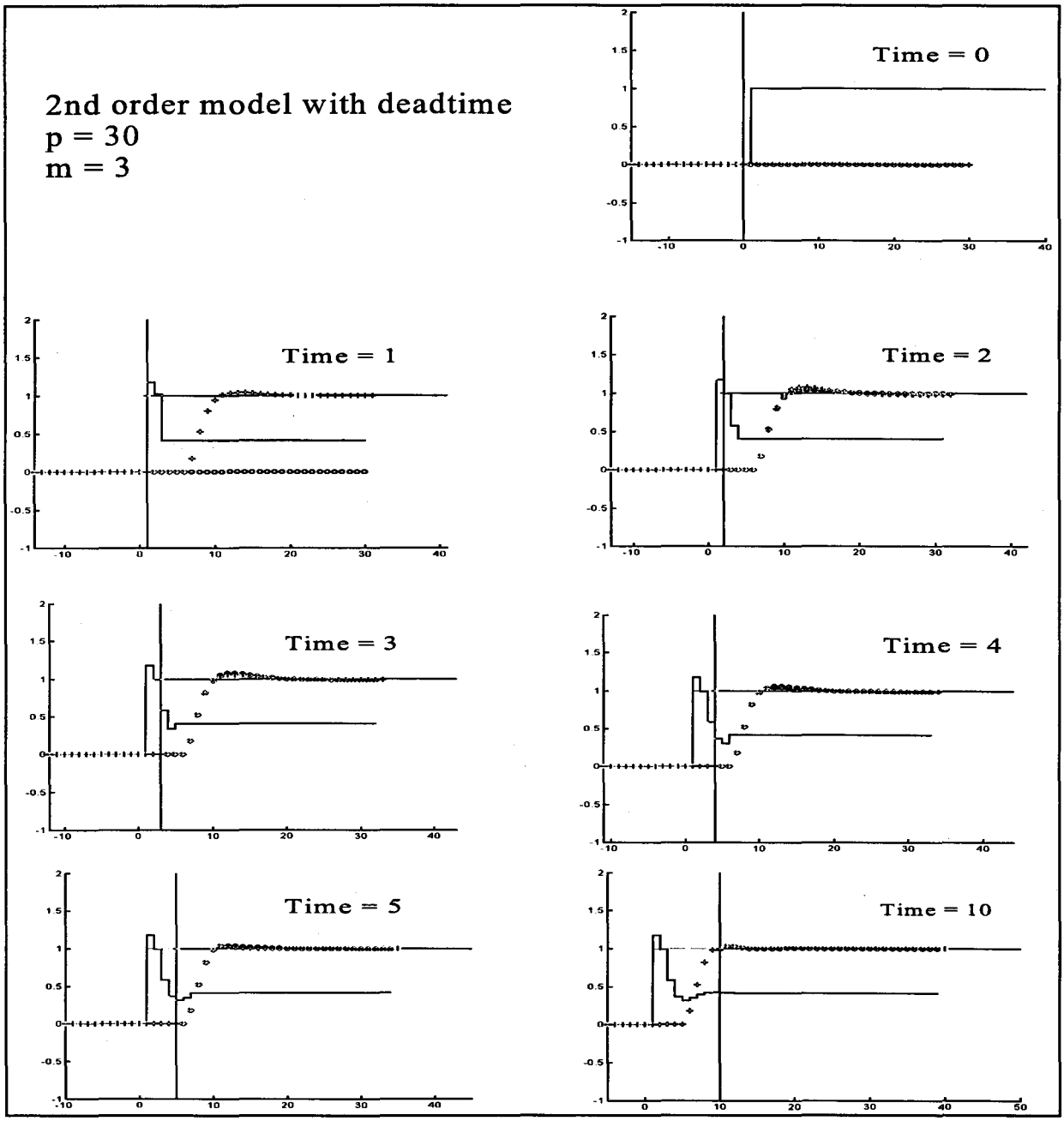

Figure 3.1: MPC control moves implemented on a SISO system. The preferred output is a unit step at time=1, the control moves calculated by the MPC algorithm are shown by the solid line, the estimated response at the previous time step by the circles and the estimated response at the actual time step by the crosses.

Since MPC uses models to predict future responses of the process for possible inputs it is very important to have reliable models. Furthermore MPC is a discrete time method and thus the choice of the sampling time also is of great importance. Too small a sampling time will drive the computing effort to astronomical height, where as too large a sampling time will result in poor control of the process since important features (short in time) are left out of the models.

Generally each model predictive controller consists of the following parts:

- a model of the process to make predictions;
- a desired reference trajectory (or setpoint);
- a performance criterion which has to be minimized;
- a computational algorithm for finding the optimal control moves.

The model of the process needed for MPC usually is in the form of step responses or impulse responses (but parametric models such as ARMAX models can also be used). In essence MPC is designed to handle linear, time invariant processes, but extensive research is done on modified versions of MPC can be set to handle non-linear, time variant processes.

3.3 The MPC algorithm

A short description of the MPC algorithm will now be given, but first the concept of step responses will be treated.

Consider a linear, time invariant process with inputs u(k) and outputs y(k). Each possible input sequence over the total control horizon can be described as a sum of shifted step inputs, and the output is a sum of the corresponding step responses over the total prediction horizon. Let $u_s(k)$ denote the unit step function. Then any input u(k) can be written as:

$$u(k) = \sum_{i=-\infty}^{k} \Delta u(i)\ u_s(k-i) \qquad \textbf{(3.1)}$$

where $\Delta u(k) = u(k)-u(k-1)$. The output can be denoted as:

$$y(k) = \sum_{i=-\infty}^{k} \Delta u(i)\ s_{k-i} = \sum_{i=0}^{\infty} s_i\ \Delta u(k-i) \approx \sum_{i=1}^{p-1} s_i\ \Delta u(k-i) + s_p\ u(k-p) \qquad \textbf{(3.2)}$$

with:
- s_x the step response of the output y to a step on the input u at time step x,
- s_p the step response of the output y to a step on the input u at the prediction horizon, p.

The last relation is used for the prediction part of MPC.

Let $y^*(k|k-1)$ be the predicted value of y(k) at a time k-1, using all the data available before time k-1. The influence of $\Delta u(k-1)$ on y(k) is $s_1\Delta u(k-1)$. So the prediction can be written in matrix notation as:

$$\begin{bmatrix} y^*(k|k-1) \\ y^*(k+1|k-1) \\ \vdots \\ y^*(k+n-2|k-1) \\ y^*(k+n-1|k-1) \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 1 \end{bmatrix} \begin{bmatrix} y(k-1|k-1) \\ y(k|k-1) \\ \vdots \\ \vdots \\ y(k+n-2|k-1) \end{bmatrix} + \begin{bmatrix} s_1 \\ s_2 \\ \vdots \\ \vdots \\ s_n \end{bmatrix} \Delta u(k-1) \quad \textbf{(3.3)}$$

or in more simple form:

$$Y(k|k-1) = M\ Y(k-1|k-1) + S^u\ \Delta u(k-1) \quad \textbf{(3.4)}$$

If the process also has some measured disturbances and the step responses of the output y to the MD's (d) are known (S^d), Equation 3.4 becomes:

$$Y(k|k-1) = M\ Y(k-1|k-1) + S^u\ \Delta u(k-1) + S^d\ \Delta d(k-1) \quad \textbf{(3.5)}$$

An important feature of MPC is the prediction horizon *p*; this is the number of steps over which the responses to manipulated variables (MV's) and measured disturbances (MD's) are calculated. Another basic feature of MPC is the control horizon *m*, this the number of steps over which the inputs are varied in order to gain an appropriate control sequence. In general only the first calculated control step is applied to the system, and after that a next control step is calculated again. Generally the prediction horizon is about ten times as big as the control horizon.

In order to find the appropriate (or the optimal) control sequence a performance criterion is defined. Usually a desired trajectory of the output is given for the first p time steps; R(k+1) = $[r(k+1),r(k+2),...,r(k+p)]^T$. A possible performance criterion would be:

$$\min_{\Delta u(k),\Delta u(k+1),...,\Delta u(k+m-1)} \sum_{i=1}^{p} ((y_p(k+i|k) - r(k+i))^2 = \min_{\Delta U(k)} \|y_p(k+1) - R(k+1)\|^2 \quad \textbf{(3.6)}$$

A more general approach is to also take into account the magnitude of the control steps to be made and the path of the trajectory compared with the desired trajectory, both weighed by a factor which can be tuned to each specific problem. This results in the following criterion:

$$\min_{\Delta U(k)} \| \Gamma^y\ [Y_p(k+1) - R(k+1)] \|^2 + \| \Gamma^{du}\ \Delta U(k) \|^2 \quad \textbf{(3.7)}$$

where:
- Γ^y weight factor for the following of the desired trajectory
- Γ^{du} weight factor for the magnitude of the control steps

The weighing of the step size of the inputs rather than the absolute value of the input was chosen, because the first option results in a more fluent control of the plant, whereas the

second option will drive the inputs to their lower constraints. In other words: weighing of the absolute value of the inputs will constrain the possible solutions by putting the inputs as close as possible to their minimum, which is not necessarily the optimal solution in terms of production.

The solution of this minimization problem can be expressed analytically by setting the derivate of the performance criterion to zero. The solution is:

$$\Delta U(k) = (S_p^{uT}\Gamma^{yT}\Gamma^{y}S_p^{u} + \Gamma^{duT}\Gamma^{du})^{-1}S_p^{uT}\Gamma^{yT}\Gamma^{y}(M_pY(k|k) + S_p^{d}\Delta d(k) - R(k+1)) \quad \textbf{(3.8)}$$

The MPC algorithm can be summarized as follows:

1. Do not vary the inputs and disturbances for at least p time steps
2. Measure the outputs and initialize the prediction as

$$Y(0|0) = [\hat{y}_1(0),\hat{y}_2(0),\cdots,\hat{y}(0)_p]^T$$

3. Measure the change in disturbance Δd(0), set k=0
4. Set k=k+1
5. Measure the outputs and the changes in disturbance Δd(k)
6. Calculate the predicted output
7. Correct the prediction for the measurement of the actual output:

$$Y(k|k) = Y(k|k-1) + K_F\,(\hat{y}(k) - y^*(k|k-1))$$

8. Determine the optimal control action sequence
9. Apply the first control action of the sequence to the process
10. Goto step 4

The previous can easily be adapted to MIMO systems by changing the ones in the M matrix to unity matrices and the zeros to n_y x n_y matrices of zeros. In the same manner the matrices S^u and S^d consist of matrices instead of scalars. In the computation of the optimal control all inputs and outputs are considered simultaneously and no decoupling is needed.

3.4 Constrained MPC: the QP problem

As noted before MPC is a technique that can handle constraints. In case of a constrained problem the optimisation is not an analytical solution, but at least a linear programming problem solving algorithm is needed to find the optimal control moves. The advantage of using a quadratic programming problem (QP) instead of a linear programming problem (LP)

is that the QP algorithm tends to be easier to tune and results in smoother responses than the LP problem (see [BOS91]). Furthermore the QP problem allows the MPC controller also to take into account the absolute value of the inputs (i.e. $\|u\|^2$) by setting a weight factor Γ^u for the magnitude of the inputs. This tuning parameter is not used if the control problem does not ask for a minimization of the input variables.

Three type of constraints can be incorporated: constraints on the inputs, the outputs and on the changes in the inputs at each time step:

$$\begin{aligned} u_{low} \le u(k) \le u_{high} \quad & k=1,2,\cdots \\ |\Delta u(k)| \le \Delta u_{\max} \quad & k=1,2,\cdots \\ y_{low} \le y(k) \le y_{high} \quad & k=1,2,\cdots \end{aligned} \tag{3.11}$$

The upper and lower bounds may vary with time, but they usually will be constant.
The constraints can be made soft by defining an extra border, say ϵ and analogously a weight factor. This allows the MPC controller to be more flexible when needed.

The QP problem can be described as follows:

$$\begin{aligned} \min_x \quad & \frac{1}{2}x^T Hx - g^T x \\ so\ that \quad & Cx \le c \end{aligned} \tag{3.12}$$

with:
- H the Hessian matrix,
- g the gradient vector,
- C the inequality constraint matrix,
- c the inequality constraint vector.

The solution vector x minimizes $\frac{1}{2}x^T Hx - g^T x$, satisfying the inequality constraint $Cx \le c$. The solution to this problem does not always exist, therefore the QP problem is called a feasible path problem.

The QP formulation for the constrained MPC problem is:

$$\begin{aligned} \min_{\Delta U(k)} \quad & \|\Gamma^y[Y_p(k+1) - R(k+1)]\|^2 + \|\Gamma^{du}\Delta U(k)\|^2 \\ so\ that \quad & C^u \Delta U(k) \ge C(k+1|k) \end{aligned} \tag{3.13}$$

From this it follows that:

$$H = S_p^{uT}\Gamma^{yT}\Gamma^{y}S_p^{u} + \Gamma^{uT}\Gamma^{u}$$

$$G(k+1|k) = S_p^{uT}\Gamma^{yT}\Gamma^{y}(R(k+1) - M_pY(k|k) - S_p^{d}\Delta d(k))$$

$$C(k+1|k) = \begin{bmatrix} u(k-1)-u_{high}(k) \\ \vdots \\ u(k-1)-u_{high}(k+m-1) \\ u_{low}(k-1)-u(k-1) \\ \vdots \\ u_{low}(k+m-1)-u(k-1) \\ -\Delta u_{\max}(k) \\ \vdots \\ -\Delta u_{\max}(k+m-1) \\ -\Delta u_{\max}(k) \\ \vdots \\ -\Delta u_{\max}(k+m-1) \\ M_pY(k|k) + S_p^{d}\Delta d(k) - Y_{p_{high}}(k+1) \\ -M_pY(k|k) - S_p^{d}\Delta d(k) + Y_{p_{low}}(k+1) \end{bmatrix}, \quad C^{u} = \begin{bmatrix} -I_L \\ I_L \\ -I \\ I \\ -S_p^{u} \\ S_p^{u} \end{bmatrix}, \quad I_L = \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & & & \vdots \\ 1 & 1 & 0 & \cdots & & 0 \\ 1 & 1 & 1 & \cdots & & 1 \end{bmatrix} \tag{3.14}$$

It is this form of the MPC controller that is implemented in the simulations further on in this report.

Chapter 4 Outlines of MPC for melt index control

4.1 The goal of the MPC control scheme

The goal of designing the MPC control scheme is to design an automatic controller for the melt index during grade changes and normal operation at the plant. The MPC controller should reduce the costs involved in the grade changes by decreasing the time needed for a grade change and thus decreasing the amount of degraded product.

4.2 Modelling the melt index

From literature it is known that designing a white model for the melt index is very difficult [AUL90]. Since white modelling of the melt index is still not possible, dynamic black box modelling has been tried as an alternative. It proved to be very difficult to reach good dynamic black box models because the available data was closed loop plant process data. The dynamic modelling was almost impossible because of strongly variable time delays imposed on the system caused by different ways of operating the separator level in effort to control the extruder as constantly as possible (also see Chapter 2). Also, it was not possible to do a wide range of new experiments at the plant for identification purposes. For these reasons, trying to build a dynamic black box model describing the melt index was discarded as a possible modelling option after considerable effort. It appeared that the residence time and mixing effects in the separator were too time-dependent, and thus too great a disturbance for proper dynamic black box modelling.

From the modelling effort on dynamic black box models, more and more insight was gained in the process of producing polyethylene in a tube reactor. It became clear that, because of the speed of the polymerization reaction, a local melt index was produced in the reaction zones of the tube reactor, dependent on local reactor quantities such as peak- and bottom temperatures, the modifier concentration and the total reactor mass flow (i.e. pressure drop). The assumption that the melt index directly follows from the properties of the gas mixture is in agreement with results of others, see [AUL91]. The dynamical behaviour of the melt index can thus be reduced to the dynamical behaviour of the properties of the gas mixture in the tube reactor, and of course the dynamical influence of the separator and extruder (i.e. holdup and mixing effects). This is the reason why a statistical melt index model is developed, describing the melt index directly after the tube reactor.

It should also be noted that an extensive part of the dynamic behaviour of the melt index that is measured at the end of the extruder is determined by the residence time and mixing effects

introduced by the separator and extruder. These dynamic influences can be estimated from experiments performed at the plant in order to estimate the PID-control behaviour of the peak temperatures (see later on in this chapter). From the experiments the dead time introduced by the separator and extruder can be estimated. This gives information about how to transform the melt index directly after the tube reactor in order to compare this melt index with the melt index measured at the end of the extruder.

In a statistical model the signs of the parameters can be technologically explained. The modifier concentration should have a positive influence on the melt index, since more modifier will lead to smaller polymer chains and shorter chain branches, resulting in a higher melt index. The length of the up going parts of the temperature profile in the tube reactor should also have a positive influence on the melt index. This can be explained from the fact that the inlet temperature of the tube reactor is constant, and thus a longer up going part will result in a higher average temperature in that part of the temperature profile, which results in more reactions and thus shorter polymer chains, and a higher melt index. The temperature after the preheater can be seen as the zeroth bottom temperature. The pressure in the suction section of the compressor should have a negative influence on the melt index, since increasing the pressure in the suction section will result in a higher total reactor flow, which in its turn is responsible for a lower average pressure in the tube reactor. The total effect of this on the melt index is negative (see also Chapter 2). The opposite goes for the temperature in the suction section of the compressor, because a rise in the temperature in the suction section will result in a lower total reactor mass flow.

Statistical analysis of plant process data over a 4 months period has led us to the following model for the melt index as a function of the reactor properties:

$$\begin{aligned} \ln(mi) \;=\; & a * [modifier] \\ & + b * (T_{peak1} - T_{preh}) \\ & + c * (T_{peak2} - T_{bottom}) \\ & - d * p_{comp} \\ & + e * T_{preh2} \\ & + f * T_{comp} \\ & - g \end{aligned} \qquad \textbf{(4.1)}$$

with:
- mi — the melt index,
- [modifier] — the modifier concentration,
- T_{peakx} — the peak temperatures,
- T_{bottom} — the bottom temperature,
- p_{comp} — the pressure in the suction section of the compressor,
- T_{comp} — the temperature in the suction section of the compressor,
- T_{preh} — the temperature after the preheater.

The statistical properties of the presented model are shown in Appendix B. This model was accepted because both the coefficient of determination (0.97597)and the adjusted coefficient of determination (0.95251) are close to the maximum value of 1, and the T-values we see that

all the model coefficients are significant within 5%. Furthermore none of the variables are significantly correlated. From the variance inflation factor it is clear that the constant term is by far the variable responsible for the variance in the model. Thus in case of an offset of the model, this parameter should be adapted.

4.3 Using the melt index model in the model predictive controller

The melt index model as described in Equation 4.1 contains the following variables: the modifier concentration, the temperature and pressure of the suction section of the compressor, the temperature after the preheater, the peak temperatures in the tube reactor and the bottom temperature in the tube reactor. The modifier concentration can be modelled by using the modifier model. Thus the modifier flow and the flow of the purge are used as manipulated variables (MV's). The peak temperatures of the tube reactor are PID-controlled by setpoint, as is the temperature after the preheater. Thus the peak temperatures and the temperature after the preheater also are MV's. The temperature and pressure in the suction section of the compressor cannot be controlled, so these are used as measured disturbances (MD's) in the model for controlling the melt index. The bottom temperatures are a result of the peak temperatures, the temperature and flow of the chilled water in the cooling jacket around the tube reactor and the total reactor mass flow. Since the bottom temperatures are largely dependent of so many variables, and a good model describing the bottom temperatures was not available, it is not convenient to use these in a model of the melt index for MPC control structures for simulation. Since the bottom temperatures are measured at the plant, they might be used as measured disturbances (MD's) in an MPC control structure implemented at the plant. Summarizing the following variables were used in the melt index model for the MPC controller:

- MV's:
  - modifier flow,
  - flow of the purge,
  - average of the peak temperatures,
  - temperature after the preheater unit,
- MD's:
  - temperature in the suction section of the compressor,
  - pressure in the suction section of the compressor.

This results in the following statistical model describing the melt index:

$$\begin{aligned} \ln(mi) \;=\; & a * [modifier] \\ & + b * T_{peak} \\ & - c * p_{comp} \\ & + d * T_{preh} \\ & + e * T_{comp} \\ & - f \end{aligned} \tag{4.2}$$

with:
- mi — the melt index,
- [modifier] — the modifier concentration,
- T_{peak} — the average peak temperature,
- p_{comp} — the pressure in the suction section of the compressor,
- T_{comp} — the temperature in the suction section of the compressor,
- T_{preh} — the temperature after the preheater.

In order to get all the parameters acceptable in a technological way the peak temperatures were lumped together in the average of the peak temperatures. This was done because the peak temperatures usually are controlled by setting the same setpoint for all the peak temperatures at the same moment. The other parameters in the model were found to be technologically right.

The statistical properties of the model are described in Appendix B. This model is accepted since both the coefficient of determination (0.97598) and the adjusted coefficient of determination (0.95254) are close to the maximum value of 1 and the T-values are significant within 5%. From the variance inflation factor it can be seen that the constant term in the model is by far the most responsible variable for the variance in the model. Thus in case of model errors this parameter should be adjusted first. Furthermore no significant correlations between the variables could be detected.

4.4 Using step response models in controlling the melt index

As stated above, the peak temperatures and the temperature after the preheater are controlled by setpoint, since the installed PID-controllers for these variables are sufficiently well tuned. Experiments at the plant show that when a change in setpoint is made for the peak temperatures, the setpoint is reached quite fast. This is due to the automatic PID-control of the initiator pumps, fed by the preferred setpoint of the peak temperatures. For this reason, the step response of the melt index to a unit step in the peak temperatures is assumed to be a first order step response with a fast settling time and a gain which is equal to the constants found in the statistical melt index model. It is assumed that the temperature after the preheater has the same kind of step response as the peak temperatures, and the same settling time as the peak temperatures, since the heating capacity of the preheater only operates in a very limited area, and its influence on the melt index is the same kind as that of the peak temperatures.

As described in Chapter 2, the temperature and the pressure in the suction section of the compressor uniquely determine the total reactor mass flow. It is assumed that the settling time of these two quantities will be similar to that of the peak temperatures. This was done so because the total reactor mass flow can change almost instantaneously, and is only slightly dependent on the total residence time of the tube reactor.

The modifier concentration are modelled by using the incoming modifier flow and the flow of the purge. By multiplying the step responses found from the modifier model with the parameters from the statistical model, the modifier flow and the flow of the purge are used directly in

controlling the melt index.

The control design as describe above is schematically shown in Figure 4.5, the step responses referred to in Figure 4.5 are more explicitly shown in Figure 4.6.

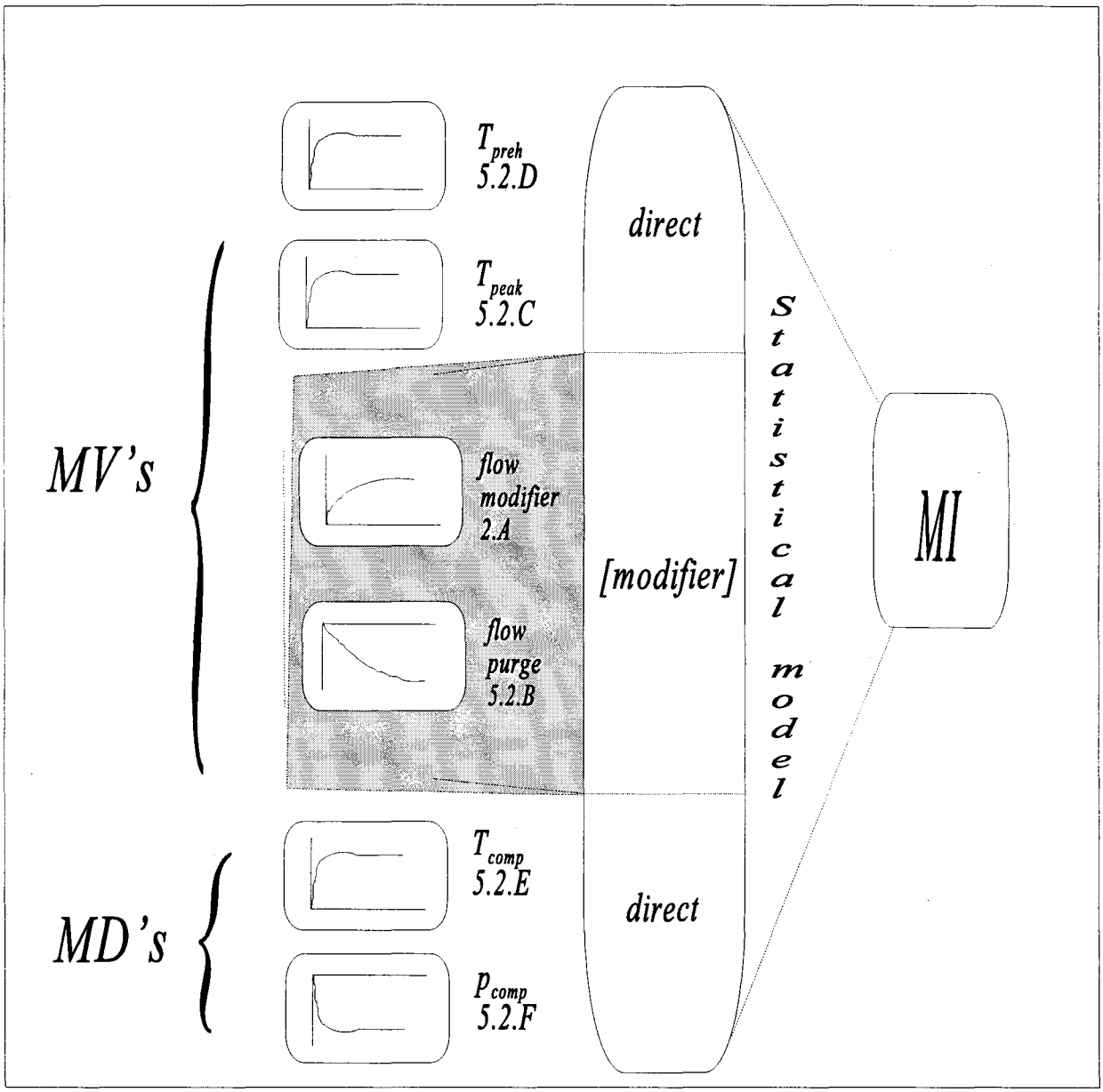

Figure 4.1: the controller design for controlling the melt index by means of MPC.

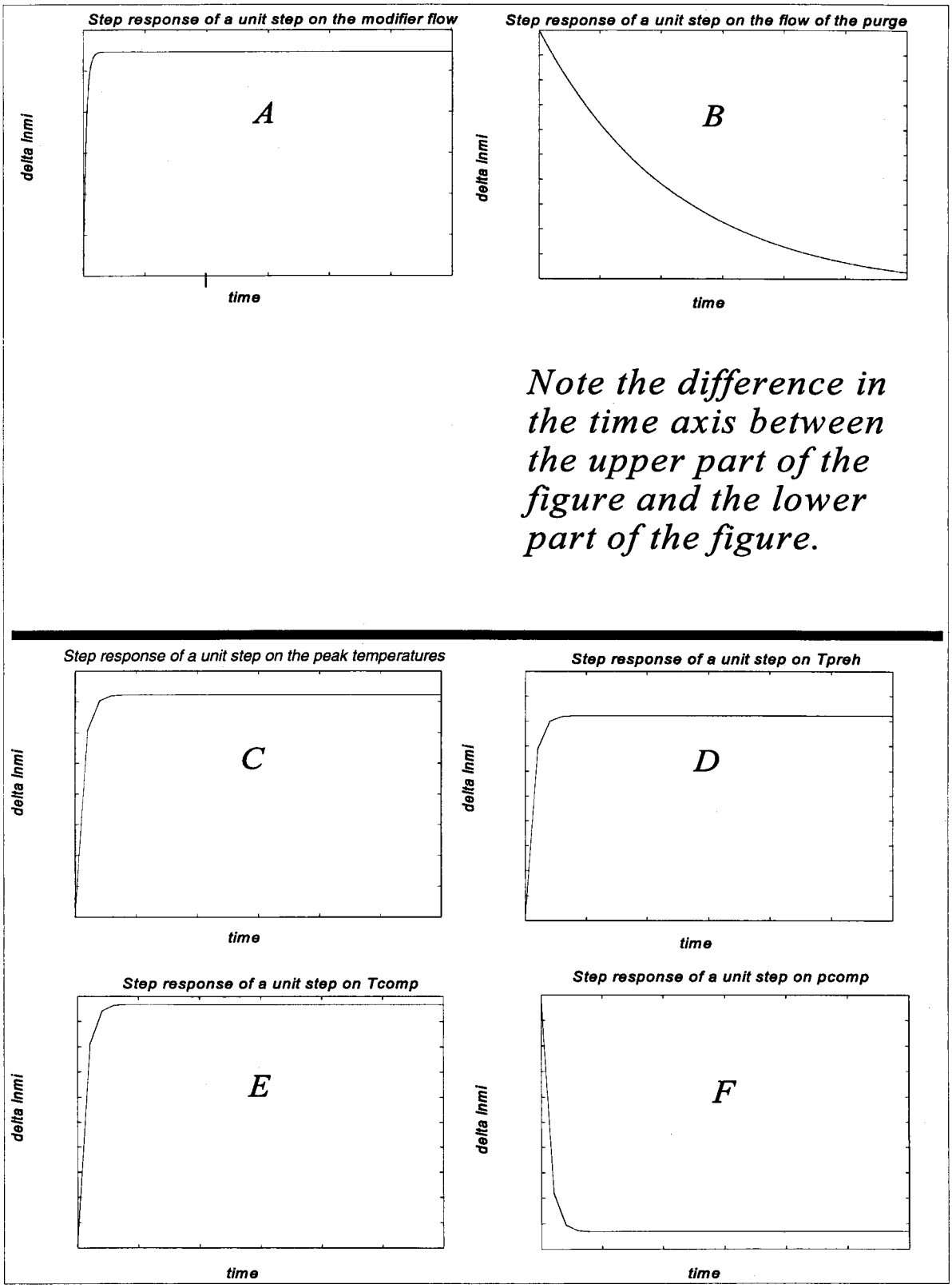

Figure 4.2: the step responses for the melt index from unit steps on the MV's and MD's.

The settling times of the flows were checked in an earlier study in PRIMAL. In these studies actual plant data was used, and the flows were filtered with a first order filter with the appropriate settling times. This way the modifier concentration was predicted and showed a good fit on the actual measurements from the plant. Thus the settling times were accepted.

4.5 The planned simulations

As stated before, the goal of this project is to design an automatic model predictive controller for controlling the melt index during grade changes and steady state operation of polyethylene production. For this reason, the general layout of the experiments is the following: starting out in a steady state production a change in setpoint is given for the melt index and the constraints of the peak temperatures (according to the recipe of the next grade to be produced). After these changes the simulation continues until again a steady state production is reached.

The most beneficial aspect of model predictive control of the melt index during grade changes should be the use of the difference in the speed of changes in the modifier concentration and the temperatures in the tube reactor. Since the modifier concentration has a larger settling time than the peak temperatures, the effect of changes in the modifier concentration can easily be compensated by controlling the peak temperatures, resulting in very fast grade changes.

This control strategy can be clarified by assuming a negative setpoint step on the melt index: a decrease in the melt index setpoint will ask for lower values of the modifier concentration and peak temperatures. A possible (perhaps optimal) control strategy would be to lower the modifier concentration at an early stage and keeping the melt index on the previous setpoint by means of increasing the peak temperatures. At the time of the setpoint change of the melt index, the peak temperatures can be lowered very fast in comparison to the rate of change in the modifier concentration, resulting in a fast decrease of the melt index towards the new value. Since the modifier concentration is already at the preferred lower level, the peak temperatures can be directed faster to their preferred setpoint, which in turn is optimal for the other product qualities such as density and brightness.

For finding the optimal control strategy for the grade changes attention had to be paid during the simulations to other tuning parameters for the MPC control problem, such as:

- the influence of the setting of the weight factors on the outputs and the change in the inputs (Γ^{y} and Γ^{du}),
- the influence of the length of the prediction and control horizon (p and m),
- the necessity and influence of ramps on the constraints and reference trajectories,
- the influence of errors in the measured disturbances.

Experiments were performed according to the experimental design as show in Table 4.1. The most important results of the experiments are shown and discussed in Chapter 5.

Table 4.1: experimental design for the simulations in Matlab. In the cells of the table all the possible values of the parameters are given. The experimental design exists of all possible combinations for the parameters.

grade change from # to #	Γ^{y}	Γ^{du}	p	m	ramp time on constraints	plant/model mismatch
1 to 4	30,10,5,1	10,1,0.1	a,b,c	d,e,f	g,h,i	yes, no
2 to 4	30,10,5,1	10,1,0.1	a,b,c	d,e,f	g,h,i	yes, no
6 to 2	30,10,5,1	10,1,0.1	a,b,c	d,e,f	g,h,i	yes, no
12 to 1	30,10,5,1	10,1,0.1	a,b,c	d,e,f	g,h,i	yes, no

Initially, all possible combinations of settings were used for simulation, but if the results of a simulation were very bad (i.e. infeasibility of the QP-problem in Matlab or the MPC controller was very sluggish) because of the parameter settings, this type of experiment was left out in further simulations. So for example, if the settings like $\Gamma^{y} = 30$ and $\Gamma^{du} = 10$ led to poor results in setpoint tracking of the MPC controller, then all the other experiments to follow with $\Gamma^{y} \leq 30$ and $\Gamma^{du} = 10$ were not performed. It is thus assumed that the MPC controller will show the same performance for different control problems (i.e. different grade changes) under the same settings of the MPC controller.

In order to see how the MPC controller responded to variable measured disturbances, coloured noise was created on the temperature and the pressure in the suction section of the compressor (i.e. the only two MD's). The noise was given an amplitude of 1% of the mean operating values at the plant and was generated by the random function in Matlab. This generally resulted in the signal drifting around the mean value with an amplitude of 5% of the mean value.

An error in the measured disturbances was simulated by adding 1 time or 4 times the noise on the measured disturbances (i.e. the temperature and pressure in the suction section of the compressor) to the model describing the plant in the simulations. The model used for the MPC controller was not adapted for these additional disturbances, and thus a kind of model error was introduced.

In total 148 experiments were performed.

Chapter 5 The simulations in Matlab

5.1 General

As described in Chapter 4 the simulations in Matlab were designed to gain more knowledge about the behaviour of the MPC controller in during grade changes in particular and more generally also during steady state operation of the plant. The influence of the tuning parameters for the MPC control problem has also been investigated, since this is necessary for good MPC control performance. In this chapter also some other experiments are discussed in order to compare the performance of the designed MPC controller for the melt index with the way operators control the plant at present. The results concerning the performance of the MPC controller design for melt index control during grade changes and steady state operation of the plant are described in Chapter 5.6.

First attention is paid to the influence of the setting of the weight factors on the outputs and the change in the inputs (Γ^{y} and Γ^{du}), the influence of the length of the prediction and control horizon (p and m), the necessity and influence of ramps on the constraints and reference trajectories and the influence of disturbances (or plant/model mismatch) in Chapter 5.2 to 5.5. Also some conclusions will be drawn. More general conclusion and discussion of the implementation of the controller can be found in Chapter 6 of this report.

5.2 The effect of the tuning parameters Γ^{y} and Γ^{du}

From the performed experiments it became clear that increasing the ratio Γ^{y} / Γ^{du} will increase the setpoint tracking performance of the MPC controller. It was also seen that the new steady state values for the inputs, after the grade change, are not the same. This is due to the fact that the control problem is not properly dimensioned: there are too many inputs available to control one output. The over dimension over the control problem shows itself in the different end temperatures for the peak temperatures and the temperature after the preheater. This difference can be avoided by setting the very stringent constraints on several of the inputs, however, this would significantly diminish the possibilities of control for the MPC controller.

If the factor Γ^{y} / Γ^{du} is too small, the speed of the grade change will be determined by the ramp set on the constraints of the melt index. In the experiments it was found that a value of 10 to 100 for Γ^{y} / Γ^{du} gives the best performance of the MPC controller during grade changes.

5.3 The effect of the tuning parameters p and m

From the performed experiment it can concluded that selecting a too small control horizon with respect to the prediction horizon will decrease the performance of the MPC controller in terms of speed and accuracy of the setpoint tracking of the output during grade changes. This is due to the fact that setting the prediction horizon much higher than the control horizon will give the MPC controller a large amount of evaluation points for the setpoint tracking error and only a small amount of control moves to track the setpoint. During grade changes this mis-match in the amount of control moves is clearly visible in terms of unstable behaviour of the MPC controller.

If the prediction and control horizon get too low, the performance of the MPC controller will significantly decrease. This can be explained by the fact that setting the prediction and control horizon below time needed to describe the dynamic behaviour of the peak temperatures and the temperature after the preheater are not accounted for by the MPC controller.

The unstable behaviour of the MPC controller arising from too small control horizons can be explained as follows. If the control horizon is set too low with respect to the prediction horizon, the MPC controller cannot deal with the change in setpoint seen by the prediction horizon, since it only has very few control moves (i.e. the control horizon) to deal with it.

Furthermore, increasing the prediction horizon, while keeping the control horizon at a constant value, will improve the output setpoint tracking performance of the MPC controller. Yet, it should be noted, that if the prediction horizon is set very high this leads to poor performance during grade changes: due to the large amount of evaluation points for the setpoint tracking error the errors made just after the preferred grade change have significantly less influence on the control moves than the far greater amount of points further in (prediction) time. This will result in poorer setpoint tracking performance of the MPC controller during grade changes.

5.4 The influence of ramps on constraints

There are two reasons for using ramp on constraints:

- keeping the solution of the QP-problem in Matlab feasible. The ramp on the constraints of the melt index was necessary to prevent the QP-problem from getting infeasible, due to overly stringent constraints. This happens when the constraints also are changed stepwise and the implemented control moves are insufficient to direct the melt index between the new constraints (i.e. the constraints are overly stringent).
- setting additional constraints of the peak temperatures and the flow of the purge. As stated before the peak temperatures do not only influence the melt index but also the density and brightness of the polyethylene, and thus should be exact at the value described in the recipe of the produced grade.

Since the QP algorithm in Matlab is a so called feasible path algorithm, the constraints put on the MPC problem should never be overly stringent. If the constraints are overly stringent the QP algorithm in Matlab either lets go of one or more constraints or becomes instable. Since almost none of the possible grade changes can be reached within one unit of sampling time setting the upper and lower constraints for the melt index to the recipe value directly after the grade change will result in an infeasible QP problem in Matlab. For this reason the relevant constraint for the melt index (i.e. the upper if a negative change in melt index required, and the lower if a positive change in melt index is required) is ramped to its new setpoint. The other constraint was set directly to its new setpoint. Several ramping times were placed on the ramps for the melt index constraint in the MPC controller.

Setting a ramp on either the upper constraint of the melt index (in case of a decrease in the setpoint for the melt index during a grade change) or on the lower constraint (in case of an increase) shows us another aspect of ramps on constraints. When the tuning of the MPC controller is very sluggish, the constraints set on the outputs (and of course the inputs if relevant) will determine the speed of the control moves (and therefore also the setpoint tracking performance in terms of speed) during grade changes.

5.5 The effect of measured disturbances

In order to check the performance of the MPC controller under more realistic circumstances with respect to the measured disturbances, a coloured noise with an amplitude of 1% was put on the measured disturbances (the temperature and the pressure in the suction section of the preheater). From the performed simulations it became clear that the MPC controller can deal with measured disturbances quite adequately.

In order to check whether the MPC controller can deal with an error in the measured disturbances by means of the filtering factor of the MPC controller, simulations were performed in which an error on the measured disturbances was introduced by additionally putting four times the measured disturbance on the plant measurement of the melt index, and not compensate for these disturbances in the internal MPC melt index model. The filter factor for correcting the plant/model mismatch was set on 1% and 10% of the model error. The model error is determined by subtracting the calculated value of internal MPC melt index model from the measured value from the plant. Setting the filter factor for correction the errors due to plant/model mismatch high enough will result in good performance of the MPC controller.

5.6 Comparison between MPC control and present operator control

In Figure 5.1 a simulation of a grade change is shown. As described before the melt index directly at the end of the tube reactor is simulated, and not the melt index as it is measured at the end of the extruder. In order to compare the behaviour of the MPC controller with operator control, the melt index is delayed and filtered according to the expected behaviour of the separator and extruder, as is described in Chapter 4. This way the dynamic influence of the separator and extruder is accounted for and the melt index resulting from MPC control can be compared with the melt index resulting from operator control.

In Figure 5.2 the control performance of operator control at the plant is shown and compared with the adapted MPC control performance.

From Figure 5.2 it can be seen that the performance of the MPC controller is about 2 times faster than the performance of the operator control. It is also clear that the ramping time for the upper constraint on the melt index is chosen to small, since the simulated melt index at the end of the extruder does not stay below this upper constraint. Thus for the application of the MPC controller at the plant the ramping time for constraints on the melt index should be higher (see Figure 5.2). Furthermore it is clear that in case of operator control the melt index does not necessarily has to be between the constraints, whereas this is always the case at MPC control. Thus MPC control will result in more pure grades during steady state production.

From Figure 5.1 it can be seen that the melt index at the end of the tube reactor changes rather fast from one grade to another. If the dynamic influence in terms of mixing effects in the separator could be minimized, then this speed of change of the melt index would also appear, with some delay, at the end of the extruder. This can be reached by minimizing the level in the separator before, during and after the grade change. This is a point for further investigation.

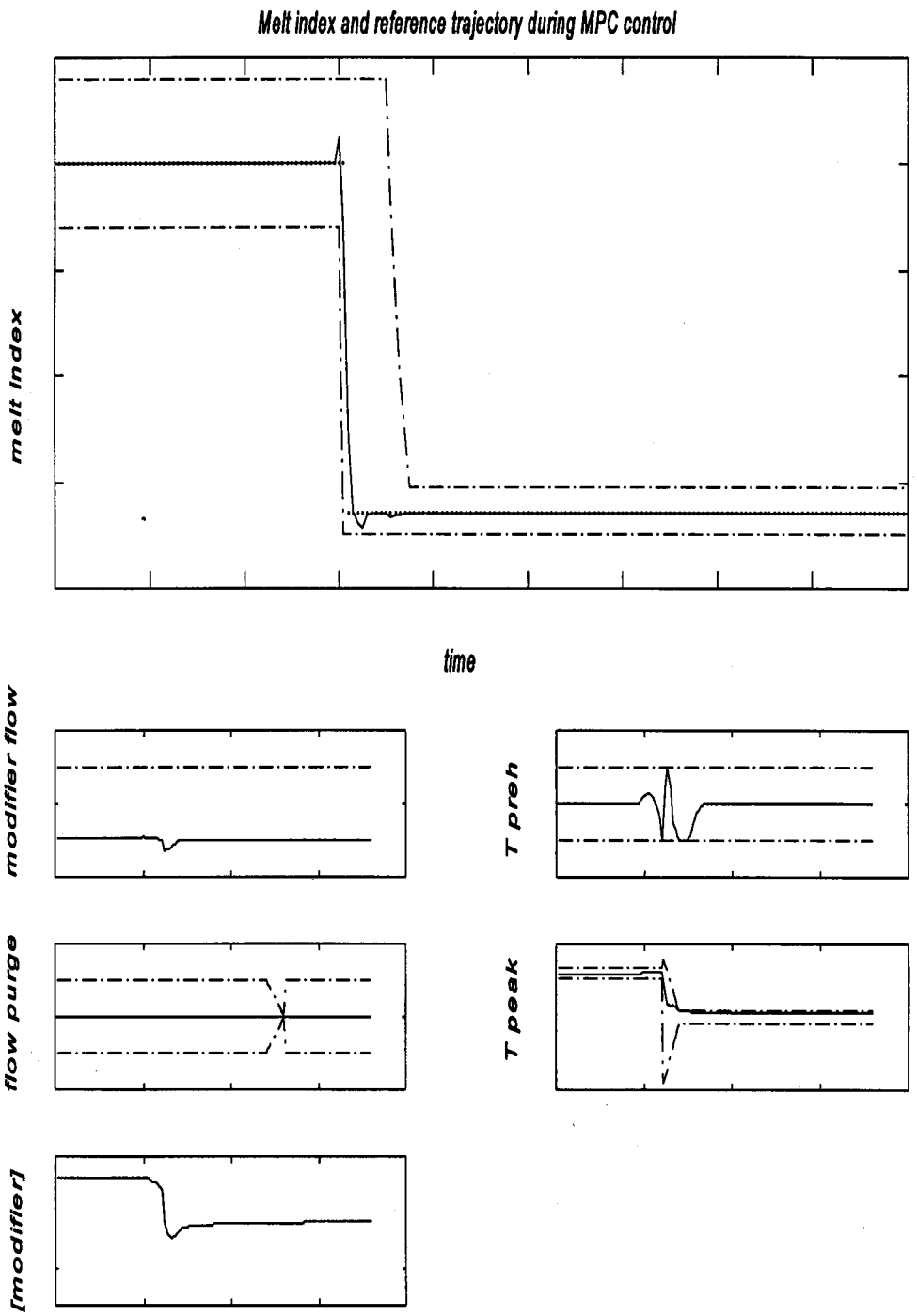

Figure 5.1: the performance during grade change of the MPC controller. The constraints are shown in the dashed/dotted lines. The setpoint is shown in the dotted line.

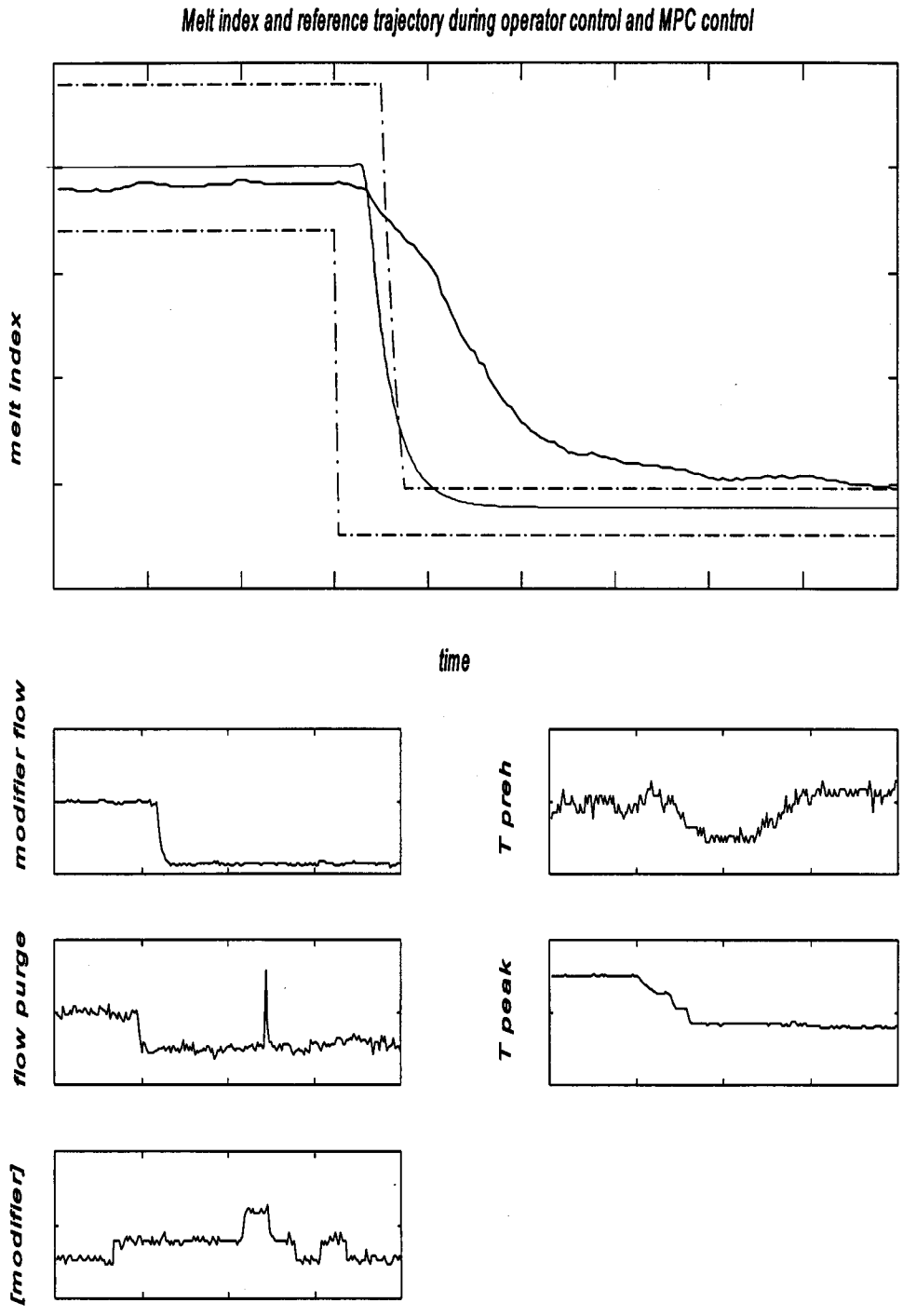

Figure 5.2: the performance during grade change by operator control of the plant compared with the most probable MPC control performance. The setpoint is shown in the dotted line.

Chapter 6 Discussion and Conclusions

6.1 Tuning of the MPC controller

From the results of Chapter 5 we see that the setpoint tracking performance of the MPC controller is greatly influenced by the ratio of Γ^{y} and Γ^{du}. Setting Γ^{y} above 10 and Γ^{du} at 0.1 gives a good performance of the MPC controller. When setting Γ^{y} above 100, sometimes the performance of the MPC controller will decrease. This decrease is due to the settings of the prediction horizon: since the simulations are focused on melt index control during grade changes, setting the prediction horizon far greater than the average time needed for a grade change will result in infeasibilities of the QP problem in Matlab. This can be illustrated by the following example. Let the present simulation time be somewhere before the grade change and the prediction horizon stretch out all over the grade change, and the control horizon stops before the grade change. Then, generally, there won't be any set of control moves possible to set the output (the melt index) to the preferred value (reference trajectory) over the total prediction horizon. In Matlab this results in unstable control before and during the grade change, or even in an infeasible QP problem.

In case of an error in the measured disturbances, the setting of the filter factor for the model error is interesting. From the experiments it can be concluded that setting the filter factor at a higher value will result in a better adaptation of the internal model, and therefore a better control performance. A good performance under realistic measured disturbances was found with a filter factor of 0.1; this means that the internal model is adapted with 10% of the measured error.

6.2 Performance of the MPC controller in simulations

From the experiments shown in Chapter 5 it can be seen that when well tuned, the MPC controller is capable of performing every grade change within a very small amount of time relative to the time needed for grade changes under operator control. Even the peak temperatures can be directed to the preferred setpoint within the same time by setting a ramp on the constraints. It is here that appear some new tuning parameters for this specific MPC controller. One could direct the peak temperatures directly to the new setpoint by setting a direct ramp, but another strategy would be to set the constraints on the peak temperatures to the maximum values, so that the peak temperatures can be used to compensate for changes in the concentrations of the modifier and in a final instance use the speed of change of the peak temperatures to get a very fast grade change.

Also the performance of the MPC controller in steady state operation was tested. Simulations were performed with 4% plant/model mismatch by feeding the MD's 4 time extra to the model of the plant. It appears that the MPC controller easily can handle disturbances that might occur during steady state control of the plant.

The ramps on the constraints are necessary to keep the QP problem in Matlab solvable. As stated before, the time needed for a grade change (which is partially determined by the settings of the ramp time of the constraints) and the settings of the prediction and control horizon determine whether the MPC controller in Matlab will remain stable, and whether the QP problem will remain feasible.

6.3 Implementing MPC in melt index control at the plant

From Chapter 5 can be seen that in simulations the grade changes take place about 10 times faster than under operator control. This seems a lot, but it also is a wrong perception since the MPC simulation calculates the melt index directly behind the tube reactor and not at the extrusion di-plate of the extruder, so the residence time and the mixing effect occurring in the separator and the extruder are not taken into account. Compensating for these effects the time needed for the grade changes would be about 20% less then under operator control. Yet, an optimal control strategy would include lowering the level in the separator before and during a grade change, resulting in a plug flow. This plug flow has the positive effect that the grade change measured at the end of the extruder will show the same dynamic behaviour as the one realised at the end of the tube reactor.

6.4 MPC control versus a multi variable PID control structure

An MPC control structure has some advantages in comparison with a multi variable PID control structure:

- the MPC controller can handle adaptation of the model parameters, which can be identified in an off-line application. This way the model used by the MPC controller will always be very accurate,
- the MPC control structure is easily expandable to control more outputs than only the melt index, such as the brightness and density of the polyethylene. Implementing more controlled variables in a PID structure will ask for decoupling of variables, and will increase the complexity of the PID control structure,
- the MPC controller can also be expanded to use more inputs. The only thing needed for implementing other inputs is the influence of these inputs on the melt index in the form of step responses. Again adding other inputs to a multi variable PID control structure would imply a lot of additional rules and decoupling of PID control loops.

Another point of interest is that the MPC control structure will alway minimize the time needed for a grade change, whereas the time needed for a grade change in a multi variable PID control structure is totally determined by the ramp time settings of the different control variables.

6.5 Conclusions

From the previous discussion it can be concluded that the exact tuning and design (i.e. the use of ramps on constraints) of an MPC controller is largely dependent on the kind of control problem that should be handled by the MPC controller. In this particular case the time needed for the grade changes (which is actually determined by the ramp time of the constraints) determines the settings of the prediction and control horizon. Only the weight factors Γ^{y} and Γ^{du} are seemingly independent of the structure of the control problem, but as described above these are related to the feasibility of the QP problem in case of badly chosen prediction and control horizons.

MPC control of the melt index during grade changes will have two benefits for the control of the plant. In the first place all the grade changes become independent of the actual reactor settings and are performed in a reproducible way without operator interference. Secondly MPC in cooperation with optimal control of the separator and extruder will significantly decrease the time needed for grade changes. Dependent on the gain in time achievable by minimizing the level in the separator, the time needed for a grade change could be reduced with approximately 50%.

6.6 Points for further investigation

Before implementing an MPC controller for controlling the melt index during polyethylene production some further investigations should be done, such as:

- the exact settings of the constraints on the melt index and the input before, during and after grade changes,
- the influence of the prediction and control horizon on the feasibility of the QP problem and the stability of the MPC controller,
- development of an improved control strategy for the level of the separator, in order to reduce the residence time and mixing effects on the eventually produced melt index during grade changes,
- the use of the bottom temperatures as measured disturbances in the melt index model could improve the performance of the melt index model.

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Appendix A The radical polymerization reactions

In this Appendix the reactions related to the radical initiator are shown. The following steps are present in the radical polymerization process: initiation, propagation, termination, inter-transfer and intratransfer. Each of these reaction types is treated below.

A.1 Initiation

The initiators used for the production of polyethylene usually are organic peroxides which will separate into two radical composites at a sufficiently high temperature, and the radicals will react with the ethylene and start a polymer chain:

$$\begin{aligned} R_1\text{-}O\text{-}O\text{-}R_2 &\rightarrow R_1\text{-}O\bullet + \bullet O\text{-}R_2 \\ R_x\text{-}O\bullet + H_2C{=}CH_2 &\rightarrow R_xO\text{-}CH_2\text{-}CH_2\bullet \end{aligned} \qquad \textbf{(A.1)}$$

This can also be denoted in the following way:

$$\begin{aligned} M_0 &\xrightarrow{k_d} 2fM_0^* \\ M_0^* + M &\xrightarrow{k_i} M_1^* \end{aligned} \qquad \textbf{(A.2)}$$

with:
- M_0 the initiator,
- M_0^* the radical from the initiator,
- M the monomer,
- M_1^* the first step in the polymer chain,
- k_d the reaction rate coefficient for the decomposition of the initiator into two radicals,
- k_i the reaction rate coefficient for the initial polymerization reaction.

The reaction rate coefficients can generally be written as:

$$k_x = k_\infty e^{-\frac{E_a}{RT}} \qquad \textbf{(A.3)}$$

with:
- k_x a reaction rate coefficient
- k_∞ a constant factor,
- E_a the activating energy of the reaction,
- R the gas constant,
- T the absolute temperature.

A.2 Propagation

The propagation reaction is the main reaction in the reaction scheme for the production of polyethylene. By adding an ethylene molecule, a macro-radical is formed which is very reactive:

$$R_x\text{-}O\bullet + H_2C\text{=}CH_2 \rightarrow R_x\text{-}O\text{-}CH_2\text{-}CH_2\bullet \qquad \textbf{(A.4)}$$

or alternatively:

$$M_x^* + M \xrightarrow{k_p} M_{x+1}^* \quad , x \geq 1 \qquad \textbf{(A.5)}$$

with:
- M_x^* the radical polymer containing x monomers,
- k_p the reaction rate coefficient for the propagation reaction.

A.3 Termination

Whenever two radicals meet a termination reaction will take place. There are two possibilities for termination reactions:

$$\begin{aligned} R_x\text{-}CH_2\text{-}CH_2\bullet + \bullet CH_2\text{-}CH_2\text{-}R_y &\rightarrow R_x\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}R_y \\ R_x\text{-}CH_2\text{-}CH_2\bullet + \bullet CH_2\text{-}CH_2\text{-}R_y &\rightarrow R_x\text{-}CH_2\text{-}CH_3 + R_y\text{-}CH\text{=}CH_2 \end{aligned} \qquad \textbf{(A.6)}$$

or alternatively:

$$M_x^* + M_y^* \xrightarrow{k_t} M_{x+y} \qquad \textbf{(A.7)}$$

with: • M_{x+y} either a polymer with a chain length of x+y monomers or two polymers with chain lengths of x and y monomers respectively,
• k_t the reaction rate coefficient for the termination reaction.

The first reaction is called recombination, the second disproportioning.

A.4 Intratransfer

Reactions in which the radical is replaced within the same molecule are called intratransfer reactions. These reactions are an explanation to the existence of short and long chain branches (SCB's and LCB's, see also Figure 2.1):

$$R_x-CH_2-CH_2-CH_2\bullet \rightarrow R_x-\underset{\bullet}{CH}-CH_2-CH_3 \qquad \textbf{(A.8)}$$

The amounts of long and short chain branches determine polymer qualities such as density and melt index. If the radical is replaced to another carbide atom in the same molecule where the polymerization continues one speaks of intertransfer reactions. Intertransfer reactions merely replace the growing location of a polymer.

Appendix B The statistical melt index models

B.1 Some statistical properties

In determining whether to accept a model or not a number of statistical properties were analysed. In the following a short description of the relevant statistical properties will be given.

The adjusted coefficient of determination, R^2_{adj}, gives a value between 0 and 1. A high value of R^2_{adj} indicates a good fit, a low value a poor fit. The adjusted coefficient of determination is defined by [MON91]:

$$R^2_{adj} = \frac{M_{tot} - M_{res}}{M_{tot}} = 1 - \frac{(1 - R^2)(o - d)}{o - q} \qquad \textbf{(B.1)}$$

with:
- R^2_{adj} the adjusted coefficient of determination,
- M_{tot} the total mean square,
- M_{res} the residual mean square,
- o the number of experiments,
- d 1 if the model contains a constant term, otherwise 0,
- q the number of model terms,
- R^2 the coefficient of determination.

The Variance Inflation Factor (VIF) gives information about the amount of variance in the model explained by the different model parameters. If VIF is big for one of the variables, this variable is responsible for most of the variance in the model (see [MYR86]).

The T-value shows the significance of the different model terms. The T-value is given by [DEM87]:

$$T = \frac{B_i}{SE(B_i)} \qquad \textbf{(B.2)}$$

with:
- T the T-value,
- B_i the ith coefficient of the model,
- $SE(B_i)$ the standard error of the ith coefficient in the model.

Further more some graphical ways of analysing a model were used. The histogram shows the frequency distribution of the residuals. If the model is proper, the peak of the histogram is at

zero, and the residuals normally distributed. In addition with a normal probability plot (a plot in which the residuals are plotted on a cumulative normal probability scale) it gives information about systematic errors that might otherwise have been overlooked. The normal probability plot should show a straight line, indicating that the model is properly built.

B.2 The general melt index model

Below some results of a linear regression performed in SPSS for Windows [SPS88] are shown. The coefficients in the model are codes as follows:

- LNMI the natural logarithm of the melt index,
- MODIF the modifier concentration,
- DIFF1 the difference between peak temperature 1 and the temperature after the preheater,
- DIFF2 the difference between peak temperature 2 and bottom temperature 1,
- TPREH the temperature after the preheater,
- TCOMP the temperature in the suction section of the compressor,
- PCOMP the pressure in the suction section of the compressor.

```
Equation Number 1    Dependent Variable..   LNMI

Variable(s) Entered on Step Number
   1..     TCOMP
   2..     MODIF
   3..     PCOMP
   4..     DIFF2
   5..     TPREH
   6..     DIFF1

Multiple R            .97597
R Square              .95252
Adjusted R Square     .95251
Standard Error        .19185

Analysis of Variance
                    DF        Sum of Squares       Mean Square
Regression           8          68112.28087        8514.03511
Residual         92250           3395.36235           .03681

F =  231321.33147       Signif F =  .0000

---------- Variables in the Equation -----------

Variable        VIF          T      Sig T

MODIF          3.177    564.774   .0000
DIFF1         25.317    156.830   .0000
DIFF2         11.062     22.156   .0000
PCOMP          1.097    -59.104   .0000
TPREH          1.366     60.536   .0000
TCOMP          1.173     19.425   .0000
(Constant)              -81.857   .0000
```

From the model data above we see that both the coefficient of determination (0.97597)and the adjusted coefficient of determination (0.95251) are close to the maximum value of 1. This implies that the model fit is rather good. From the T-values we see that all the model coefficients are significant within 5%. It can also be seen that the constant term is responsible for most of the variance in the model.

From the correlation diagram it is clear that none of the variables are significantly correlated. From the histogram and the normal probability plot of the general melt index model it can clearly be concluded that the residuals have a normal distribution, and that most likely the model does not have any systematic deficiencies.

B.3 The melt index model used for MPC

Below some results of a linear regression performed in SPSS for Windows [SPS88] are shown. The coefficients in the model are codes as follows:

- LNMI the natural logarithm of the melt index,
- MODIF the modifier concentration,
- SUMPEAK the average of the two peak temperatures,
- TPREH the temperature after the preheater,
- TCOMP the temperature in the suction section of the compressor,
- PCOMP the pressure in the suction section of the compressor.

```
Equation Number 1    Dependent Variable..    LNMI

Variable(s) Entered on Step Number
   1..     TCOMP
   2..     MODIF
   3..     PCOMP
   4..     TPREH
   5..     SUMPEAK

Multiple R            .97598
R Square              .95254
Adjusted R Square     .95254
Standard Error        .19135

Analysis of Variance
                    DF        Sum of Squares        Mean Square
Regression           6          67397.82063        11232.97011
Residual         91702           3357.82733              .03662

F =  306771.52898        Signif F =  .0000
```

---------- Variables in the Equation ----------

Variable	VIF	T	Sig T
MODIF	1.931	770.468	.0000
PCOMP	1.088	-52.696	.0000
SUMPEA	2.439	621.692	.0000
TPREH	1.103	5.099	.0000
TCOMP	1.071	24.297	.0000
(Constant)		-120.761	.0000

From the model data above we see that both the coefficient of determination (0.97598) and the adjusted coefficient of determination (0.95254) are close to the maximum value of 1. This implies that the model fit is rather good. From the T-values we see that all the model coefficients are significant within 5%. It can also be seen that the constant term is responsible for most of the variance in the model. From the correlation diagram it can be seen that none of the variables are significantly correlated. From the histogram and the normal probability plot of the residuals of the melt index model used for MPC it is clear that the residuals are normally distributed and from that most likely the model does not have any systematic deficients.

Appendix C List of the used symbols

Below an overview of the symbols uses in the report will be given. The symbols are given in alphabetical order, the Greek characters are placed first, the mathematical symbols are at the end of the list. The variables used in the Matlab programs are not listed here, since those are explicated in the program listing itself.

Γ^{du}	weight factor on the change in the inputs for the MPC controller
Γ^{u}	weigth factor for the absolute value of the inputs for the MPC controller
Γ^{y}	weigth factor for the setpoint tracking for the MPC controller
$\Delta d(k-1)$	change in measured disturbances at time *k-1*
$\Delta u(k)$	change in inputs at time *k*
Δumax	constraint on the maximum change in the inputs
ϵ	weight factor for soft constraints
η	viscosity
$\phi_{m,recycle}$	recycle flow from the separator
$\phi_{m,modifier}$	fresh modifier flow
$\phi_{m,purge}$	flow of the purge
$\phi_{m,ethylene}$	fresh ethylene feed to the system
$\phi_{m,R}$	total reactor mass flow
$\phi_{modifier}$	fresh modifier flow
B_i	ith statistical parameter in a statitstical model
c	vector containing the constraint for the MPC controller
C	matrix selecting the constrained variables for the MPC controller
d	1 if the model contains a constant term, otherwise 0
DIFF1	peak temperature # 1 - temperature after the preheater
DIFF2	peak temperature # 2 - bottom temperature # 1
E_a	activating energy for a reaction
g	vector for selecting the setpoint tracking in the MPC controller
H	Hessian matrix for the MPC controller
k	time *k*
k|k+1	estimation of state on time *k+1* at time *k*
k_d	reaction rate coefficient for the decomposition reaction of the catalist
K_f	filter factor for the error made by the MPC controller
k_i	reaction rate coefficient for the initiation reaction
$k_{modifier}$	reaction rate coefficient for the conversion of the modifier
k_p	reaction rate coefficient for the propagation reaction
k_t	reaction rate coefficient for the termination reaction
k_x	general reaction rate coefficient
k_∞	general reaction rate coefficient at infinite temperature
LNMI	the natural logatihm of the melt index
m	control horizon for the MPC controller

M	monomer (ethylene)
M	matrix putting all the predicted values on time step ahead in the MPC controller
M_0	non-reactive initiator
M_0^*	reactive initiator
M_1^*	first step in the polymer chain
mi	melt index
M_{res}	residual mean square
M_{tot}	total mean square
M_{x+y}	polymer chain containing x+y monomers
M_x^*	reactive polymer chain containing x monomers
n	prediction horizon
o	number of experiments
p	prediction horizon
p_{comp}	pressure in the suction section of the compressor
PCOMP	pressure in the suction section of the compressor
p_R	pressure in the reactor
q	number of model terms
$r(k+1)$	value of the reference trajectory for the outputs at time $k+1$
$R(k+1)$	matrix for the reference trajectory over the prediction horizon at time $k+1$
R^2	coefficient of determination
R_{adj}^2	adjusted coefficient of determination
S^d	matrix containig the step responses of the measured disturbances
$SE(B_i)$	the standard error in the ith parameter of a statistical model
S^u	matrix containig the step responses of the inputs
SUMPEAK	average of the two peak temperatures
s_x	step response of the output to a step on input x
T	T value of a parameter in a statistical model
T_{bottom}	bottom temperature
T_{comp}	temperature in the suction section of the compressor
TCOMP	temperature in the suction section of the compressor
$T_{peak1,2}$	peak temperatures
T_{preh}	temperature after the preheater
TPREH	temperature after the preheater
T_R	temperature in the reactor
$u(k)$	value of the inputs at time k
uhigh	upper constraints on the inputs
ulow	lower constraint on the inputs
$u_s(k)$	unit step function
$y(k)$	output at time k
$Y(k\|k-1)$	prediction of the outputs for time k at $k-1$
$y^*(k\|k-1)$	prediction of the outputs for time k at $k-1$
yhigh	upper constraints on the outputs
ylow	lower constraints on the outputs
$y_p(k+1)$	prediction of the output for time $k+1$
$y_p(k+i\|k)$	prediction of the output for time $k+1$ at k
[modifier]	modifier concentration