A comparative study of conventional and pipeless batch plants

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Award date:
1997

A Comparative Study of Conventional and Pipeless Batch Plants

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WPA 420159

Master's thesis

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Eindhoven, October 1997

Thanks to Bastiaan van de Kerkhove for his company
and fruitful cooperation during this study.

Summary

In the Sections Systems Engineering of the Department Mechanical Engineering of Eindhoven University of Technology, research concerning modelling industrial systems is performed. This research concerns a modern type of chemical plant, the pipeless plant. By means of two case studies a comparison between pipeless plants and conventional batch plants is made.

First an overview is given concerning the possible types of plants in the chemical industry. From this comparison the pipeless plants appear to be the most flexible type of plant. For this reason the pipeless plant is discussed extensively. It is important to compare the conventional batch plant and the pipeless batch plant, not only concerning the qualitative aspects but also the quantitative aspects. This is done by means of two case studies.

The first case study, the zero wait case study, is a fictitious plant, where a zero-wait transfer policy is applied. Models of both a conventional batch plant and a pipeless plant have been made using the χ specification language. With these models some simulations with different constraints have been made.

The second case study is based upon an existing process of DSM Andeno, the 'FATGE'-process. The existing (conventional) plant and a pipeless version have been modelled in χ. Using simulations a comparison between the conventional batch plant and the pipeless plant has been made.

Quantitatively the pipeless plant has a lot of advantages as compared to the conventional batch plant. From the case studies it appears that the possibility of debottlenecking of the pipeless plant is a big advantage when deploying new products. The degree of difficulty of the modelling of conventional and pipeless batch plants turns out to be almost the same.

Table of Symbols

symbol	explanation
δ	throughput
δ_b	maximum throughput
φ	flowtime
φ_1	minimum flowtime
t_l	lead time
w	work in process
w^*	optimal work in process

Prefixes

letter	meaning
t	time
n	number of

Suffixes

letter	meaning
s	list
t	tuple
u	set

Abbreviations

abbreviation	meaning
sep	separation
reac	reaction
sr	separation ready

Identifiers

identifier	**explanation**
wip	work in progress
x	reactor (pipeless) or batch (conventional)
r	recipe

Contents

1 Introduction **1**

1.1 Scope of the Assignment 1

1.2 Outline 1

2 Chemical Plants **3**

2.1 Chemical Plants in General 3

2.2 Batch Plants 3

3 Pipeless Plants **7**

3.1 Qualitative Aspects of the Pipeless Plant 8

3.2 Qualitative Design of Pipeless Plants 8

3.3 Optimization of Pipeless Plants 11

4 The Zero-wait Case Study **15**

4.1 Description of the Process 15

4.2 Conventional Batch Plant 16

Description of the System 16

Model in χ 16

4.3 Pipeless Plant 20

Description of the System 20

Model in χ 20

4.4 Simulation Results 22

4.5 Evaluation 24

5 The 'FATGE'-process **27**

5.1 Description of the Process 27

5.2 Conventional Batch Plant 28

Description of the System 28

Models in χ 29

5.3 Pipeless Batch Plant 34

Description of the System 34

Model in χ 36

5.4 Simulation Results 38

5.5 Evaluation 41

6 Conclusions and Recommendations **43**

6.1 Conclusions 43

6.2 Recommendations for Further Research 44

Bibliography **47**

A Terminology **49**

B Zero-wait Model of the Pipeless Plant **53**

C Simulation Results of the Zero-wait Study **57**

D Description of the 'FATGE'-process **59**

E Model of the Pipeless 'FATGE'-process in χ **65**

F Results of the 'FATGE'-project **71**

G The Kinidine Synthesis **75**

Chapter 1

Introduction

1.1 Scope of the Assignment

The need for flexibility arises more and more in the industry. This research project concerns the flexibility of the chemical industry, by means of pipeless plants. The idea of pipeless plants was already applied in Japan and in France. Currently DSM is interested in the concept too. It is important to deliberate the advantages and disadvantages of the pipeless plant. This is done by means of a comparison of conventional batch plants and pipeless plants.

1.2 Outline

In Chapter 2 an overview is given concerning the possible types of plant in the chemical industry. The pipeless plant is one of the possibilities and is discussed extensively in Chapter 3. By means of the zero-wait case study the pipeless plant is compared with the conventional plant. This case study can be found in Chapter 4. An existing process of DSM Andeno, the 'FATGE'-process, is the basis of another comparison of pipeless plants and conventional batch plants, which is discussed in Chapter 5. In Chapter 6 some conclusions and recommendations for further research are presented.

In Appendix A some terminology will be explained. In Appendix B the χ-specification of the zero wait model of the pipeless plant can be found. The results of the zero wait case study are presented in Appendix C. Appendix D contains an accurate description of the 'FATGE'-process, the model of the pipeless 'FATGE'-plant is presented in Appendix E. The results of the FATGE-case study can be found in Appendix F. Finally an initial start is made concerning the DSM Kinidine Synthesis, which can be found in Appendix G.

Chapter 2

Chemical Plants

2.1 Chemical Plants in General

The chemical industry is concerned with the conversion of raw materials into a tremendous diversity of chemical products. It is the most expanding industry world-wide. The great emphasis on research and development in this branch, is responsible for this strong growth [Hea96]. In the Netherlands, the chemical industry is responsible for about 17 percent of the total industrial activity [VNC96]. In the UK and the USA this quantity is approximately three times higher.

Chemical plants can be divided into batch plants, continuous plants or a combination of the two. Both batch plants and continuous plants bring advantages and disadvantages about. Chemicals manufactured only in small quantities are usually made by batch operations. Batches can be measured very accurately, but the temperature control can be problematic. The equipment of batch processes is much more expensive. In continuous plants much less material is in process, resulting in a smaller chance to ruin large quantities of product. The major force in the decision to use a continuous plant rather than a batch plant when production is increasing, is the lower cost per unit of production.

Another motive to choose for a certain type of plant is the flexibility. Continuous plants appear to be very rigid. A small change in the production recipe might lead to a radical change of equipment. In the framework of this research we are interested in chemical plants which are flexible to changing consumer demands, so we focus on chemical batch plants.

2.2 Batch Plants

By means of the degree of recipe similarity an operating strategy can be determined. When a plant is designed for two or more products, with small changes in recipe, the

plant can be classified as multi-product plant. In a multi-purpose plant two or more products with significantly different recipes are manufactured. Another division can be made by means of the campaign length. When the time lost due to product change-overs is small compared to the production time, a campaign length is long. In [Rek90] a division of different operating strategies is made using differences in campaign lengths, which is made visible in Figure 2.1. Continuous plants generally are flow-shops, while every operating strategy can be applied to chemical batch plants. In most literature no clear distinction is made between job-shops and flow-shops on the one hand and multi-product and multi-purpose plants on the other hand. Therefore this way of categorizing will not be used in this research.

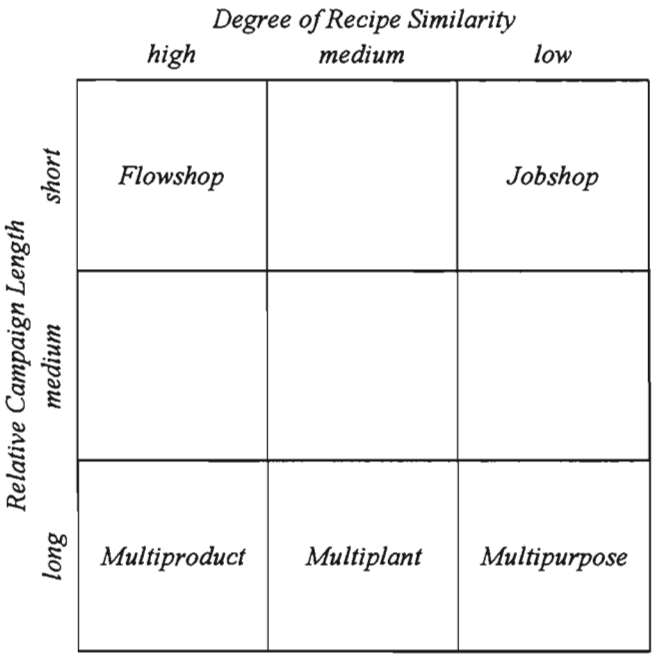

Figure 2.1: Operating strategy space

Lately four general concepts of multi-product plants have been developed: the standard multi-product plant (SMPP), the modular multi-product plant (MMPP), the multi-product plant with transfer panels (TMPP) and the pipeless plant (PP) [Teb97]. A characteristic in which the concepts differ is the flexibility. Three types of flexibility are especially important in this relation [FRS96]:

- structure flexibility - the ability of a system to adapt to changing functional demands by changing the connections between the elements of the system;
- assortment flexibility - the ability of a system to manufacture different products, without essential changes in the elements of the system;

- capacity flexibility - the ability to come up to changing demands in capacity.

The equipment of a standard multi-product plant is selected on the basis of a beforehand known range of products. As a result of the large amount of equipment needed to produce all kind of products, the utilization of some equipment might be very poorly. As with the conventional batch plant, all equipment is fixed and connected by pipelines, which brings about a low structure and capacity flexibility. The assortment flexibility on the other hand is very high.

Modular multi-product plants often consist of a fixed reactor. With modules (compact process equipment) it is possible to make a desired process layout around the fixed reactor. For this reason the modules usually are mobile. The modules are connected with pipes and standardized connection systems. Because the modules have to be mobile, the size of the equipment used is restricted. Due to the almost unlimited ways of building up process routes, the structure flexibility is high, however the capacity flexibility is low due to the limited size of the modules. The assortment flexibility is average.

Transfer panels are used to connect the equipment in a multi-product plant with transfer panels. Groups of equipment are connected with pipelines to these transfer panels, making it possible to interconnect almost all of the process equipment. A problem arising with the use of transfer panels is the inaccurate connection of equipment. The introduction of new equipment should be no problem, for it only has to be connected to the transfer panel. As a result of this, the TMPP has a high structure flexibility. A problem of the TMPP plant is the cleaning of the pipelines. Materials used in the plant have to be pumped easily and adequate solvents must be available. The multi-product plant with transfer panels has a high capacity flexibility combined with a moderate assortment flexibility.

In a Pipeless plant no pipelines are necessary to transport the materials from process operation to process operation. Mobile vessels containing the product transport the material from one cell to the other. The transport is mostly done by Automated Guided Vehicles (AGVs). A major problem occurring when using the pipeless plant concept is the connection of the pipelines and energy supplies between the mobile vessel and the fixed cell. Pipeless plants can be specially useful when a wide range of raw materials has to be used or if the materials are hard to be pumped. The range of readily available cells is somewhat limited, but efforts are made to expand the number of different cells. As a result of the limited number of available cells, the structure flexibility is low, but potentially high. The capacity flexibility is high because different kinds of mobile vessels can be used. The assortment flexibility of pipeless plants is high.

In Table 2.1 an overview concerning the different concepts and their degrees of flexibility is given. The multi-product plant with transfer panels seems to be the best concept. The structure flexibility of pipeless plants is low, but, as mentioned above, potentially high. This means that in future the pipeless plant might be the most flexible concept.

	Structure flexibility	Assortment flexibility	Capacity flexibility
SMP	−−	++	−−
MMPP	++	o	−
TMPP	++	o	++
PP	− (++)*	++	++

−− very low − low o average + high ++ very high
*good expectations in future

Table 2.1: An overview of the basic multi-product concepts

Chapter 3

Pipeless Plants

In Figure 3.1 an example of a pipeless plant is given. The pipeless batch process is intended to come towards the desired degree of flexibility and to minimize the piping. First some advantages of pipeless plants will be described. Furthermore both the qualitative and the quantitative design (optimization) is dealt with in this chapter. Because optimization of the design phase goes together with the optimization of the scheduling, this is treated together.

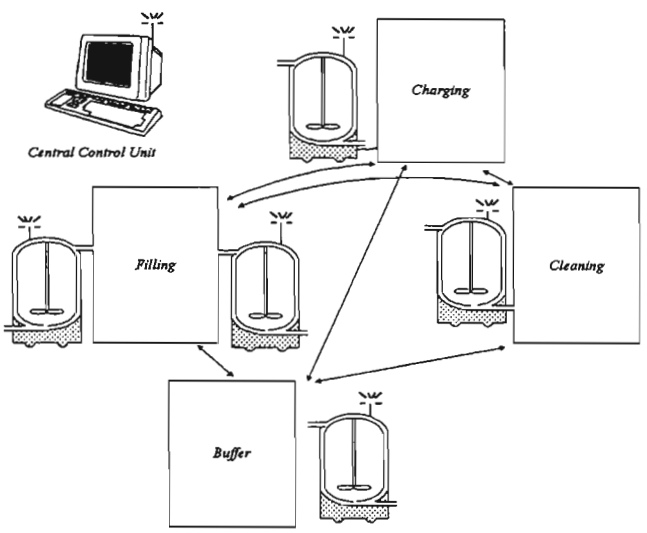

Figure 3.1: An example of a pipeless plant at a given moment

3.1 Qualitative Aspects of the Pipeless Plant

First of all it is obvious that the maze of piping is avoided when a pipeless plant is used. As a result of this one can prevent product contamination and pipe cleaning [Niw94]. Furthermore the different kinds of flexibility to which a pipeless plant comes up should be mentioned. The structure flexibility - the ability of a system to adapt to changing functional demands by changing the connections between the elements of the system - is very big in a pipeless plant, because only the route of the reactor changes. The ability of a system to manufacture different products, without essential changes in the elements of the system - the assortment flexibility - also is a big advantage of the pipeless plant. The same applies to the capacity flexibility - the ability to come up to changing demands in capacity. An additional benefit is that it is possible to get a new product onto the market in the shortest possible lead times [Niw93].

Another advantage is the safety aspect. Because the dosage is automated and therefore more accurate, just as the process control, the process can be controlled better than in conventional plants. Consequently it is not longer necessary to deploy a lot of people, even an unmanned plant belongs to the possibilities.

If a batch fails, the losses are less than in a conventional batch plant, simply because the batch sizes of the pipeless plant are usually smaller. As far as the equipment concerns, it can be said that the pipeless batch plant often requires smaller equipment, due to the smaller batch sizes. The pumps often are smaller too, because process materials have to be pumped over smaller distances.

Of course the pipeless plants brings disadvantages about too. One of them is the high costs of the reactors. They have to be leak proof, regardless of the number of connections. The positioning of the reactors is a very accurate process and therefore not very cheap. Another disadvantage is the constant supply of gas or liquid. When a gas or liquid has to be added constantly to a reactor, even when the reactor is transported from one cell to the other, it is almost inevitable to carry a tank with the reactor. Finally it can be said that the control signals, which often have to be sent wireless, have to be very reliable, which brings higher costs about. More about the control and transport can be found in the following section.

3.2 Qualitative Design of Pipeless Plants

As the pipeless plant has to be controlled centrally, control signals have to be sent from and to the vessels and the cells. Signals between the vessels and the central control unit might be given via the cells using optical wires or wireless directly to the vessels. In existing plants only emergency signals are transmitted wireless [Niw91]. The signals to and from the cells can be transmitted via wires. Mostly optical wires are applied, because the control signals have to be transmitted with a very high reliability.

To obtain a flexible plant, the conventional process-operations have to be redivided. Depending on the (expected) product-assortment, one conventional operation might be split up into two or more cells. When two or more operations are sequential for every product, they might be joined together in one cell.

Another important element in the design phase is the conveyance of the reactors. Generally spoken three basic concepts can be distinguished [Lin85]:

- unrestricted, completely free to move;
- area restricted, completely free to move within a certain area;
- line restricted, restricted to a certain track.

Unrestricted conveyance is the most flexible type of transport. The most important examples of unrestricted conveyance are trucks and automatic guided vehicles (AGVs). Only AGVs can operate without the intervention of people. In the case of area restricted conveyance one can think about cranes. The advantage of cranes is that vertical movements are almost as easy as horizontal movements. A big disadvantage is that two cranes operating in the same area easily might conflict. That is why cranes are not suitable for pipeless plants. The line restricted concept can be split up into circular and linear tracks. When a circular track is used, the cells are in a fixed order, which is anything but flexible. The most important examples of linear tracks are the conveyor and the on track AGV. The disadvantage of conveyors is that the speed of the vessels carried by the conveyor is not free to choose. In case of AGVs the speed is only limited to the maximum speed of the engine. On one track the first vessel (on a AGV) stands still while the other (on the same track) is moving. In the case of a conveyor this is not realizable.

In Figure 3.2 an overview of the different conveyance possibilities of vessels is given, as a function of the flexibility. The types of conveyance most suitable for application in pipeless plants are colored gray. When the plant has to be designed as flexible as possible, the choice for AGVs is obvious. Now a more detailed comparison can be made between on-track AGVs and off-track AGVs. Of course off-track AGVs are more flexible. The positioning of on-track AGVs is easy, while off-track AGVs require position control. Another point is that off-track AGVs are difficult to be made explosion-proof. This is because the AGVs are powered by batteries, and it is impossible to recharge them in an explosion-proof area. When the choice between on-track and off-track AGVs has been made, one have to choose whether the AGVs are built in the vessels or are separate from the vessels. The built-in AGV brings higher costs about when many vessels are used. A disadvantage from the separate AGV is the disconnection of the vessel and the AGV.

Therefore, the type of transport should be determined according to the products being manufactured in the plant. One should take into account that the mobile vessels might

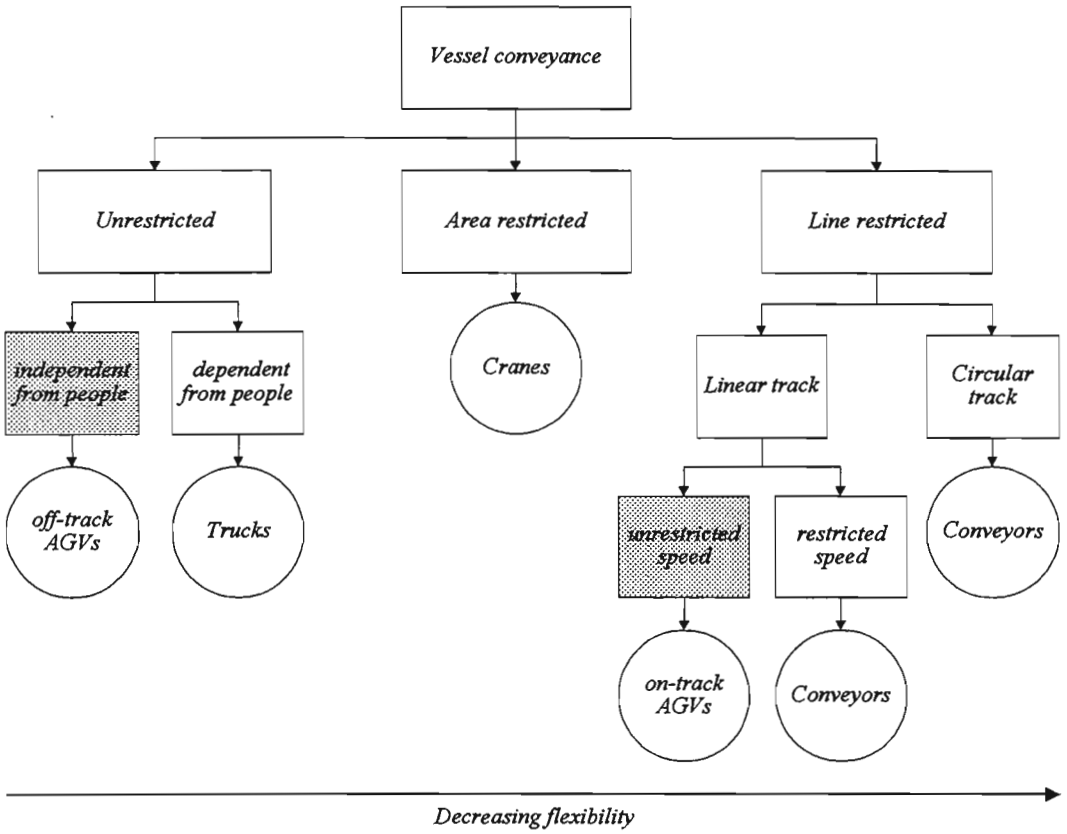

Figure 3.2: Types of conveyance and their flexibility

hamper each other. This can be prevented by using enough transportation area and making use of priority rules.

Because of the mobility of the vessels the cells must have a good accessibility. When a vessel is in the cell it has to be connected to the unit. This means that first of all an accurate positioning of the vessel is necessary. The power is either taken from the batteries the vessel is carrying or from the cell. In an explosion proof environment it is difficult to design a suitable connection for the last mentioned situation. Depending on the utilization various pipe-connections can be applied [Niw93]. When the pipes have to be used for powders, an inflation seal type connection should be applied. A sleeve type connection is best applied for nontoxic liquids, while leakproof connections (eventually with a lever-lock system) should be used for toxic or flammable liquids, because they pose problems if they leak. Fasten flange connections have to be applied when high pressure gasses have to be transported trough the pipelines. The different connection-type are made visual in Figure 3.3.

Another important aspect is the design of the vessel. It is possible to construct a lot

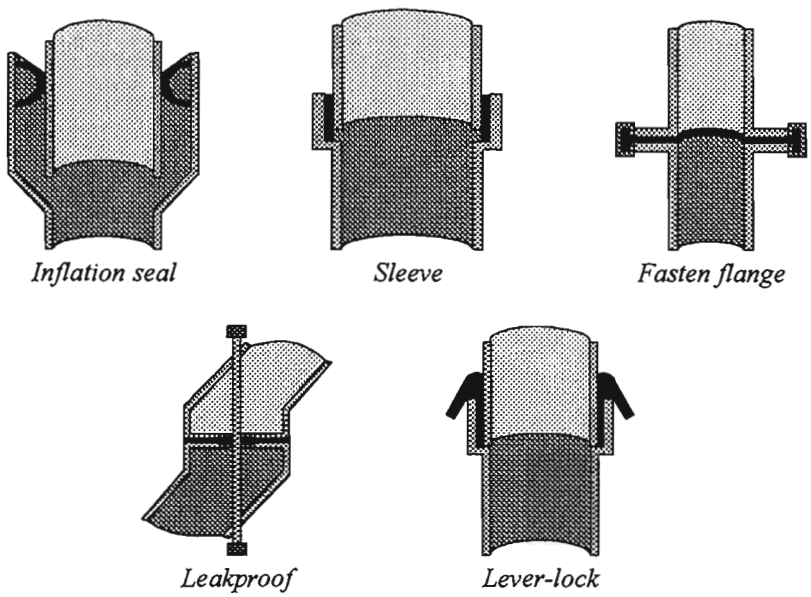

Figure 3.3: Different connection types

of operations in the vessel, like for example an agitator. For the heating of the vessel a steam-jacket can be used. Furthermore a consideration should be made to use a closed or an open vessel. In the latter case it is possible to work under pressures different from atmospheric pressure. When the vessel has to be made completely leak-proof, a magnetic agitator can be considered, which avoids expensive seals.

3.3 Optimization of Pipeless Plants

Since pipeless plants are concerned with multi-products, the scheduling of the plant has a large economical impact. In the design of a pipeless plant one comes across problems concerning the number of vessels and cells. More and more research is dedicated to the optimization of pipeless plants in both the design and the scheduling stage. This can be observed on the basis of the number of articles concerning this subject sent in lately. In this section some basic algorithms for design and scheduling are presented.

Most algorithms for this purpose are founded on linear programming (LP). LP assumes a linear objective function and linear constraints. The continuous decision variables are restricted to non-negative values. The most applied solution method is the simplex algorithm. In mixed-integer linear programming (MILP) problems a subset of the decision variables consists of integers. The solution of a MILP problem can be found using the branch-and-bound method [Van97]. Nonlinear programming (NLP) assumes a nonlinear objective function, nonlinear equations and nonlinear constraints. Using

sequential quadratic programming (SQP) or the reduced-gradient method a solution for NLP problems can be found [NS96]. When a subset of the decision variables of a NLP problem consists of integers, a mixed-integer non-linear programming (MINLP) problem is obtained. A MINLP problem can be solved by two methods: the generalized benders decomposition and the outer-approximation.

Scheduling can be dynamic or predictive [GR97b]. In the first case routing decisions are made progressively. Predictive scheduling can be necessary in case of zero-wait policy, and might result in very good utilization of resources. Disadvantages of predictive scheduling in comparison with dynamic scheduling are the rigid computations, not taken into account possible malfunctioning, and the complexity of the computations.

In the design of flowshops, and so a lot of conventional plants, the equipment size can be calculated using MINLP. When only standard equipment sizes are available and not continuous sizes as assumed in the latter case, MILP can be applied. When a mixed product campaign is used in a flowshop the scheduling can be optimized on the basis of NLP. In chemical industry it might be important that a product goes to the next operation without waiting, which is called zero-wait. When clean times are taken into account or zero-wait policies are used, the scheduling becomes more difficult. In this case so called cyclic scheduling has to be applied. Cyclic scheduling is a method in which cycle times play an important part [BGW97].

The scheduling of jobshops brings more difficulties about. The short-time scheduling of pipeless plants is described in [KPS93] and [PRS95]. On the basis of small examples, large MILP models are obtained making use of state-task networks (STNs). STNs are networks containing the batch operations ("tasks") and the stores, intermediate and final products ("states"). In case of pipeless plants not only in the scheduling phase optimization has to be applied, but also in the design phase, where the number of vessels and the number of units have to be determined. Because there are strong interactions between the design and layout of pipeless plants and the scheduling of the plant operations, as well as the utilization of the plant, those three stages should be involved in one optimization process [GR97a]. In Figure 3.4 the interactions between the three stages are made visible.

In the design stage the number of units and vessels, the layout of cells and the nominal demand can be determined on the basis of the product-recipes, the vessel and cell types and the potential demand over nominal horizon. Using the obtained data the vessel and cell utilization as well as the production quantities can be calculated. Unexpected events and parameter variation during simulation might lead to a new scheduling, which can influence the design phase because of the changed vessel and unit utilization.

A typical dynamic scheduling is obtained using dispatch rules. A dispatch rule is a routine that makes a decision about the next action to take, based on the current state of the system. In [GR97b] dispatch rules are applied on a pipeless plant. In comparison with MILP (predictive) scheduling, dispatch rules appear to perform poorly. After having included information from the MILP schedule, a better result is achieved.

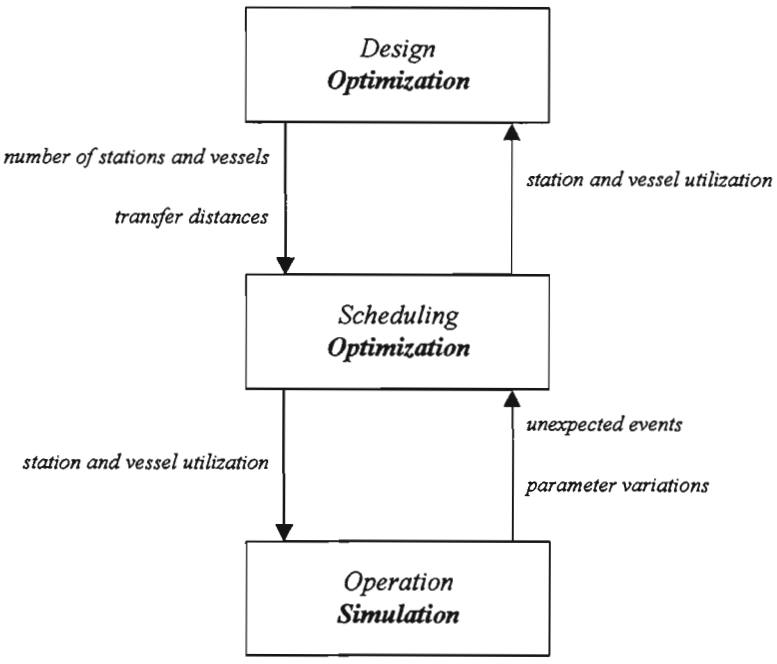

Figure 3.4: Simultanuous design, scheduling and operation

As the optimization in both design and scheduling phase appears to be very complicated, within the framework of this research most optimization is done on the basis of simulation. Dispatch rules have been applied in both the zero-wait case study and the FATGE-process. Nevertheless the use of MILP in both the scheduling and the design phase will most likely give better results.

Chapter 4

The Zero-wait Case Study

In order to compare the conventional batch plant with the pipeless batch plant, a type of process that is found often in the

chemical industry is tested on both kinds of plants. The process will be referred to as the zero-wait process and is a hypothetical example. In a zero-wait process the operations have to follow up each other immediately. This might occur when for example the product has to be dried immediately after the reaction is finished. In Figure 4.1 three Gantt charts are depicted, showing the three different transfer policies [BGW97]. The first one, zero-wait, was already explained above. The transfer policy with no intermediate storage,which means that the product can wait in the last process, when the following process is not available yet, leads to shorter cycle times, as can be seen in the picture. An unlimited storage (product can wait in buffers between operations) brings in the shortest cycle times. In this chapter only zero-wait transfer will be dealt with in the shape of both a conventional batch plant and a pipeless plant.

4.1 Description of the Process

The process is quite simple: first the product undergoes a reaction and then immediately afterwards a separation step (zero-wait). Four different products with different reaction and separation times are used. Only product 2 undergoes the complete procedure two times.

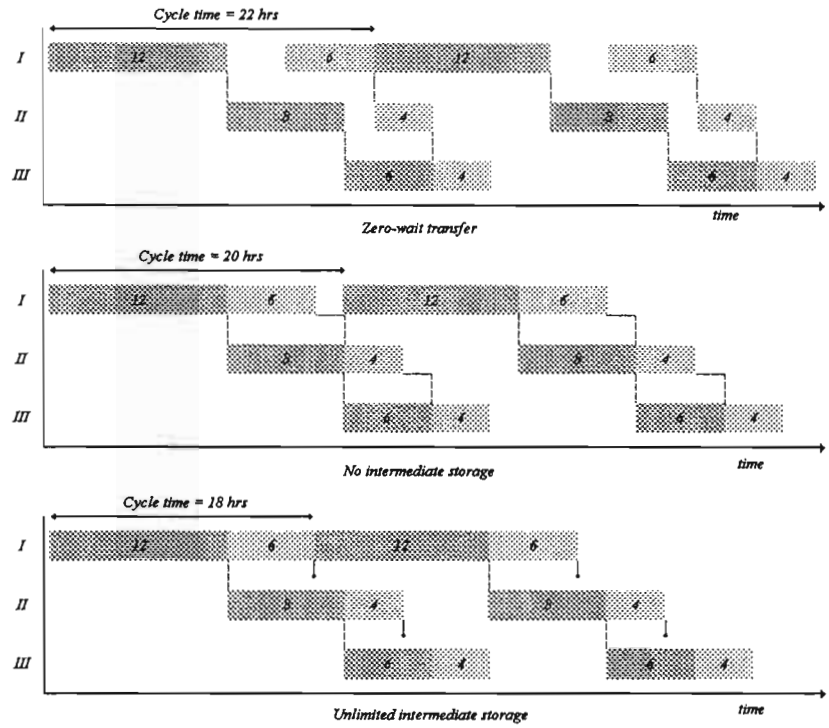

Figure 4.1: Transfer policies

4.2 Conventional Batch Plant

Description of the System

The conventional plant consists of a number of reactors and one separation section. When a product has left the reactor, the reactor has to be cleaned when a different product is about to enter the reactor. The number of reactors has been determined by means of debottlenecking. The system is most optimal when three reactors are used.

Model in χ

While the models are simplified representations of reality, and because the plant is invented by the authors, some assumptions and simplifications have been made:

- the reactions do not cause any changes in volume;
- during separation no changes in volume take place;

- buffers are assumed to have infinite capacity;
- transport time between different sections is negligible.

The conventional batch plant consists of three reactors and a separation section. Initially orders are sent by the combined order generator/WIP-controller G to the buffer B. From this buffer the products are sent to the reactors R. The final process the product undergoes is in the separation section S. The product is collected in the exit process E. In Figure 4.2 an iconic representation of the plant can be found.

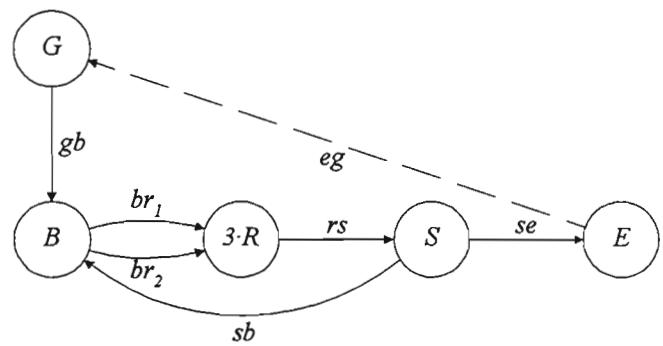

Figure 4.2: Iconic representation of the conventional batch plant

This model is designed so, that it is easy to introduce more reactors. This is done by using bundles, indexes and counters [Roo96]. The specification of the system is as follows:

syst $ZWCBP =$
$[\![\ G :: \text{Generator},\ B :: \text{Buffer},\ R :: \text{Reactor}^3,\ S :: \text{Separator},\ E :: \text{Exit}$
$,\ gb, eg, sb, se : !?\ \text{batch},\ br_1 : !?^3\ \text{prodnr},\ br_2, rs : !?^3\ \text{batch},\ i : \text{nat}$
$|\ G(gb, eg, w_{max}) \parallel B(gb, sb, br_1, br_2) \parallel$
$\parallel i : [0,3) : R.i(br_1.i, br_2.i, rs.i)$
$\parallel S(rs, se, sb) \parallel E(se, eg)$
$]\!]$

xper $= [\![\ ZWCBP\ ]\!]$

The types used in this model are defined below:

type	prodnr	= nat	Product-type
,	starttime	= real	Start-time
,	ordernr	= nat	order-number
,	firstrun	= bool	first run boolean
,	batch	= prodnr × starttime × ordernr × firstrun	

Process G generates the orders and is responsible for the maintenance of a constant WIP level. As long as the user defined WIP-level is not reached ($wip < wip_{max}$), process G generates an order, using a discrete uniform distribution. The order is sent to the buffer B ($gb!\langle \sigma\, v, \tau, n, \text{true}\rangle$). When a product leaves the plant, a signal is received from process E ($eg?$), after which the WIP level is adjusted.

$$
\begin{array}{l}
\textsf{proc Generator}(gb : !\,\text{batch},\ eg : ?\,\text{void},\ wip_{max} : \text{nat}) = \\
[\![\ v : \longrightarrow \text{int},\ n : \text{ordernr},\ wip : \text{nat} \\
|\ wip := 0;\ v := \text{dun}(0,4);\ n := 1 \\
;\ *[\ wip < wip_{max};\ gb!\langle \sigma\, v, \tau, n, \text{true}\rangle \longrightarrow wip := wip + 1;\ n := n + 1 \\
\quad [\!] \qquad\qquad ;\ eg? \qquad\qquad\quad \longrightarrow wip := wip - 1 \\
\quad] \\
]\!]
\end{array}
$$

Process B represents the buffer. Products are sent to the reactors when possible. Products are received from the order generator G ($gb?x$) or, in case of product 2, from the separation section ($sb?x$). When the wait-time has expired ($\Delta\, t_{sr} - \text{treac}(\text{hd}(xs).0) - \tau$), a product can be sent to the reactor ($send := \text{true}$). When the boolean $send$ is set true, a product is sent to the reactor which is empty ($br.i!\,\text{hd}(xs)$). The clean time t_c becomes 0.25 when a product was in the reactor different from the product. Finally the time on which the separation section is available (t_{sr}) is calculated.

$$
\begin{array}{l}
\textsf{proc Buffer}(gb, sb : ?\,\text{batch},\ br_1 : !^3\,\text{prodnr},\ br_2 : !^3\,\text{batch}) = \\
[\![\ x : \text{batch},\ xs : \text{batch}^*,\ t_{sr}, t_w : \text{real},\ i, j : \text{nat},\ send, ready : \text{bool} \\
|\ xs := [\,];\ t_{sr} := 0;\ p := \langle 5,5,5\rangle;\ t_c := 0;\ send := \text{false};\ ready := \text{false} \\
;\ *[\qquad\qquad gb?x \qquad\qquad\qquad\qquad \longrightarrow xs := xs +\!\!+ [x] \\
\quad [\!] \qquad\qquad sb?x \qquad\qquad\qquad\qquad \longrightarrow xs := xs +\!\!+ [x] \\
\quad [\!]\ \neg send \wedge \text{len}(xs) > 0;\ \Delta\, t_{sr} - \text{treac}(\text{hd}(xs).0) - \tau \longrightarrow send := \text{true} \\
\quad [\!]\ i : send \wedge \neg ready \quad ;\ br_2.i!\,\text{hd}(xs).0 \qquad\quad \longrightarrow ready := \text{true};\ j := i \\
\quad [\!]\ send \wedge ready \qquad ;\ br_1.j!\,\text{hd}(xs) \qquad\quad \longrightarrow xs := \text{tl}(xs) \\
\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\quad ;\ t_{sr} := \text{treac}(x.0) + \text{tsep}(x.0) + \tau \\
\quad] \\
]\!]
\end{array}
$$

Function treac returns the product dependent reaction time, while function tsep returns the separation time on the basis of the product:

$$
\begin{array}{l}
\textsf{func treac}(x : \text{int}) \rightarrow \text{real} = \\
|\ [\ x = 0 \longrightarrow 16 \\
\quad [\!]\ x = 1 \longrightarrow 14 \\
\quad [\!]\ x = 2 \longrightarrow 8 \\
\quad [\!]\ x = 3 \longrightarrow 6 \\
\quad] \\
]\!]
\end{array}
$$

```
func tsep(x : int) → real =
| [ x = 0 ⟶ 4
  [] x = 1 ⟶ 6
  [] x = 2 ⟶ 9
  [] x = 3 ⟶ 7
  ]
]|
```

Process R represents a reactor. First a product is received from the buffer ($br\_i_1 \,?\, x$). When the reaction is completed ($\Delta\,\text{treac}(x.0)$), a clean time t_c is computed if necessary. When the product is sent away ($rs\_i \,!\, x$), the reactor is cleaned ($\Delta\, ct$), after which the reactor is ready to receive a new batch.

```
proc Reactor(br_i1 : ? prodnr, br_i2 : ? batch, rs_i : ! batch) =
[| x : batch, p_n, p_o : prodnr, t_c : real
| p_o := 5
; *[ br_i1 ? p_n ;
   ; [ x.0 = p ∨ p = 5 ⟶ t_c := 0
     [] x.0 ≠ p ∧ p ≠ 5 ⟶ t_c := 0.25
     ]
   ; Δ t_c ; br_i2 ? x ; Δ treac(x.0) ; p := x.0
   ; rs_i ! x
   ]
|]
```

Process S represents the separation section. After a product is received from one of the reactors ($j : rs.j \,?\, x$), the wait time is calculated. While the separation time is stochastic, the product dependent separation time is added to a sample of a normal distribution. Now two things might occur: the wait time expires ($\Delta\, t_w - \tau$), or a new product enters the separation section ($j : rs.j \,?\, y$). In the latter case the part of the product that has not been processed yet is thrown away. When a product of type 2 was processed for the first time, (that is when $x.3$ is false), it is sent back to the buffer B ($sb \,!\, x$), else the product is sent to the exit process E ($se \,!\, x$).

```
proc Separator(rs ?^3 batch, se, sb : ! batch) =
[[ x, y : batch, b : bool, v : → real, tw : real, j : nat
| v := nor(0, 0.05); b := true
; *[ [ b  → [ j : rs.j ? x → skip ]
     [] ¬b → x := y
     ]
   ; t_w := tsep(x.0) + σ v + τ
   ; [ j : rs.j ? y → b := false
     [] Δ t_w − τ   → b := true
     ]
   ; [ ¬(x.0 = 2 ∧ ¬x.3) → se ! x
     [] x.0 = 2 ∧ ¬x.3   → x.3 := true; sb ! x
     ]
   ]
]]
```

In the exit process E the product is collected. The process is quite straightforward: after a product has been received ($se\,?\,x$), a signal $eg\,!$ is sent to the WIP-controller G indicating that a product has left the system.

```
proc Exit(se : ? batch, eg : ! void) =
[[ x : batch
| [ se ? x; eg ! ]
]]
```

4.3 Pipeless Plant

Description of the System

The pipeless plant consists of a reaction buffer and a separation section. The reaction buffer is a cell where a number of mobile reactors are processed at the same time. The separation section however can only process one batch at a time. Because the batches have become smaller, both the reaction and the separation times have become smaller.

Model in χ

While the models are simplified representations of reality, and because the plant is invented by the authors, the same assumptions and simplifications have been made as in the previous section. For reasons of clarity they are mentioned here again:

- the reactions do not cause any changes in volume;

- during separation no changes in volume take place;
- buffers are assumed to have infinite capacity;
- transport time between different sections is negligible.

The pipeless plant consists combined order generator/WIP-controller G. Orders are sent to the vessel buffer VB. Vessels are sent to the reaction buffer RB. Finally the product is separated in the separation section S and collected in the exit process E. In Figure 4.2 an iconic representation of the plant can be found. Because the bigger part of this model is almost the same as the model of the conventional batch plant (see Section 4.2), only the most important processes are described in this section. A complete description of the specification can be found in Appendix B.

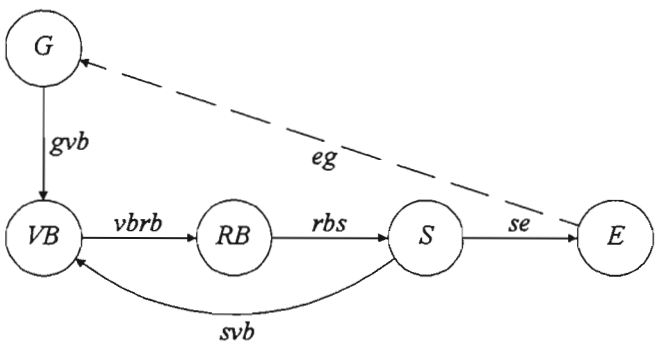

Figure 4.3: Iconic representation of the pipeless batch plant

In process VB, the vessel buffer, the vessels are waiting to be processed. When possible a vessel is sent to the reaction buffer RB. After a product is received from the order generator G ($gvb?x$) or from the separation section S ($svb?x$), the product is put into the list ($xs +\!\!+ [x]$). When vessels are waiting ($\text{len}(xs) > 0$), and it is possible to send a product to the next section ($\Delta\, t_{sr} - \tau - \text{treac}(\text{hd}(xs).0)$), the product is removed from the list ($x := \text{hd(xs)};\ xs := \text{tl}(xs)$) and sent to the reaction buffer RB ($vbrb!x$). Finally the time at which the separation section is ready is calculated ($t_{sr} := \tau + \text{treac}(x.0) + \text{tsep}(x.0)$).

$$
\begin{array}{l}
\textbf{proc}\ \text{VesselBuffer}(gvb, svb : ?\,\text{batch},\ vbrb : !\,\text{batch}) = \\
[\![\ x : \text{batch},\ xs : \text{batch}^*,\ t_{sr} : \text{real} \\
\mid\ xs := [];\ t_{sr} := 0 \\
;\ [\qquad\qquad gvb?x \qquad\qquad\qquad\qquad \longrightarrow x.3 := x.0 \neq 2;\ xs := xs +\!\!+ [x] \\
\ \ [] \qquad\qquad svb?x \qquad\qquad\qquad\qquad \longrightarrow xs := xs +\!\!+ [x] \\
\ \ [] \ \text{len}(xs) > 0;\ \Delta\, t_{sr} - \tau - \text{treac}(\text{hd}(xs).0) \longrightarrow x := \text{hd(xs)};\ xs := \text{tl}(xs) \\
\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad ;\ vbrb!x;\ t_{sr} := \tau + \text{treac}(x.0) + \text{tsep}(x.0) \\
\ \ ] \\
]\!]
\end{array}
$$

Process RB represents the reaction buffer. This is one cell where several vessels can be processed. When a vessel is received from the vessel buffer VB ($vbrb\,?\,x$), it is put in a sorted list, together with the time at which the reaction is completed ($rs := \text{insert}(rs, \langle x, \tau + \text{treac}(x.0)\rangle, \text{crit})$). The list is sorted so, that the product that is ready first, is on the head of the list. When the reaction time has expired ($\Delta\,\text{hd}(rs).1 - \tau$), the product is removed from the list ($x := \text{hd}(rs).0\,;\, rs := \text{tl}(rs)$) and sent to the separation section S ($rbs\,!\,x$).

$$
\begin{array}{l}
\textsf{proc ReactionBuffer}(vbrb : ?\,\text{batch},\ rbs : !\,\text{batch}) = \\
[\![\ rs : \text{reac}^*,\ x : \text{batch} \\
\mid\ rs := [\,] \\
;\ [\qquad\qquad vbrb\,?\,x \qquad\qquad \longrightarrow rs := \text{insert}(rs, \langle x, \tau + \text{treac}(x.0)\rangle, \text{crit}) \\
\quad [\!]\ \text{len}(rs) > 0\,;\ \Delta\,\text{hd}(rs).1 - \tau \longrightarrow x := \text{hd}(rs).0\,;\, rs := \text{tl}(rs)\,;\, rbs\,!\,x \\
\quad] \\
]\!]
\end{array}
$$

4.4 Simulation Results

In order to compare the conventional batch plant and the pipeless plant, four different simulation runs have been made, for both types of plants. First a mixed product campaign is applied, first with two products and after that the product assortment was expanded to four products. The same is done whit a single product campaign, for a campaign length of 100 batches. An extensive overview of the results can be found in Appendix C. In Table 4.1 a short description of the results is represented.

The batch size of the conventional batch plant was set to 100 liters independent from the type of product. The yield of the pipeless plant has to be as big as the yield of the conventional batch plant when an optimal WIP level is maintained, in order to get a good comparison of both kinds of plant. To obtain this goal a batch size of 47 liters is applied to the pipeless plant.

		w^* [# batches]	yield [ltr/hr]
Conv. batch plant	mixed product campaign - 2	3.8	18.6
	mixed product campaign - 4	2.5	10.8
	single product campaign - 2	3.5	17.7
	single product campaign - 4	2.4	11.0
Pipeless plant	mixed product campaign - 2	5.6	18.6
	mixed product campaign - 4	2.5	8.3
	single product campaign - 2	5.6	17.7
	single product campaign - 4	2.8	8.7

Table 4.1: Results of the zero wait case study

The reactors of the conventional plant have to be cleaned when product is changed. The cleaning time is set at 15 minutes. In the pipeless plant the reactors have to be cleaned at the end of the process, but this is left out of the model, because when a clean and empty reactor is always available, cleaning does not influence the results.

The results of the simulation runs will be discussed one by one:

- First the mixed product campaigns will be described. When 2 products are deployed in the conventional batch plant the yield is higher than when 4 products are brought into action. This is because the plant was optimized for products 1 and 2 only by debottlenecking. When products 3 and 4 are introduced to the plant, the separation section becomes the bottleneck. As a result of this the optimal WIP level becomes only 2.5, which means that the third reactor is used hardly or not. The pipeless plant shows a bigger decrease of the yield when the two extra products are deployed. The separation section is not occupied continuously, as can be seen in Figure 4.4, in contrast to the separation section of the conventional batch plant. When the batch-size is adapted, the yield can be optimized. In this case the pipeless plant is less favorable than the conventional batch plant. On

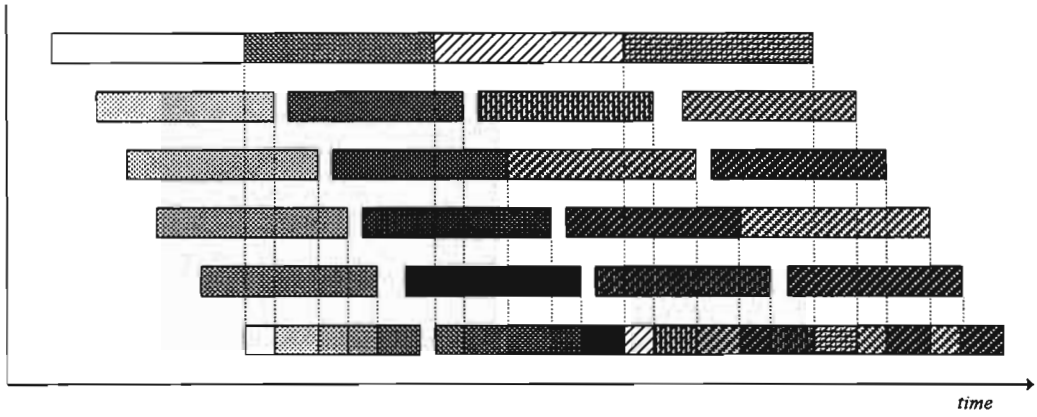

Figure 4.4: Gantt chart of pipeless plant, mixed product production, two products

the other hand, suppose only products 3 and 4 where deployed, and the pipeless plant was optimized so that the yields of both types of plants are equal. When now product 1 and 2 are brought into action as extra products, the pipeless plant is in the advantage. This is because the separation section is loaded less now.

- When the single product campaign is applied on both plants it can be seen that the results of the pipeless plant and the conventional batch plant are almost equal, when products 1 and 2 are deployed. This is just a coincidence. The yield of the pipeless plant decreases because the separation section is not occupied continuously, as can be seen in Figure 4.5. The conventional batch plant should

be faster now, because of the fact that the reactors have to be cleaned less. For the same reason as found for the pipeless plant, the yield decreases.

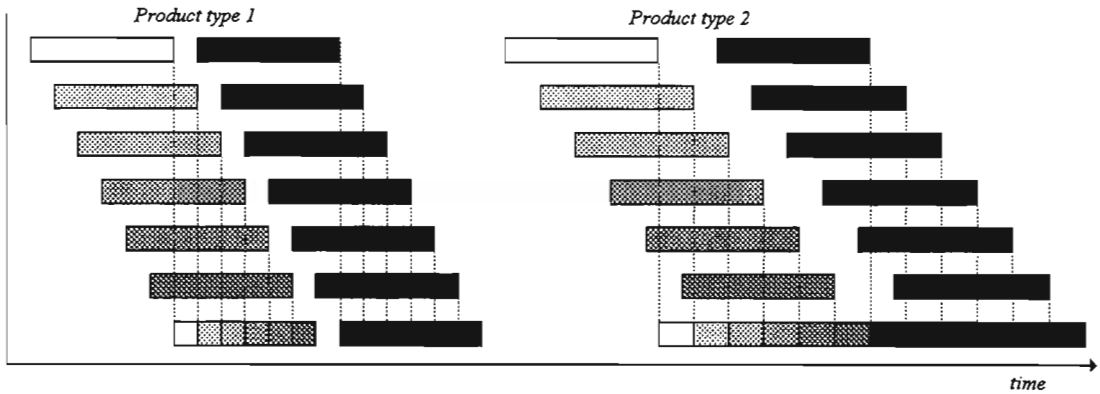

Figure 4.5: Gantt chart of pipeless plant, single product campaign, two products

When products 3 and 4 are introduced as extra products, the same story as told about the mixed product campaign applies.

4.5 Evaluation

As far as the control concerned, no big differences between pipeless and conventional batch plant can be found. For the design of the model this does not apply. Particularly the buffer of the conventional batch plant is a complicated process comparing to the other processes. This can be attributed to the choice in which reactor the product has to be put in. The products of the pipeless plant already are in their reactors, so no difficulties concerning that can occur.

From this case it becomes obvious that when first the complete product assortment is known the pipeless plant can be used optimal. When this is not possible, the choice between conventional and pipeless strongly depends on the bottleneck of the system.

In this case the bottleneck can be the separation section or the reaction section. Because the separation section is a conventional part of the pipeless plant (the product is put in the separation machine and is not in its reactor anymore), this section can not be optimized. In that case the conventional plant might be better, because the bigger batch sizes compensate partly for the losses made because of the bottleneck. When the bottleneck is the reaction section, the pipeless plant can be optimized and will be better than a conventional plant.

When no conventional elements exist in the pipeless plant, the plant can always be optimized.

The differences between single product campaign and mixed campaign strongly depend on the product recipes and the cleaning times, so that no conclusive view can be given about this subject. A big advantage of single product campaign is the ability to respond quickly to demands of the customer. One of the disadvantages of single product campaign in case of the conventional batch plant is the cleaning of the reactors during the process. In the pipeless plant cleaning can be done outside the production.

Chapter 5

The 'FATGE'-process

In order to obtain more qualitative information about the difference between pipeless plants and conventional batch plants, an existing process of DSM Andeno is specified. First a short description of the process will be given. After a description of the conventional process, a pipeless batch plant of the same process is designed. Both variants are specified in χ as described in Section 5.2. On the basis of those specifications some were simulations executed, from which the results will be discussed at the end of this chapter.

5.1 Description of the Process

The intermediate 2-formylaminothiazolyl-4-glyoxylic acid ethyl ester ('FAT-Glyoxylic acid Ester' or 'FATGE'), is prepared by the manganese-catalyzed air oxidation of 'FATA-Ester' [PTR90]. The reaction scheme of the main-process is presented in Figure 5.1.

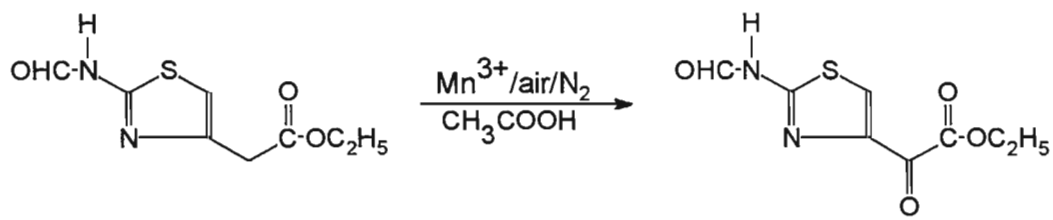

Figure 5.1: Reaction scheme of the 'FATGE' process

First manganese diacetate tetrahydrate and acetic anhydride in acetic acid are heated to reflux. After having cooled down the suspension, potassium permanganate is added in small portions and held at reflux. The obtained catalyst solution is cooled and the 'FATA-Ester' is added. Air is spouted through the mixture continuously. To keep

the reaction system out of the explosion range, nitrogen is blown through the reaction mixture at the same time. When the reaction is nearly complete a second quantity of 'FATA-Ester' is charged. After a while 'FATGE' crystallizes from the reaction mixture. When the reaction is complete, the product is isolated by centrifugation, where it is washed successively with acetic acid, water and acetone. Finally the product is dried.

5.2 Conventional Batch Plant

Description of the System

In this section a description of the conventional 'FATGE' process is given. A more accurate description of the process can be found in Appendix D. In Figure 5.2 a process flow scheme of the conventional 'FATGE' process is given as used for this research. The product flow is as follows: First raw materials are added into the glass lined reactor. The glass condensers export the escaping gasses. After the reaction, the product is put in the centrifuge. After that operation, the main product (the 'FATGE') is sent to the vacuum drier. The remainder is pumped via a glass lined tank into the distiller, represented by a glass lined tank with a glass condenser. The first part of the distillate, the primary cut, is sent back to the glass lined tank to be processed with the next batch, while the second part (the main cut) is collected for further recycling. The suspension that is still in the tank is sent to neutralization.

The glass lined reactor is supposed to be empty and clean. Acetic acid is added. The next step is the addition of manganese-(II)-acetate,tetrahydride, which has to be done while the agitator and the nitrogen-flow are turned on. Now the acetic anhydride can be added, also with the nitrogen-flow turned on. The reaction mixture is heated to reflux and held at reflux for a while. Then the product is cooled down, while a high nitrogen-flow is applied. When the desired temperature is reached, the potassium permanganate is added in small portions. After having stirred and ventilated with nitrogen for a while, the product is heated to reflux as quickly as possible and held at reflux for a certain time. When the product mixture is cooled down (nitrogen flow turned on), the 'FATA-Ester' can be added. Now air is blown into the reactor for a long time through a dip pipe. To prevent from explosion, the nitrogen flow has to be turned on, in order to keep the oxygen-degree under a safe percentage. To obtain a homogenous reaction the agitator has to be turned on. After a long time the next batch 'FATA-Ester' is added, after which the same conditions are valid as for the first batch. When the reaction is complete, the product is cooled down. The reaction mixture is dried in a spindrier. Every portion has to be washed with acetic acid, city water and acetone. Finally the product is dried in a vacuum spin drier.

Meanwhile the acetic acid mother liquors are distilled in the AcOH recovery. The first part will be distilled with the next motherbatch, the second part is collected for further recycling, while the remainder is abandoned in the neutralization.

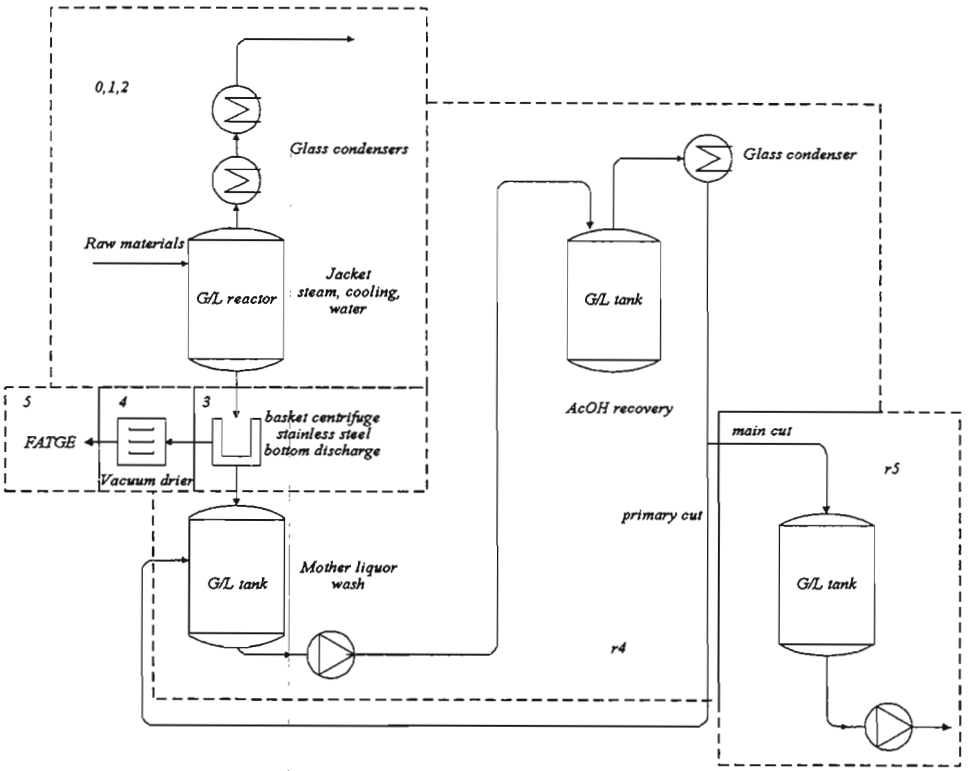

Figure 5.2: Process-flow of the conventional 'FATGE' process

Models in χ

In order to compare the conventional and the pipeless batch plant, models are designed so, that they are as much the same as possible. The same recipes r_1, r_2 and r_r can be applied in both models. The models are very simple compared to reality. The processes are represented by their time-duration only. All events are modeled discrete. Changes in volume, for example, only occur when the accompanying process has been finished. Assumptions made for the models are:

- Transport always takes the same time, regardless of the next destination of the product.
- All apparatuses are supposed to work properly.
- The capacity of the apparatuses is big enough to process one entire batch at a time.

System *CBP* consists of a combined order-generator/WIP-controller G, a reactor R, a junction controller J, three operation sections O and two exit-processes E. An iconic

representation of the system is given in Figure 5.3. In this figure it can also be seen that system O is built of two processes: process B representing storage tanks, and process P, representing the actual process operation.

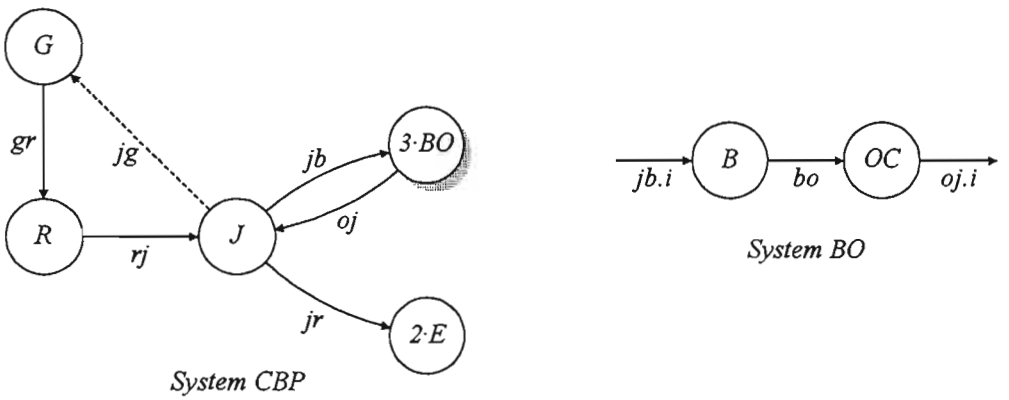

Figure 5.3: Iconic representation of system *CBP*

The declaration of the system is as follows:

$$
\begin{array}{l}
\textsf{syst } CBP = \\
[\![\ G :: \text{Generator},\ R :: \text{Reactor},\ J :: \text{Junction},\ E :: \text{Exit}^2,\ BO :: \text{Cell}^3 \\
,\ gr, rj : !\,?\ \text{product},\ oj, jb\,!?^3\ \text{product},\ je : !\,?^2\ \text{product},\ jg : {}^{\sim},\ i, j : \text{nat} \\
|\ G(jg, gr, w_{max}) \parallel R(gr, rj) \parallel J(rj, oj, je, jb, jg) \\
\parallel i : [0,2) : E.i(je.i) \\
\parallel j : [0,3) : O.j(jb.j, oj.j) \\
]\!]
\end{array}
$$

$$
\textsf{xper } = [\![\ CBP\ ]\!]
$$

The types used in the specifications is as follows:

type	ordernr	= nat	serial number
,	starttime	= real	time at which an order is generated
,	vol	= real	volume of product
,	opnr	= nat	operation number
,	proctime	= real	process-time
,	volchange	= real	change in volume
,	operation	= opnr × proctime × volchange	
,	recipe	= operation*	
,	ptype	= int	type of product
,	product	= recipe × vol × starttime × ordernr × ptype	

As can be seen in the type-declaration, a recipe consists of a list of operations and is product specific. In this case recipes for two different products are described (r_1 and r_2). Recipe r_r is meant for the recycling of acetic acid. As can be seen in the type-declaration, a recipe consists of operations. The first element of the operation indicates which operation has to be undergone. In Table 5.1 the corresponding operations numbers are described. The numbers can be found back in the process flow of the 'FATGE'-plant, Figure 5.2.

opnr	operation	acetic acid recovery
0	filling	
1	refluxing	
2	oxidation reaction	
3	drying (centrifuge)	
4	vacuum drying	distillation
5		to exit-tank

Table 5.1: Operation numbers and the accompanying operations

An example of the recipes as used for the simulations can be found below:

$$
\begin{aligned}
\textsf{const}\ \ r_1 = {} & [\langle 0,75,1467\rangle, \langle 1,130,0\rangle, \langle 0,25,8\rangle, \langle 1,290,0\rangle, \langle 0,5,40\rangle, \langle 2,480,0\rangle \\
& , \langle 0,20,40\rangle, \langle 2,1015,0\rangle, \langle 3,215,-1476\rangle, \langle 4,630,-12\rangle \\
&] \\
,\quad r_2 = {} & [\langle 0,75,1467\rangle, \langle 1,130,0\rangle, \langle 0,25,8\rangle, \langle 1,290,0\rangle, \langle 0,5,40\rangle, \langle 2,480,0\rangle \\
& , \langle 0,20,40\rangle, \langle 2,1015,0\rangle, \langle 3,215,-1476\rangle, \langle 4,630,-12\rangle \\
&] \\
,\quad r_r = {} & [\langle 4,475,-876\rangle, \langle 5,0,0\rangle]
\end{aligned}
$$

Process G represents a combined order-generator/WIP-controller. As long as the WIP-level, which is defined by the user, is not reached ($wip > 0$), an order is generated. The product-type is determined by a discrete uniform distribution (in this case: dun$(0,2)$). When a product has left the system, a signal ($jg?$) is received from the junction-controller.

$$
\begin{aligned}
&\textsf{proc}\ \text{Generator}(jg : ?\,\text{void},\ gr : !\,\text{product},\ wip_{max} : \text{nat}) = \\
&[\![\ wip : \text{nat},\ r : \text{recipe},\ rt : \text{recipe}^2,\ v : \longrightarrow \text{int},\ s : \text{ptype},\ n : \text{ordernr} \\
&|\ n := 1;\ v := \text{dun}(0,2);\ rt := \langle r_1, r_2\rangle;\ wip := 0 \\
&;\ s := \sigma\, v;\ r := rt.s \\
&;\ *[\ wip < wip_{max};\ gr\,!\,\langle r, 0, \tau, n, s\rangle \longrightarrow n := n+1;\ wip := wip+1;\ s := \sigma\, v;\ r := rt.s \\
&\quad [\!]\qquad\qquad jg?\qquad\qquad \longrightarrow wip := wip - 1 \\
&\quad] \\
&]\!]
\end{aligned}
$$

Process R represents the reactor, where the filling, the refluxing and the oxidation reactions take place. First the product enters the reactor ($gr\,?\,x$). As long as the operation-number agrees with an operation that takes place in the reactor ($x.0.0 < 3$), the operation is carried out ($\Delta\, r.1$). After having adapted the volume ($x.1 := x.1 + r.2$), the first element of the recipe is removed ($x.0 := \mathrm{tl}(x.0)$).Now the next operation can take place. The product is sent out of the reactor ($rj\,!\,x$) when the operation number of the following route exceeds 2.

```
proc Reactor(gr : ? product, rj : ! product) =
[[ x : product, r : operation
| *[ gr ? x; *[ x.0.0 < 3 ⟶ r := hd(x.0); Δ r.1; x.1 := x.1 + r.2; x.0 := tl(x.0) ]
   ; rj ! x
   ]
]]
```

Process J, the junction controller, is the most complicated process of the system. In this process it is estimated where the product has to go to. After having received a product from the reactor ($rj\,?\,x$) or from an other operation ($j : oj.j\,?\,x$), the product is put at the end of a list, together with the time the product will arrive at the next cell ($ys := ys +\!\!+ \langle x, \tau + 5 \rangle$). The transport trough the pipelines is assumed to last 5 minutes. When this transportation time has expired ($\Delta\, \mathrm{hd}(ys).1 - \tau$), the product is sent to the next cell. When the recipe is empty ($\mathrm{len}(x.0) = 0$), the product is ready, so that it can be sent to the exit-process ($je.0\,!\,x$). Because the product has left the system now, a signal to the WIP-controller is sent ($jg\,!$), indicating that the WIP-level has to be adjusted. When the recipe is not empty, it depends on the first element of the first route, where to sent the product to ($r := x.0.0$). In the case that $r = 4$, the main-product is sent to the drier ($jo.1\,!\,x$), while the remainder is sent to the acetic acid recycling (represented by $r4$ in Figure 5.2), after having adapted the volume and the recipe ($x.0 := r_\tau$; $x.1 := 1976$; $jo.2\,!\,x$). Finally the element is removed from the list ($ys := \mathrm{tl}(ys)$).

```
proc Junction( rj : ? product, oj : ?^3 product
             , je : !^2 product, jo : !^3 product
             , jg : ! void
             ) =
[[ x : product, ys : ⟨product × proctime⟩, r : ws
```

```
| ys := []
; *[                    rj ? x              ⟶ ys := ys ++ ⟨x, τ + 5⟩
  [] j :                oj.j ? x            ⟶ ys := ys ++ ⟨x, τ + 5⟩
  []     len(ys) > 0  ; Δ hd(ys).1 − τ      ⟶ x := hd(ys).0
                                             ; [ len(x.0) = 0 ⟶ je.0 ! x ; jg !
                                               [] len(x.0) > 0 ⟶ r := hd(x.0)
                                                                 ; [ r = 3 ⟶ jo.0 ! x
                                                                   [] r = 4 ⟶ jo.1 ! x
                                                                               ; x.0 := r_τ
                                                                               ; x.1 := 1976
                                                                               ; jo.2 ! x
                                                                   [] r = 5 ⟶ je.1 ! x
                                                                   ]
                                               ]
                                             ; ys := tl(ys)
  ]
||
```

Process E, the exit-process is valid for both the main product and the acetic acid that is to be recovered . The process is quite straightforward: it only receives a product from the junction controller J. The contents of product x can be used for calculation of for example lead times and throughput (not specificated here).

```
proc Exit(je : ? product) =
|[ x : product
| *[ je ? x ]
]|
```

System O represents an operation unit, consisting of storage-tanks, brought together in process B, and one operation process P.

```
syst Cell(jb : ? product, oj : ! product) =
|[ BT :: BufferTanks, O :: Operation, bo : product
| BT(jb, bp) || O(bp, pj)
]|
```

In process BT the storage tanks of the process operation are modeled. When a product is received ($jb ? x$), it is put in at the back of the list ($xs := xs ++ [x]$). As long as the list is not empty, the process tries to send a product to the process operation O ($\text{len}(xs) > 0$; $bp ! \text{hd}(xs)$), after which the list is updated ($xs := \text{tl}(xs)$). For the pumping from and to the tanks no delay is taken into account, because this time is used in the operations.

```
proc Buffer(jb : ? product, bp : ! product) =
[[ x : product, xs : product*
| [                jb ? x          ⟶ xs := xs ++ [x]
  [] len(xs) > 0; bp ! hd(xs) ⟶ xs := tl(xs)
  ]
]]
```

Process O is the actual operation process, as indicated by its operation number, which can be found in Table 5.1. After a product is received ($bp\,?\,x$), the operation is started. When the operation is ready ($\Delta\, r.1$), the volume is adapted ($x.1 := x.1 + r.2$). After the recipe has been updated, the product is sent back to the junction controller J ($pj\,!\,x$).

```
proc Operation(bp : ? product, pj : ! product) =
[[ x : product, r : route
| *[ bp ? x; r := hd(x.0); Δ r.1
   ; x.1 := x.1 + r.2; x.0 := tl(x.0); pj ! x
   ]
]]
```

5.3 Pipeless Batch Plant

Description of the System

For the design of a pipeless 'FATGE' batch plant, a very important choice is the redivision of the processes. This is often a dilemma: to obtain maximal flexibility a fine division is desired, while the design is easier when assigning all functions to one cell. In Figure 5.4 the different process steps are pictured.

The first choice was to make a filling cell, where all different products can be added. This choice was made for reasons of flexibility: when a new product is introduced, only the filling cell needs to be adapted, not the other cells, at least as far as the addition of material is concerned. Step 5,6 and 7 have been combined in one reflux cell. This is because of the fact that heating to reflux and holding at reflux demand the same equipment. The cooling of the vessel is added to this cell, because it brings only a small adaptation of the cell about. Furthermore it often occurs that the cooling unit has to be turned on, to adjust the temperature. Step 7, agitating, can be done in the reflux cell too. For the actual reaction (which occurs two times: in step 14 and 16) one cell is allocated, because a connection for air supply is needed. Step 17 (cooling down) can be done in the same cell, because the necessary equipment is present yet. Centrifuging and washing occur on the same time, and thus have to be allocated in one work cell. The vacuum drier forms one cell. The same applies for the distiller. A problem occurring is the addition of nitrogen. According to the log-sheets of the original process, nitrogen has to be added constantly for example between step 7 and 9, while the steps are allocated in

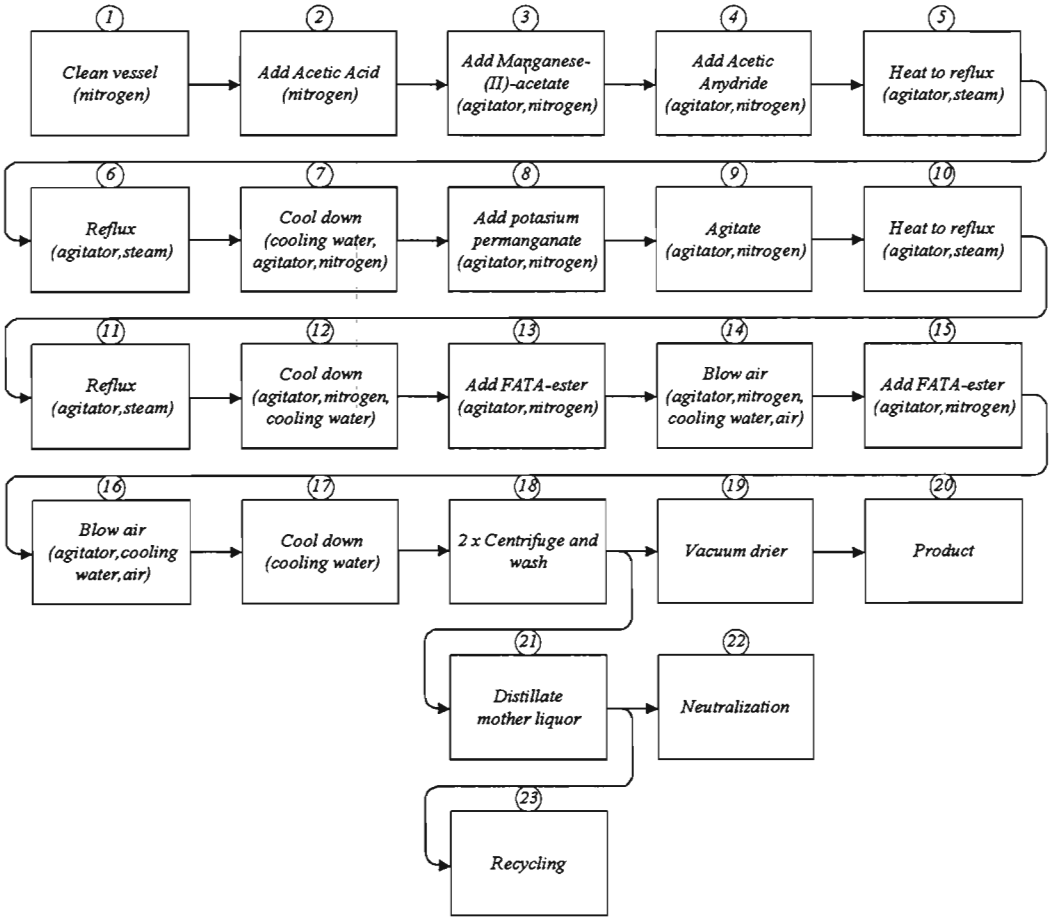

Figure 5.4: Analyzed process steps

different cells, which means that the vessels have to be transported. Supplying nitrogen to the vessel during transport can be done in two different ways: connecting the vessel via a flexible pipe to a nitrogen supplier or carrying the supplier with the vessel. The first solution is difficult to realize because the vessels drive all over, so that the pipes might be confused. The second solution is difficult to realize because flows of 50 to 70 [m^3/hr] have to be realized, which means that a very big reservoir is needed, under high pressure. Fortunately it appears that the nitrogen flow is not necessary. In the conventional process it is applied to keep the oxygen volume percentage under a certain value. When the vessel is designed leak-proof, and in the vessel is an overpressure, the oxygen volume percentage will stay at a certain value. Designing the vessel leak-proof means the applying of leak-proof connections (as discussed in Section 3.2). Of course it is possible to design leak-proof conventional reactors too. The drive shaft of an agitator does not bring leaks about, when a magnetic agitator is applied. When the oxygen

volume percentage exceeds a certain value, the vessel can be brought to an 'emergency' cell, with a fixed nitrogen supply unit.

The possible transportation techniques have already been discussed in Section 3.2. Because a high degree of flexibility is demanded, the AGVs are preferred. The use of a conveyor is dissuaded from, because of the job-shop layout of the pipeless plant. The choice between vessels fixed on or separate from the AGVs is not important for the model and depends on the costs and possible expansions of the plant. The same applies for the choice between on-track and off-track AGVs.

Model in χ

The specification of the pipeless 'FATGE' plant in χ looks a lot like the specification of the conventional plant. This is a result of the fact, that the transport and the operations are not modelled at a big grain size. Transport using vessels looks a lot like transport through pipelines at this level. The same applies for the operations. The actual operation of a pipeless plant is represented by a delta-command, the same is valid for the model of the conventional batch plant. A big difference between the two models is the reactor R of the conventional batch plant, which is replaced by three cells in the pipeless plant. As every cell consists of different units, while the operation processes of the conventional batch plant consist of simply one unit, the process representing the cell has changed the most. Therefore only this process will be dealt with in this section. A complete specification of this model can be found in Appendix E.

The assumptions specifically made for this model are:

- the AGVs are supposed not to hinder each other;
- the number of vessels in the entire system is always big enough to come up to the demands.

As can be seen in the iconic representation of the model (Figure 5.5), the system consists of a combined order-generator/WIP-controller G, a transport controller T, comparable with the junction controller J of the conventional process, two exit-processes E and six cells C, comparable with the operation units O of the conventional process. A cell consists of a buffer B, where vessels waiting to be processed are parked, and the actual process cell OC. The operation cell OC consists of a number of units, and is therefore able to process more than one vessel at the same time.

When the number of vessels in the process cell is smaller than the maximum ($n < nr$), the process is able to receive a vessel ($bp\,?\,x$). A product is put in a list ($ys := \text{insert}(ys, \langle x, \tau + x.0.1\rangle/\text{conv}(pr, f), \text{crit})$), sorted at the finishing-time of the process ($\tau + x.0.1$). When the processing-time has expired ($\Delta\,\text{hd}(ys).1 - \tau$), the volume and the recipe of the vessel are adjusted ($x.1 := x.1 + x.0.0.2/f$; $x.0 := \text{tl}(x.0)$). Then

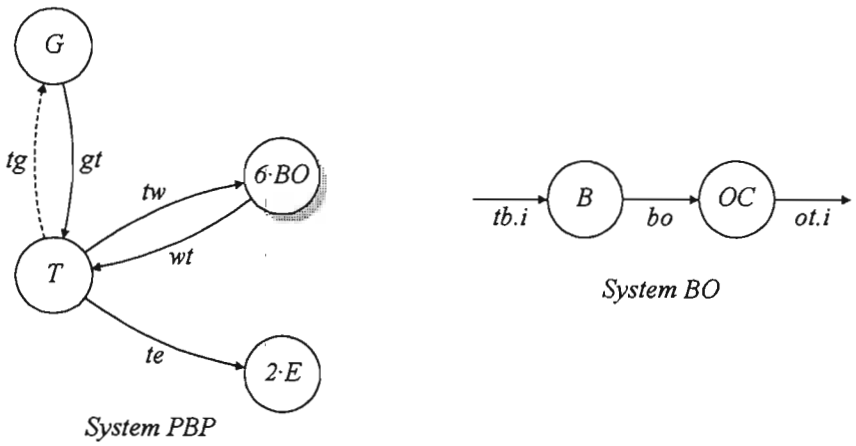

Figure 5.5: Iconic representation of system *PBP*

the product is sent back to the transport controller T $(pt\,!\,x)$, after which the list is updated $(ys := \mathrm{tl}(ys))$.

$$
\begin{array}{l}
\textsf{proc}\ \mathrm{OperationCell}(bp : ?\,\mathrm{vessel},\ pt : !\,\mathrm{vessel},\ nr : \mathrm{nat},\ f : \mathrm{real},\ pr : \mathrm{nat}) = \\
[\![\ x : \mathrm{vessel},\ ys : \langle \mathrm{vessel} \times \mathrm{proctime} \rangle,\ n : \mathrm{nat} \\
\mid\ ys := [\,];\ n := 0 \\
;\ *[\ n < nr \quad ;\ bp\,?\,x \qquad\qquad \longrightarrow ys := \mathrm{insert}(ys, \langle x, \tau + x.0.1/\mathrm{conv}(pr, f) \rangle, \mathrm{crit}) \\
\qquad\qquad\qquad\qquad\qquad\quad ;\ n := n + 1 \\
\quad [\!]\ \mathrm{len}(ys) > 0;\ \Delta\,\mathrm{hd}(ys).1 - \tau \longrightarrow x := \mathrm{hd}(ys).0;\ x.1 := x.1 + \mathrm{hd}(x.0)/f \\
\qquad\qquad\qquad\qquad\qquad\quad ;\ x.0 := \mathrm{tl}(x.0);\ pt\,!\,x;\ ys := \mathrm{tl}(ys);\ n := n - 1 \\
\quad] \\
]\!]
\end{array}
$$

The function crit is applied for the insertion of products in a sorted list. This function is defined as follows:

$$
\begin{array}{l}
\textsf{func}\ \mathrm{crit}(x, y : \langle \mathrm{product} \times \mathrm{proctime} \rangle) \rightarrow = \mathrm{bool} \\
[\![\ \uparrow x.1 \leq y.1\ ]\!]
\end{array}
$$

The function conv is needed to convert the process time indicated in the recipe to the real process time. Only in the case of the drier and the distiller the process time is divided by the user-defined factor f. This factor represents the ratio of the batch volumes of the conventional process and the pipeless process. When the natural pr is 0, the operation is batch size independent, when pr is 1, the factor f has to be applied.

```
func conv(pr : nat, f : real) → real =
|[ [ pr = 0 ⟶ ↑1
  [] pr = 1 ⟶ ↑f
  ]
]|
```

5.4 Simulation Results

In order to compare both types of plants with each other, the yield of the pipeless batch pants is set equal to that of the conventional batch plant. The yield of product 1 (the 'FATGE') is 11.12 [ltr/hr]. The pipeless plant has to be optimized for this production. On the basis of the greatest common divisor of the operation times, the number of units of each cell is calculated. This means that a cell with a long operation time consists of more units than a cell with a short operation time. Since the process times of the spindrier and the distillation section depend on the batch-size, the following iterative calculation method is applied. The reactors of the pipeless plant are smaller than the reactors of the conventional batch plant, so that a factor is applied, in order to keep the same recipes. Initially a factor 10 is assumed, which means that the batches of the pipeless plant are 10 times smaller than the batches of the conventional plant. After having determined the optimal WIP level, using the method as described in Appendix A, the yield of product 1 is determined, after which the factor is changed in order to obtain the same yield as in the case of the conventional batch plant. Now the number of units per cell is determined again, and the cycle starts again. When finally the yield of the pipeless plant is equal to the yield of the conventional batch plant, the optimal WIP level is 10, while the volume factor is 7.74. The number of units per cell can be found in Table 5.2. An extended overview of the results can be found in Appendix F.

cell	Filling	Reflux	Air	Centrifuge	Spin Drier	Distilation
units	1	2	6	1	1	1

Table 5.2: Number of units per cell

In order to determine the influence of an extra product on both plants, a fictitious product is brought into action. The product is almost the same as product 1, the 'FATGE', except for the vacuum drying time, which has been doubled. The recipe for this product, further referred to as product 2, is as follows:

$$
\begin{aligned}
r_2 = [\ & \langle 0,75,1467\rangle, \langle 1,130,0\rangle, \langle 0,25,8\rangle, \langle 2,480,0\rangle, \langle 0,5,40\rangle, \langle 1,290,0\rangle \\
, \ & \langle 0,20,40\rangle, \langle 2,1015,0\rangle, \langle 3,215,-1476\rangle, \langle 4,1230,-12\rangle \\
]
\end{aligned}
$$

For both the pipeless plant and the conventional batch plant three simulations have been made. In the first run only product 1 is brought into action, in the second run only product 2. In the third run both products are produced, maintaining a ratio 1:1.

The results of the three runs with the conventional batch plant can be found in Table 5.3.

Conventional Batch Plant			
product	w* [# batches]	yield 1 [m^3/hr]	yield 2 [m^3/hr]
1	1.42	1.993	0
2	1.72	0	1.969
1&2	1.57	1.007	0.960

Table 5.3: Results of the conventional batch plant for product 1 and 2

The optimal WIP level is higher when only product 2 is deployed than when only product 1 is brought into action. This is due to the higher flow time of product 2, when a low WIP level is applied. The optimal WIP level in the case where both products are deployed lies between the two other optimal WIP levels. The explanation for this is as follows: the maximum throughput of both products is the same, while they both have the same bottleneck. The minimum flow time of product 1 is lower than the minimum flow time of product 2, the difference is exactly 630 minutes. When both products are deployed in the same run, the maximum throughput is still the same, irrespective of the ratio. The minimum flow time however depends on the ratio the products are deployed at. In this case the ratio is 1:1, so the minimum flow time, and so the optimal WIP level, is exactly the average of the results of the first two runs.

The same product is applied to the pipeless plant. The results of the simulations can be found in Table 5.4.

Pipeless Batch Plant			
product	w* [# batches]	yield 1 [m^3/hr]	yield 2 [m^3/hr]
1	10.02	2.012	0
2	10.35	0	2.028
1&2	10.18	1.06	1.00

Table 5.4: Results of the pipeless plant for product 1 and 2

As can be seen no big differences comparing to the conventional batch plant are obtained. This is because the plant is optimized for product 1, where the degree of occupation of the vacuum drier was only 32 %. When product 2 is deployed, this value becomes 64, because product 2 stays twice as long in the vacuum drier as product 1, so the degree of occupation is twice as big. When both products are deployed, the degree of occupation of the vacuum drier lays between the two earlier found values, because the ratio is 1:1, which means that product 1 is produced as much as product 2. An overview of the degrees of occupation of cells during the three runs can be found in Table 5.5.

Since the conventional batch plant and the pipeless plant have different bottlenecks, it is useful to look at the following product:

product	w* [# batches]	Filling	Reflux	Air	Centrifuge	Vacuum Drier	Distillation
1	10.02	49	81	96	83	32	24
2	10.35	48	80	95	82	64	24
1&2	10.18	49	82	96	83	48	24

Table 5.5: Degrees of occupation of the pipeless plant for product 1 and 2

$$r_3 = [\ \langle 0,75,1467\rangle, \langle 1,1300,0\rangle, \langle 0,25,8\rangle, \langle 2,480,0\rangle, \langle 0,5,40\rangle, \langle 1,290,0\rangle \\ ,\ \langle 0,20,40\rangle, \langle 2,1015,0\rangle, \langle 3,215,-1476\rangle, \langle 4,630,-12\rangle \\ ]$$

This product is compared to product 1. The difference in the recipes can be found in the first reflux, which is 10 times longer for product 3. Again simulations have been made for both the pipeless and the conventional batch plant. In the first run only product 1 is deployed, in the second run only product 3. In the third run both products are brought into action, maintaining a ratio 1:1. The results of the three runs with the conventional batch plant can be found in Table 5.6.

Conventional Batch Plant			
product	w* [# batches]	yield 1 [m^3/hr]	yield 3 [m^3/hr]
1	1.42	1.993	0
3	1.27	0	1.26
1&3	1.32	0.78	0.74

Table 5.6: Results of the conventional batch plant for product 1 and 3

As can be seen the optimal WIP level of product 3 is lower than in the case of product 1. This can be declared as follows: the minimum flow time becomes longer, while the first reflux time is 10 times longer than formerly. The maximum throughput on the other hand becomes lower, because the bottleneck is enlarged now. The optimal WIP level becomes lower on balance, together with the yield of product 3. When both products are brought into action, the yields are quite low.

The pipeless plant initially shows the same changes. When however the plant is optimized, which means an extension of two units in the reflux cell, the results become much better, because there is no queue in front of the reflux cell. The results of the runs can be found in Table 5.7.

In Table 5.8 the degrees of occupation for the different cells can be found. The optimized pipeless plant obviously leads to a better occupation of the reflux and air cells.

In this case only the pipeless plant is optimized after the addition of an extra product. This is realistic, while optimizing the conventional plant should lead to the building of one or more expensive reactors. The optimization of the pipeless plant only demands extra units in the cells, which often means some extra connections from existing machines.

Pipeless Batch Plant			
product	w* [# batches]	yield 1 [m^3/hr]	yield 3 [m^3/hr]
1	10.15	2.012	0
3	4.44	0	0.51
1&3	6.02	0.455	0.418
1&3 opt.	11.84	0.89	0.9

Table 5.7: Results of the pipeless plant for product 1 and 3

product	w* [# batches]	Filling	Reflux	Air	Centrifuge	Vacuum Drier	Distillation
1	10.1	48.5	81.3	96.1	82.7	32.2	24.3
3	4.44	12.0	76.3	23.9	20.6	8.0	6.0
1&3	6.0	20.5	80.4	40.7	35.0	13.6	10.3
1&3 opt.	11.8	41.7	84.2	83.1	71.7	28.0	21.1

Table 5.8: Degrees of occupation of the pipeless plant for product 1 and 3

By means of the results it can be said that the pipeless plant stands out more positive against conventional batch plant, when optimization is applied after the addition of an extra product. The most important motive for this is, that the adaptation of a conventional plant is more expensive than the 'cheap' adaptation of a pipeless plant.

5.5 Evaluation

The control of both plants is easy in both cases. The conventional batch plant is a flowshop, so that no difficult choices have to be made concerning the product route. The pipeless plant is designed so, that a reactor enters a cell when one or more units are available. When no unit is available the reactor has to wait in the buffer. As can be seen in the specification of the pipeless plant this is quite straightforward.

Concerning the design of the χ models it can be said that the models do not differ much, so the degree of difficulty for both plants is the same.

When the bottleneck of the plant is in the pipeless part of the plant purely, and there is a possibility to change the units, the pipeless plant is better than the conventional plant, concerning the deployment of new products. In that case the pipeless plant can be debottlenecked easily. It has to be said emphatically that the ability of changing the cell capacity is a necessity when the pipeless plant has to be optimized. When the bottleneck of the plant lies in the conventional part of the plant (in this case the centrifuge, the vacuum drier or the distiller), the same situation arises as described in Chapter 4, where the pipeless plant could not be optimized too. In that case it depends on the recipe of the (extra) product that has to be deployed whether the pipeless plant is better than the conventional batch plant.

Chapter 6

Conclusions and Recommendations

6.1 Conclusions

The pipeless plant brings a lot of benefits about, especially in flexibility. Quick response to demands of the customer, quick changes in capacity and the ability to manufacture a wide variety of products are important characteristics of the pipeless plant. The equipment is often smaller, due to the smaller batch sizes. Unfortunately the investment costs are somewhat higher due to the accuracy of the equipment, the control signals and the positioning of the reactors in the cells. Finally it can be said that when a gas has to be added to the reactor constantly, it is almost inevitable to put the gas tank and the transferable reactor together.

From both case studies the debottlenecking of pipeless plants appears to be a big advantage compared to the conventional batch plant. As long as the bottleneck of the plant lies within the pipeless part of the plant, it is possible to move the bottleneck by adding more units to the cells. In conventional batch plants this is also possible, but this brings much higher costs about, because instead of a few connections often a whole new reactor has to be built. When the bottleneck lies outside the pipeless part of the plant, as occurred in the zero-wait case study, and a new product is deployed, it depends on the product recipe whether it is better to use the conventional batch plant or the pipeless plant. When a wide product assortment is deployed, a lot of cleaning during the process is required in conventional batch plants, while the reactors of the pipeless plants contain one product, and cleaning of the reactor can be done off-line.

From the case study of the 'FATGE'-plant it appears that the choice between a pipeless plant and a conventional batch plant strongly depends on the products to be deployed. This is a result of the fact that the conventional batch plant is not really optimized for the current product (the reactor is a big bottleneck). When optimization should be

done after deploying a new product with the bottleneck outside the conventional part of the pipeless plant, it would be to the advantage of the pipeless plant, because of the ability of debottlenecking.

As far as the control of both plants is concerned, it can be said that no big differences can be found. When a smaller grainsize is considered, the control of the conventional batch plant is complicated, because a lot of valves have to be controlled, in order to obtain the correct route for the process material. In a pipeless plant the same can be obtained simply by telling the reactor to go to a specific cell, but the traffic control of the AGVs might bring new problems about. The design of the models in χ brought no big differences about, apart from the control processes.

6.2 Recommendations for Further Research

As debottlenecking is a big advantage of the pipeless plant, the financial consequences of adding new units to a cell should be investigated. When those costs are too high, the product assortment flexibility of the pipeless plant decreases considerably. Nevertheless those costs will be lower than in the conventional batch plant.

Debottlenecking of the conventional part of a pipeless plant is as hard as debottlenecking an existing conventional batch plant. To avoid this, one should look at the possibilities to make this part of the plant pipeless too. In the 'FATGE'-case driers and distillers belong to the conventional part of the pipeless plant. It is advisable to look at the possibilities to involve those machines to the pipeless part too, in order to create a maximal flexibility.

Because zero-wait transfer policies often occur in the chemical industry, more insight in the scheduling and optimization of zero-wait job-shops is of great importance. So far very little research in done about zero-wait in flow-shops, and articles about zero-wait job-shops are very hard to find.

When molecule reactions, heating and cooling are represented by formulas, the effects of volume scale down should be more accurate. It would be useful when those effects are researched and implemented in a hybrid χ model. In this research project only assumptions could be made concerning the scale effects.

As the constant supply of gas (or liquid) to a transferable reactor cannot be done by a fixed connection (the reactors ride all over the plant, so that flexible pipes should be confused), it is almost inevitable to transport tanks with the reactor. Some difficulties can be the high pressure and the big volume. It is advisable to investigate this subject, because it is an obstacle for the design of pipeless plants.

In Chapter 3 the optimization of was discussed. Unfortunately it was not within the framework of this research to implement an optimized scheduling, for example using

MILP or MINLP. It is recommendable to research the effects of the optimization methods. Furthermore it is advisable to make an optimization library, in order to make the optimization of χ-models more convenient.

As only a start was made concerning the Kinidine synthesis (see Appendix G) it is advisable to take a further look at this case study. It is possible to design a pipeless Kinidine plant, so a comparison between pipeless and conventional batch plant can be made by means of models of both kinds of plants.

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Appendix A

Terminology

In this chapter some terms used in this report are explained:

- the throughput $\delta(t)$ is defined as follows:

$$\delta(t) = \frac{n_{out}(t)}{t} \tag{A.1}$$

  In this equation $n_{out}(t)$ represents the number of batches that have left the system at time t. The throughput equals the average rate of departure.

- The flow time $\varphi(t)$ can be calculated as follows:

$$\varphi(t) = \frac{\sum t_l(t)}{n(t)_{out}} \tag{A.2}$$

  In this equation $n_{out}(t)$ represents the number of batches that have left the system at time t, while $\sum t_l(t)$ represents the total lead time. The lead time of a product can be calculated as follows:

$$t_l(t) = t_{out}(t) - t_{in}(t) \tag{A.3}$$

  where t_{out} is the time a batch leaves the system and t_{in} is the time a batch enters the system.

- The optimal WIP level w^* will can be calculated as described in [RBR97]. The equation of Little gives the relation between work in progress w, throughput δ and flow time φ:

$$w = \delta\varphi \tag{A.4}$$

  The maximum throughput of the system equals the maximum throughput of the bottleneck δ_b, which can be calculated. When the bottleneck is not used optimal,

the throughput decreases, so at a minimum w the throughput is still optimal. The minimum flow time is the flowtime when $w = 1$ and will be denoted as φ_1. This flow time increases when at a higher WIP level some cells are blocked by the bottleneck. There is a maximum w where the flow time is still optimal. In order to come to a WIP level where both throughput and flow time are optimal, following equation can be derived from Equation A.4:

$$w^* = \delta_b \varphi_1 \tag{A.5}$$

- The campaign length indicates the number of products of one type that are manufactured consecutively. In relation with this term two different strategies can be applied on the production: Mixed product campaign and single product campaign. A single product campaign is the production of two or more products, where campaign lengths of 1 product are maintained. Mixed product campaign on the other hand is the production with campaign length larger than one. An example will clarify those strategies: when two different products, A and B, are deployed, the production order can be ABAABABBA (single product campaign) or AAAABBBBAAAABBBB (mixed product campaign with campaign length 4).

Some terms are mixed up in literature because they have different meanings:

- the term reactor has two different meanings. When a reactor is mentioned in relation with a conventional plant, a fixed reactor is meant. With a reactor of a pipeless plant on the other hand, a mobile reactor is meant, which means, a vessel connected to its transport unit, together with all the equipment that is carried with it. In literature reactor is often replaced by vessel or tank.
- The term cell is mentioned in relation with pipeless plants. A cell is a space, equipped to execute a number of the same processes. A cell consists of units.
- A unit is a part of a cell, where one operation can be performed. In literature the term work station is often used for both cell and unit.

For reasons of clarity the terms cell and unit are illustrated in Figure A.1.

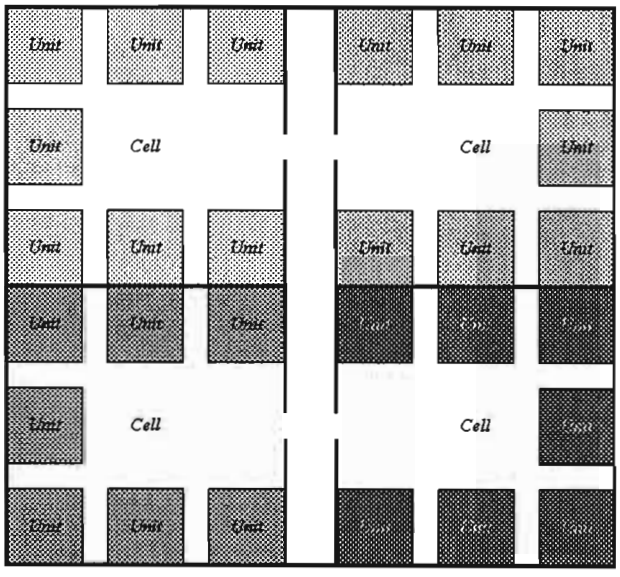

Figure A.1: A plant consisting of cells and units

Appendix B

Zero-wait Model of the Pipeless Plant

The pipeless plant consists combined order generator/WIP-controller G. Orders are sent to the vessel buffer VB. Vessels are sent to the reaction buffer RB. Finally the product is separated in the separation section S and collected in the exit process E. In Figure B.1 an iconic representation of the plant can be found. While the bigger part of this model is almost the same as the model of the conventional batch plant (see Section 4.2), only the most important processes are described in this section. A complete description of the specification can be found in Appendix B.

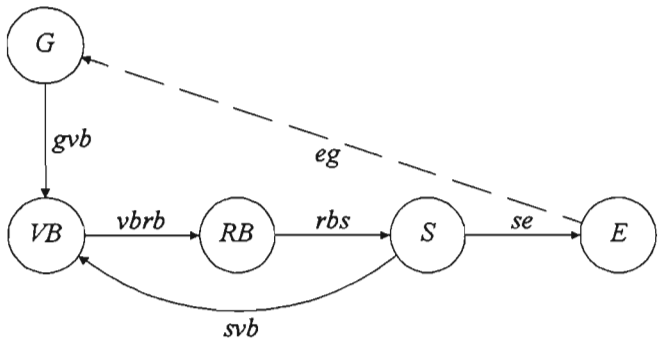

Figure B.1: Iconic representation of the pipeless batch plant

The specification of the system is as follows:

$$
\begin{array}{l}
\textsf{syst}\ ZWPBP = \\
[\![\ G :: \text{Generator},\ VB :: \text{VesselBuffer},\ RB :: \text{RectionBuffer},\ S :: \text{Separator},\ E :: \text{Exit} \\
,\ gvb, vbrb, rbs, se, svb : !\,?\,\text{batch},\ eg : \sim \\
|\ G(gvb, eg, w_{max}) \parallel VB(gvb, svb, vbrb) \parallel \\
\parallel RB(vbrb, rbs) \parallel S(rbs, se, svb) \parallel E(se, eg) \\
]\!]
\end{array}
$$

$$
\textsf{xper}\ = [\![\ ZWPBP\ ]\!]
$$

The types used in this model are defined below:

$$
\begin{array}{lll}
\textsf{type} & \text{prodnr} & = \text{nat} \\
, & \text{starttime} & = \text{real} \\
, & \text{ordernr} & = \text{nat} \\
, & \text{firstrun} & = \text{bool} \\
, & \text{batch} & = \text{prodnr} \times \text{starttime} \times \text{ordernr} \times \text{firstrun} \\
, & \text{endtime} & = \text{real} \\
, & \text{reac} & = \text{batch} \times \text{endtime}
\end{array}
$$

Process G represents the combined order generator/WIP-controller. As long as the user defined WIP-level is not reached ($wip > 0$), an order is generated and sent to the reaction buffer VB ($gvb\,!\langle\, \sigma\, v, \tau, n, \text{true}\rangle$). After that the WIP level is adjusted and the order-number is increased by one. When a product leaves the plant, a signal is received from process E ($eg\,?$), after which the WIP level is adjusted.

$$
\begin{array}{l}
\textsf{proc}\ \text{Generator}(gvb : !\,\text{batch},\ eg : ?\,\text{void},\ wip_{max} : \text{nat}) = \\
[\![\ v : \longrightarrow \text{int},\ n : \text{ordernr},\ wip : \text{nat} \\
|\ wip := 0;\ v := \text{dun}(0,4);\ n := 1 \\
;\ *[\ wip < wip_{max};\ gvb\,!\langle\, \sigma\, v, \tau, n, \text{true}\rangle \longrightarrow wip := wip + 1;\ n := n + 1 \\
\quad [\!] \qquad\qquad\qquad ;\ eg\,? \qquad\qquad\qquad \longrightarrow wip := wip - 1 \\
\quad] \\
]\!]
\end{array}
$$

In process VB, the vessel buffer, the vessels are waiting to be processed. When possible a vessel is sent to the reaction buffer RB. After a product is received from the order generator G ($gvb\,?\,x$) or from the separation section S ($svb\,?\,x$), the product is put into the list ($xs +\!\!+ [x]$). When vessels are waiting ($\text{len}(xs) > 0$), and it is possible to sent a product to the next section ($\Delta\, t_{sr} - \tau - \text{treac}(\text{hd}(xs).0)$), the product is removed from the list ($x := \text{hd}(\text{xs});\ xs := \text{tl}(xs)$) and sent to the reaction buffer RB ($vbrb\,!\,x$). Finally the time at which the separation section is ready is calculated ($t_{sr} := \tau + \text{treac}(x.0) + \text{tsep}(x.0)$).

```
proc VesselBuffer(gvb, svb : ? batch, vbrb : ! batch) =
[[ x : batch, xs : batch*, t_sr : real
| xs := []; t_sr := 0
; [                gvb ? x                          --> x.3 := x.0 ≠ 2; xs := xs ++ [x]
  []               svb ? x                          --> xs := xs ++ [x]
  [] len(xs) > 0; Δ t_sr − τ − treac(hd(xs).0) --> x := hd(xs); xs := tl(xs)
                                                       ; vbrb ! x; t_sr := τ + treac(x.0) + tsep(x.0)
  ]
]]
```

Function treac returns the product dependent reaction time, while function tsep returns the separation time on the basis of the product:

```
func treac(x : int) → real =
| [ x = 0 --> 12
  [] x = 1 --> 10
  [] x = 2 --> 4
  [] x = 3 --> 2
  ]
]]
```

```
func tsep(x : int) → real =
| [ x = 0 --> 2
  [] x = 1 --> 3
  [] x = 2 --> 4.5
  [] x = 3 --> 3.5
  ]
]]
```

Process *RB* represents the reaction buffer. This is one cell where several vessels can be processed. When a vessel is received from the vessel buffer *VB* ($vbrb\,?\,x$), it is put in a sorted list, together with the time at which the reaction is completed ($rs := \text{insert}(rs, \langle x, \tau + \text{treac}(x.0)\rangle, \text{crit})$). The list is sorted so, that the product that is ready first, is on the head of the list. When the reaction time has expired ($\Delta\,\text{hd}(rs).1 - \tau$), the product is removed from the list ($x := \text{hd}(rs).0; rs := \text{tl}(rs)$) and sent to the separation section *S* ($rbs\,!\,x$).

```
proc ReactionBuffer(vbrb : ? batch, rbs : ! batch) =
[[ rs : reac*, x : batch
| rs := []
; [                vbrb ? x          --> rs := insert(rs, ⟨x, τ + treac(x.0)⟩, crit)
  [] len(rs) > 0; Δ hd(rs).1 − τ --> x := hd(rs).0; rs := tl(rs); rbs ! x
  ]
]]
```

Function crit is needed for the insert-function in process RB. By means of this sorting criterium the products are arranged on starttime:

```
func crit(x, y : reac) → bool =
[[ ↑x.1 < y.1 ]]
```

The separation section S is the conventional part of the plant, the separation takes place in a machine, not in the mobile reactors. After a reactor is received from the reaction buffer RB ($rbs\,?\,x$), the (stochastic) wait time is calculated ($tw := \mathrm{ft}(x.0) + \sigma\, v + \tau$). From now on two things might occur: the wait time expires ($\Delta\, tw - \tau$), or a new product enters the separation section ($rbs\,?\,y$). In the latter case the part of the current product that has not been processed yet is thrown away. When a product of type 2 was processed for the first time ($x.0 = 2 \vee \neg x.3$), it is sent back to the vessel buffer VB ($svb\,!\,x$), else the product is sent to the exit process E ($se\,!\,x$).

```
proc Separator(rbs : ? batch, se, svb : ! batch) =
[[ x, y : batch, v : ⟶ real, t_w : real, b : bool
| v := nor(0, 0.05); b := true
; *[ [ b  ⟶ rbs ? x
     [] ¬b ⟶ x := y
     ]
   ; t_w := tsep(x.0) + σ v + τ
   ; [ rbs ? y    ⟶ b := false
     [] Δ t_w − τ ⟶ b := true
     ]
   ; [ ¬(x.0 = 2 ∨ ¬x.3) ⟶ se ! x
     [] x.0 = 2 ∨ ¬x.3   ⟶ x.3 := true; svb ! x
     ]
   ]
]]
```

In the exit process E the product is collected. When a product is received ($se\,?\,x$), a signal is sent to the WIP-controller G ($eg\,!$) indicating that a product has left the system.

```
proc Exit(se : ? batch, eg : ! void) =
[[ x : batch
| [ se ? x; eg ! ]
]]
```

Appendix C

Simulation Results of the Zero-wait Study

In this appendix the simulation results of the zero-wait study are presented. The results have already been discussed extensively in Chapter 4.

As described in the Terminology both throughput and flow time can be calculated, en thus the optimal WIP level. The results in this appendix however are all determined by simulation. Only 'suspicious' values have been checked by means of calculation.

In Table C.1 the simulation results concerning the conventional batch plant are represented. When dimension # is used, the number of batches is meant.

campaign	products	w [#]	φ [hr]	δ [#/hr]	w* [#]	yield [ltr/hr]	lost [%]
mixed	2	1	20	0.050	3.8	18.6	0.90
		100	533	0.187			
mixed	4	1	22	0.045	2.5	10.5	0.95
		100	890	0.112			
single	2	1	20	0.050	3.5	17.7	0.18
		100	557	0.177			
single	4	1	22	0.046	2.4	11.0	0.20
		100	898	0.110			

Table C.1: Simulation results of the conventional batch plant

In Table C.2 the simulation results concerning the pipeless plant can be found.

campaign	products	w [#]	φ [hr]	δ [#/hr]	w* [#]	yield [ltr/hr]	lost [%]
mixed	2	1	14	0.074	5.6	18.6	0.77
		100	248	0.400			
mixed	4	1	12	0.081	2.5	8.3	0.51
		100	450	0.208			
single	2	1	14	0.071	5.6	17.7	0.50
		100	242	0.397			
single	4	1	12	0.081	2.8	8.7	0.40
		100	420	0.225			

Table C.2: Simulation results of the pipeless plant

Appendix D

Description of the 'FATGE'-process

In this appendix an accurate description of the existing 'FATGE'-process is given.

The intermediate 2-formylaminothiazolyl-4-glyoxylic acid ethyl ester ('FAT-Glyoxylic acid Ester' or 'FATGE'), is prepared by the manganese-catalyzed air oxidation of 'FATA-Ester' [PTR90]. The reaction scheme of the main-process is presented in Figure D.1.

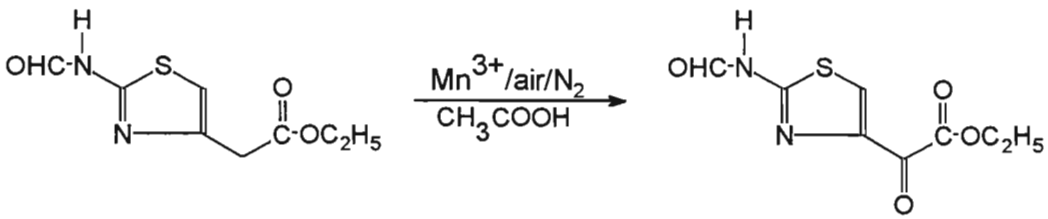

Figure D.1: Reaction scheme of the 'FATGE' process

First manganese diacetate tetrahydrate and acetic anhydride in acetic acid are heated to reflux. To this refluxing suspension potassium permanganate is added in small portions at 343-353 [K] and held at reflux for 1 hour. The obtained catalyst solution is cooled down to 341-343 [K] and the 'FATA-Ester' is added. Air is spouted through the mixture continuously. To keep the reaction system out of the explosion range (which means that the oxygen volume in the gas input should not exceed 8 volume percent), nitrogen is blown through the reaction mixture at the same time. After about 8 hours, when the reaction is nearly complete a second quantity of 'FATA-Ester' is charged. The air/nitrogen stream is maintained for about 16 hours. After a while 'FATGE' crystallizes from the reaction mixture. The temperature of the mixture is held between 343 and 355 [K]. When the reaction is complete, the product is isolated by centrifugation, where

it is washed successively with acetic acid, water and acetone. Finally the product is dried. Meanwhile the acetic acid mother liquors are distilled. The first part of the fraction is sent to incineration, the second part can be reused, the residue is sent to waste treatment.

In Table D.1 an overview can be found of the steps of the 'FATGE'-process.

Step	Time	Temp [K]	Product in	Device	Stirring [rpm]	N_2 vent. [m^3/hr]
1	0:00			K1		1
2	0:00-0:40		P1 (1170 ltr.)	K1		
3	0:40-0:50		P2 (136 kg)	K1	84	5-10
4	0:50-1:15		P3 (210 ltr.)	K1		1
5	1:15-2:10	383		K1		
6	2:10-2:45	383-391		K1		
7	2:45-3:25	348		K1		10-15
8	3:25-3:50	343-353	P4 (22 kg)	K1	124	28
9	3:50-4:20	348-353		K1	124	5-6
10	4:20-4:50	385		K1	84	
11	4:50-5:35	385-390		K1	84	
12	5:35-8:40	303		K1	84	5-6
13	8:40-8:45	<303	P5 (60 kg)	K1		15-25
14	8:45-16:45	301-311		K1	84	
15	16:45-17:05		P5 (50 kg)	K1		15-25
16	17:05-33:05	301-311		K1	84	
17	33:05-34:00	ca. 303		K1		
18	34:00-37:35		A1 (250 ltr.) A2 (290 ltr.) A3 (30 ltr.)	K1→C1		
19	37:35-41:00		A1 (250 ltr.) A2 (290 ltr.) A3 (30 ltr.)	K1→C1		
20	41:00-58:30			C1→B1		
21	58:30-61:00	291-313		B1→D		
22	61:00-69:00	313		D		
23	69:00			B2		

Table D.1: Overview of the 'FATGE'-process

In Table D.2 the details of every step are described. The codes for the products and devices are declared in Table D.3.

The acetic acid recycling process can be found in Table D.4.

In Table D.5 some details per step concerning the acetic acid recovery can be found,

Step	Detail
1	Clean K1 two times, then ventilate with N_2
2	Add P1
3	Add P2
4	Add P3
5	Heat to reflux
6	Hold at reflux
7	Cool down to 348 [K], turn of cooler at ca. 378-383 [K]
8	Add P4 in small portions
9	Hold at 348-353 [K]
10	Heat as quick as possible to reflux
11	Heat for maximal 45 minutes at reflux
12	Cool down to 301-303 [K]
13	Add P5; temperature maximal 303 [K]
14	Blow dry air through reactor
15	Add P5; temperature maximal 303 [K]
16	Blow dry air through reactor
17	Cool down to ca. 303 [K]
18	First of two portions in spindrier; muthersuds in T1 and next pumped into K2 Wash C1 with A1 and A2l; spout K1 with A3
19	Second of two portions in spindrier; muthersuds in T1 and next pumped into K2 Wash C1 with A1 and A2l; spout K1 with A3
20	Moist 'FATGE' in bundle with PE-layer
21	Dry product in vacuum spin drier at 313 [K], together with other batches
22	Dry during 8 hours
23	yield: 200 [kg]

Table D.2: Details of the 'FATGE'-process

while in Table D.6 the codes for products and devices are declared.

Code	Name
A1	Acetic acid
A2	City water
A3	Acetone
H1	Nitrogen
H2	Air
P1	Acetic acid
P2	Manganese-(II)-acetate,tetrahydride
P3	Acetic anhydride ACS
P4	Potassium Permanganate
P5	'FATA' Ester
B1	Bundle with PE-layer
B2	Steel drum
C1	Centrifuge
D1	Spin drier
K1	Glass lined reactor

Table D.3: Code names for products and devides

Step	Time	Temp. [K]	Product in	Product out	Device
1	35:45-36:55	386-387	E2 (1100 ltr.)		K1
2	36:55-37:25	387-389		E2 (50 ltr.)	
3	37:25-38:55	389-393		Er (150 ltr.)	
4	38:55-42:30				
5	42:30				

Table D.4: Overview of the acetic acid recycling

Step	Detail
1	
2	First 50 [ltr.] abandoned in the neutralization in V1
3	Further 150 [ltr.] distilled in T1 - this part will be distilled with next motherbatch
4	Yield 600 [ltr.]
5	Clean K1 using 500 [ltr.] A1 while stirring

Table D.5: Details of the acetic acid recovery

Code	Name
A1	City water
E1	Motherbatch
E2	1st batch
E3	2nd batch
K1	Vessel
T1	Tank
T2	Tank
V1	Vessel

Table D.6: Code names of products and devices of the acetic acid recovery

Appendix E

Model of the Pipeless 'FATGE'-process in χ

In this appendix the entire specification of the model of the pipeless 'FATGE' process is dealt with. In Figure E.1 an iconic representation of the model is depicted. System *PBP* of a combined order-generator/WIP-controller G, a transport controller T, two exit-processes E and six cells C. The cells are built of two processes: process B represents the buffer where the vessels waiting to be processed are parked, the actual process cell PC consists of several units. In every unit one vessel can be processed.

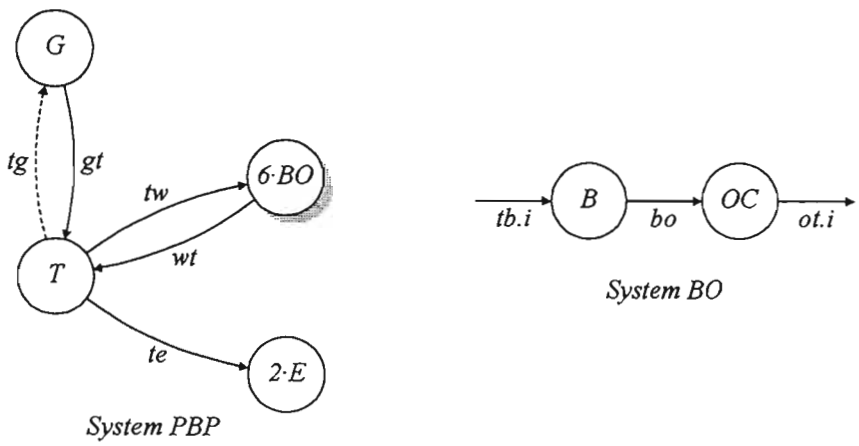

Figure E.1: Iconic representation of system *PBP*

The declaration of the system is can be found below.

```
syst PBP =
[[ G :: Generator, T :: Transport, BO :: Cell^6, E :: Exit^2
, tg : ~, gt : !? vessel, ct,tc : !?^6 vessel, te : !?^2 product, i,j : nat
| G(tg,gt,w_max) || T(gt,ct,te,tc,tg) ||
|| i : [0,2) : E.i(te.i)
|| j : [0,6) : BO.j(tc.j,ct.j)
]]

xper = [[ PBP ]]
```

The type 'vessel' is built as follows:

```
type ordernr    = nat                                          serial number
,    starttime  = real                                         time at which an
                                                               order is generated
,    vol        = real                                         volume
,    cenr       = nat                                          cell number
,    proctime   = real                                         process-time
,    volchange  = real                                         change in volume
,    operation  = cenr × proctime × volchange
,    recipe     = operation*
,    ptype      = int                                          type of product
,    product    = vol × starttime × ordernr × ptype
,    vessel     = ⟨recipe × vol × starttime × ordernr × ptype⟩
```

The product-recipes (two in this case) are defined as constants, together with the acetic acid recovery recipe:

```
const r1 = [⟨0,75,1467⟩,⟨1,130,0⟩,⟨0,25,8⟩,⟨1,290,0⟩,⟨0,5,40⟩,⟨2,480,0⟩
           , ⟨0,20,40⟩,⟨2,1015,0⟩,⟨3,215,−1476⟩,⟨4,630,−12⟩
           ]
,     r2 = [⟨0,75,1467⟩,⟨1,130,0⟩,⟨0,25,8⟩,⟨2,480,0⟩,⟨0,5,40⟩,⟨1,290,0⟩
           , ⟨0,20,40⟩,⟨2,1015,0⟩,⟨3,215,−1476⟩,⟨4,630,−12⟩
           ]
,     r_r = [⟨4,475,−876⟩,⟨5,0,0⟩]
```

Process G, the combined order-generator/WIP-controller, generates orders in by means of an empty vessel ($gt!\langle r,0,\tau,n,s\rangle$), as long as the WIP-level, which is defined by the user, is not reached ($wip < wip_{max}$). The product-type is determined by a discrete uniform distribution (in this case: dun$(0,2)$). When a product has left the system, a signal ($tg?$) is received from the transportation-controller.

```
proc Generator(tg : ? void, gt : ! vessel, wip_max : nat) =
[[ wip : nat, r : recipe, rt : recipe^2, v : ⟶ int, s : ptype, n : ordernr
| n := 1; v := dun(0,2); rt := ⟨r_1, r_2⟩; s := σ v; r := rt.s; wip := 0
; *[ wip < wip_max; gt ! ⟨r, 0, τ, n, s⟩ ⟶ n := n + 1; wip := wip + 1; s := σ v; r := rt.s
   []                 tg ?               ⟶ wip := wip − 1
   ]
]]
```

Process T represents the transportation process. In this process it is estimated which is the next destination of the vessel. When a vessel is received from the order generator G ($gt\,?\,x$) or from a cell ($ct.j\,?\,x$), the vessel is put at the end of a list ($ys +\!\!+ \langle x, \tau + 15\rangle$). When the transportation time of a vessel has expired ($\Delta\,\mathrm{hd}(ys).1 - \tau$), the vessel is sent to its next destination. When the recipe is empty ($\mathrm{len}(x.0) = 0$), the product is ready, so that it can be sent to the exit-process ($te.0\,!\,p$). Because the product has left the system now, a signal to the WIP-controller is sent ($tg\,!$), indicating that the WIP-level has to be adjusted. When the recipe is not empty, it depends on the first element of the first route, where to sent the product to ($r := x.0.0$). In the case that $r = 4$, the main-product is sent to the dryer ($jc.4\,!\,x$), while the remainder is sent to the acetic acid recycling, after having adapted the volume and the recipe ($x.0 := r_\tau$; $x.1 := 1976$; $tc.5\,!\,x$). Finally the element is removed from the list ($ys := \mathrm{tl}(ys)$).

```
proc Transport( gt : ? vessel, ct : ?^6 vessel
              , te : !^2 product, tc : !^6 vessel, tg : ! void
              ) =
[[ x : vessel, ys : ⟨vessel × proctime⟩, r : ce, p : product
| ys := []
; *[                  gt ? x          ⟶ ys := ys +\!\!+ ⟨x, τ + 15⟩
   [] j :             ct.j ? x        ⟶ ys := ys +\!\!+ ⟨x, τ + 15⟩
   []    len(ys) > 0 ; Δ hd(ys).1 − τ ⟶ x := hd(ys).0; p := ⟨x.1, x.2, x.3, x.4⟩
                                      ; [ len(x.0) = 0 ⟶ te.0 ! p; tg !
                                        [] len(x.0) > 0 ⟶ r := x.0.0
                                                        ; [ r < 4 ⟶ tc.r ! x
                                                          [] r = 4 ⟶ tc.4 ! x
                                                                   ; x.0 := r_τ
                                                                   ; x.1 := 1976
                                                                   ; tc.5 ! x
                                                          [] r = 5 ⟶ te.1 ! p
                                                          ]
                                        ]
                                      ; ys := tl(ys)
   ]
]]
```

Process E, the exit-process receives products (without the vessel) from the transport

controller T. Because this is the only function of the process, it can be wrote down quite straightforward:

```
proc Exit(te : ? product) =
[[ x : product
| *[ te ? x ]
]]
```

A cell BO consists of a buffer B, a temporary storage for vessels which have to be processed, and the process unit OC. The process cell on its turn consists of several units. Every single unit is capable to process one vessel. The number of units per cell is user defined and is fixed beforehand.

```
syst Cell(tb : ? vessel, pt : ! vessel) =
[[ B :: Buffer, OC :: OperationCell, bp : vessel
| B(tb, bp) || OC(bp, pt, nr)
]]
```

In the buffer B the vessels, waiting for their operation are parked. First a vessel is received from the transport controller T ($tb\,?\,x$) and put at the end of the list. As long as the list is not empty ($\mathrm{len}(xs) > 0$), the process tries to send a product to the operation cell OC ($bp\,!\,\mathrm{hd}(xs)$). When this succeeds, the list is updated ($xs := \mathrm{tl}(xs)$).

```
proc Buffer(tb : ? vessel, bp : ! vessel) =
[[ x : vessel, xs : vessel*
| [                tb ? x          --> xs := xs ++ [x]
  [] len(xs) > 0; bp ! hd(xs)      --> xs := tl(xs)
  ]
]]
```

The actual operation cell OC consists of a number of units, and is therefore able to process more than one vessel at the same time. When the number of vessels in the process cell is smaller than the maximum ($n < nr$), the process is able to receive a vessel ($bp\,?\,x$). A product is put in a list ($ys := \mathrm{insert}(ys, \langle x, \tau + x.0.1/\mathrm{conv}(pr, f)\rangle, \mathrm{crit})$), sorted at the finishing-time of the process ($\tau + x.0.1$). When the processing-time has expired ($\Delta\,\mathrm{hd}(ys).1 - \tau$), the volume and the recipe of the vessel are adjusted ($x.1 := x.1 + x.0.0.2/f$; $x.0 := \mathrm{tl}(x.0)$). Then the product is sent back to the transport controller T ($pt\,!\,x$), after which the list is updated ($ys := \mathrm{tl}(ys)$).

```
proc OperationCell(bp : ? vessel, pt : ! vessel, nr : nat, f : real, pr : nat) =
[[ x : vessel, ys : ⟨vessel × proctime⟩, n : nat
| ys := []; n := 0
; *[ n < nr      ; bp ? x                  ⟶ ys := insert(ys, ⟨x, τ + x.0.1/conv(pr, f)⟩, crit)
                                             ; n := n + 1
   [] len(ys) > 0; Δ hd(ys).1 − τ ⟶ x := hd(ys).0; x.1 := x.1 + x.0.0.2/f
                                             ; x.0 := tl(x.0); pt ! x; ys := tl(ys); n := n − 1
   ]
]]
```

The function crit is applied for the insertion of products in a sorted list. This function is defined as follows:

```
func crit(x, y : ⟨product × proctime⟩) →= bool
[[ ↑ x.1 ≤ y.1 ]]
```

The function conv is needed to convert the process time indicated in the recipe to the real process time. Only in the case of the dryer and the distiller the process time is divided by the user-defined factor f. This factor represents the ratio of the batch volumes of the conventional process and the pipeless process.

```
func conv(pr : nat, f : real) → real =
[[ [ pr = 0 ⟶ ↑ 1
   [] pr = 1 ⟶ ↑ f
   ]
]]
```

Appendix F

Results of the 'FATGE'-project

In this appendix the simulation results of the 'FATGE'–process are presented. The results have already been discussed extensively in Chapter 5. An explanation of the throughput, the flow time and the optimal WIP level can be found in the Terminology. As described there, both throughput and flow time can be calculated, en thus the optimal WIP level. The results in this appendix however are all determined by simulation. Only 'suspicious' values have been checked by means of calculation.

The first runs concern 2 different products: product 1, the original product and product 2, where the process time of the vacuum drying is doubled. The recipes of the products are:

$$\begin{aligned} r_1 = \; & [\langle 0,75,1467\rangle, \langle 1,130,0\rangle, \langle 0,25,8\rangle, \langle 1,290,0\rangle, \langle 0,5,40\rangle, \langle 2,480,0\rangle \\ & , \langle 0,20,40\rangle, \langle 2,1015,0\rangle, \langle 3,215,-1476\rangle, \langle 4,630,-12\rangle \\ &] \end{aligned}$$

$$\begin{aligned} r_2 = \; & [\langle 0,75,1467\rangle, \langle 1,130,0\rangle, \langle 0,25,8\rangle, \langle 2,480,0\rangle, \langle 0,5,40\rangle, \langle 1,290,0\rangle \\ & , \langle 0,20,40\rangle, \langle 2,1015,0\rangle, \langle 3,215,-1476\rangle, \langle 4,1230,-12\rangle \\ &] \end{aligned}$$

In Table F.1 the simulation results of the conventional batch plant model can be found. Table F.2 describes the simulation results of the pipeless plant. In Table F.3 the degrees of occupation of the cells of the pipeless plant can be found. When dimension # is used, the number of batches is meant.

Finally some runs with product 1, the original product and product 3, have been made. Product 3 is the has the same recipe as product 1 except for the first reflux, which lasts 10 times longer. The recipes of product 3 is:

$$\begin{aligned} r_3 = \; & [\langle 0,75,1467\rangle, \langle 1,1300,0\rangle, \langle 0,25,8\rangle, \langle 1,290,0\rangle, \langle 0,5,40\rangle, \langle 2,480,0\rangle \\ & , \langle 0,20,40\rangle, \langle 2,1015,0\rangle, \langle 3,215,-1476\rangle, \langle 4,630,-12\rangle \\ &] \end{aligned}$$

Conventional Batch Plant						
product	w [#]	φ [min]	δ [#/min]	w* [#]	yield 1 [m^3/hr]	yield 2 [m^3/hr]
1	1	2900	0.000345	1.42	1.993	0
	100	4079	0.000490			
2	1	3530	0.000284	1.72	0	1.969
	100	4081	0.000490			
1&2	1	3215	0.000312	1.57	1.007	0.960
	100	4081	0.000490			

Table F.1: Results of the conventional batch plant with product 1 and 2

Pipeless Plant						
product	w [#]	φ [min]	δ [#/min]	w* [#]	yield 1 [m^3/hr]	yield 2 [m^3/hr]
1	1	2504	0.0004	10.02	2.012	0
	100	25177	0.0040			
2	1	2588	0.0004	10.35	0	2.028
	100	24934	0.0040			
1&2	1	2546	0.0004	10.18	1.06	1.00
	100	25087	0.0040			

Table F.2: Results of the pipeless plant with product 1 and 2

In Table F.4 the simulation results of the conventional batch plant model can be found. Table F.5 describes the simulation results of the pipeless plant. In Table F.6 the degrees of occupation of the cells of the pipeless plant can be found.

product	w* [#]	Filling	Reflux	Air	Centrifuge	Vacuum Drier	Distillation
1	10.02	48.5	81.3	96.1	82.7	32.2	24.3
2	10.35	47.8	80.2	94.7	81.4	63.4	23.9
1&2	10.18	48.6	81.6	96.3	82.8	48.0	24.3

Table F.3: Degrees of occupation of the cells of the pipeless plant

Conventional Batch Plant						
product	w [#]	φ [min]	δ [#/min]	w* [#]	yield 1 [m^3/hr]	yield 2 [m^3/hr]
1	1	2900	0.000345	1.42	1.993	0
	100	4079	0.000490			
2	1	4070	0.000246	1.27	0	1.26
	100	6420	0.000312			
1&2	1	3485	0.000288	1.40	0.78	0.74
	100	4660	0.000401			

Table F.4: Results of the conventional batch plant with product 1 and 3

Pipeless Plant						
product	w [#]	φ [min]	δ [#/min]	w* [#]	yield 1 [m^3/hr]	yield 2 [m^3/hr]
1	1	2545	0.000393	10.15	2.012	0
	100	25087	0.004			
2	1	3674	0.00027	4.44	0	0.51
	100	78812	0.00121			
1&2	1	3110	0.00032	6.06	0.455	0.418
	100	49317	0.00195			
1&2 opt.	1	3110	0.00032	11.82	0.89	0.9
	100	2536	0.0038			

Table F.5: Results of the pipeless plant with product 1 and 3

product	w* [#]	Filling	Reflux	Air	Centrifuge	Vacuum Drier	Distillation
1	10.15	48.5	81.3	96.1	82.7	32.2	24.3
2	4.44	12.0	76.3	23.9	20.6	8.0	6.0
1&2	6.06	20.5	80.4	40.7	35.0	13.6	10.3
1&2 opt.	11.82	41.7	84.2	83.1	71.7	28.0	21.1

Table F.6: Degrees of occupation of the cells of the pipeless plant

Appendix G

The Kinidine Synthesis

During this investigation most attention was given to the zero-wait case and the FATGE process. In order to see of the pipeless concept could be applied to different kinds of batch processes, DSM Andeno provided the necessary data concerning the quinidinone step in the quinidine synthesis [Kin97]. This quinidine synthesis is used at the Venlo site of DSM Andeno in the Netherlands. A start is made with this synthesis to keep the investigation going. A brief survey is made of the process to see if and how it can be converted into a pipeless plant. It should be stated that no extensive research has been done for this process, so possibly no optimal solutions were found. The information represented below should give valuable starting points for the continuation of this investigation.

Description of the process

Quinine is dissolved in toluene. The toluene mixture is washed several times and subsequently distilled to remove all water. Benzophenone, KOH and NaOH are added and the reaction is started. Because of the exothermic nature of the process, the temperature will rise. After completion of the reaction the mixture is cooled and cold water is added. Again the mixture is heated. The mixture is allowed to settle and the watery alkaline layer is removed. The toluene mixture is washed several times with water to remove all alkaline.

A main extraction is performed by adding oxalate acid to the toluene mixture. This extraction is performed 5 times with different volumes of oxalic acid. To remove traces of bezophenone/benzohydrol an additional extraction is performed with clean toluene. The oxalic acid extract itself is neutralized with NaOH and subsequently cooled. To obtain the product, the extract is centrifuged. The product is collected without any washing. The fluid collected from the centrifuge is mixed with toluene and extracted with sulfuric acid. This mixture is to be treated with the next batch in the main extraction.

The quinidinone process at DSM Andeno

The actual process at the Venlo site of DSM Andeno follows essentially the same processing route as described above. Since the data about the process are in Dutch, the names of the devices used were translated into English. For the sake of clarity are the Dutch names given in brackets. The following devices are used for the quinine oxidation:

Device	Dutch name
1 Dissolver	(Oplosstander)
2 Mix vessels	(Inzetketel)
1 Emulsion vessel	(Emulsieketel)
1 Acid vessel	(Zuurketel)
1 Dissolver oxalic acid (o.a.)	(Oplosstander oxaalzuur)
2 Crystallizers	(Kristallisator)

The process is designed in order to produce 420 kg of quinidinone oxalate per twenty-four hours. Since at the site only work is done during the day, a second Mix vessel is used to allow a production of 420 kg/day. A flow sheet representation of the process is given in Figure G.1.

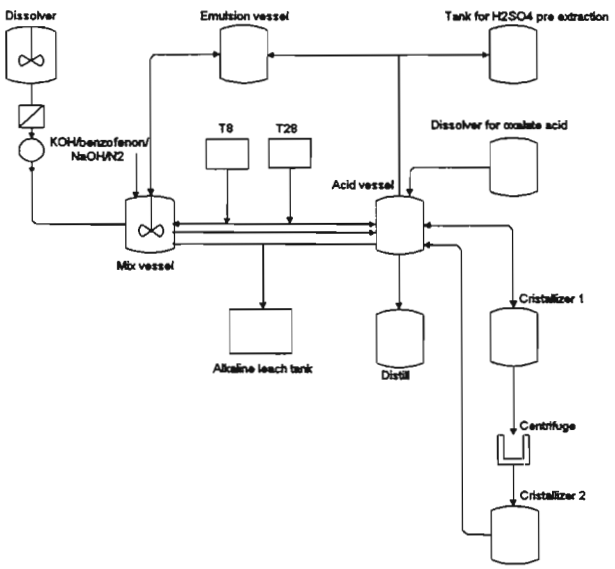

Figure G.1: Flow sheet representation of the quinidine synthesis at the Venlo site of DSM Andeno.

The operations per device are represented in Table G.1.

The processing times for each of the devices used in the quinidinone synthesis are represented in Figure G.2.

Device	Operation
Dissolver	Dissolve quinine bisulfate Fitration
Mix vessel 1	Mix quinine bisulfate sollution Wash toluene/emulsion alkaline free Distill toluene/quinine mixture
Mix vessel 2	Add benzofenone/KOH/NaOH Oxidation Wash out KOH/NaOH
Acid vessel	Sulphuric acid pre extraction Main extraction with oxalic acid Post extraction Extract liquor previous charge
Crystallizer 1	Storage main extraction Crystallization
Crystallizer 2	Storage fluid centrifuge
Centrifuge	2*2 hours centrifuge

Table G.1: Use of equipment

As with the FATGE process the quinidinone process is analyzed in all the processing steps, in order to abstract the necessary processing cells. The results of this analysis are represented in Table G.2 and further. The results are grouped by process, and consist of a brief description of the operation (Operation), the source of materials (Source), the device the operation is performed in (Device) and the facilities needed to perform the operation (Facilities).

All operations can be divided into essentially 7 processing cells. The processing cells are the following: Filling, Heat transfer, Agitation, Extraction, Settling, Emptying and Distilling. As with the FATGE process it has been pursued to obtain as many logical processing cells as possible, by combining all independent operations into one processing cell.

Although 7 independent processing cells can be derived from the process, some cells can be combined into one processing cell, without making the plant less flexible. During filling heat transfer is often needed. Although heat transfer is assigned to a separate cell is may be advisable to incorporate this operation also in the Filling cell. Because of the frequency the filling procedure is needed it may be impractical to combine filling and heat transfer into one cell. Agitation is needed at several processing cells. It should therefore be assigned to either the vessel or the relevant processing cells. Extraction and settling first require the addition of an extract material with subsequent heating and settling. The filling can be done at the Filling cell, whereas heating and settling can be performed at the Heat transfer cell, especially since settling only takes about 5 to 10 minutes. Emptying has to be assigned to a separate processing cell, for extraction is

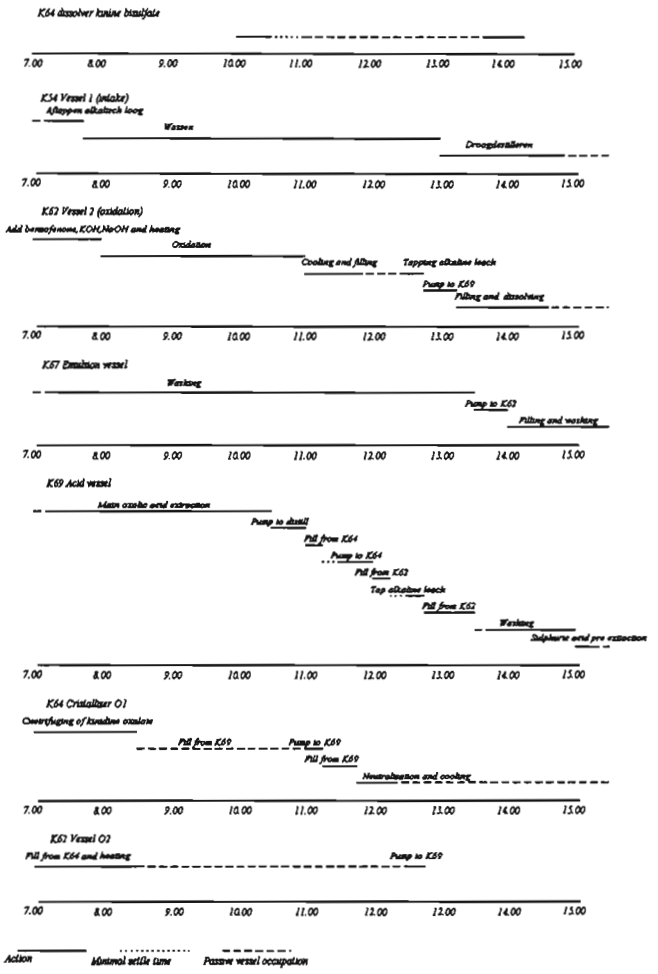

Figure G.2: Occupation in time of the devices in the kinine synthesis.

often needed in the process. The extracted products often require intermediate storage. The Emptying cell should therefore be connected to these intermediate storage tanks. Distillation only requires heat transfer with refluxing. Since the distilling facilities are only needed for a relatively short time, distillation can be assigned to the Heat transfer cells as well.

As a result only 3 processing cells remain, namely: Filling, Heat transfer and Emptying. Compared to the conventional process not much flexibility is gained. This is mainly due to the limited amount of operations needed and the fact that most of the process consists of extraction. The division of the process into processing cells to make a pipeless plant, might even be impractical. In the conventional process most of the extractions can be carried out after each other. Extraction in a pipeless plant on the other hand require the use of the Filling, Heat transfer and Emptying cells. The times needed for the

transportation between the different cells can make the process very time consuming. Besides this the Emptying cell is still mainly conventional, for it is connected to all the different intermediate storage tanks by means of piping.

It can be concluded that the use of the pipeless concept is possible for the quinidine synthesis. Due to the limited number of different processing cells needed, and the consequent introduction of extra transportation times it might however be impractical to use the pipeless concept. Without further investigation we dare state that it is possible to convert most batch processes into pipeless processes. The question only is if it is desirable.

Dissolving of the quinine bisulfate

Step	Operation	Source	Device	Facilities
1	Add quinine bisulfate		Dissolver	
2	Add water/filter earth		Dissolver	steam/agitate
3	Add toluene	Emulsion vessel	Mix vessel I	
4	Add NaOH		Mix vessel I	steam/agitate
5	Add contents Dissolver	Dissolver	Mix vessel I	steam/clean filter
6	Dissolve quinine		Mix vessel I	agitate
7	Take sample alkaline leach	Mix vessel I	Emulsion vessel	
8	Settle leach		Mix vessel I	
9	Pump alkaline leach	Mix vessel I	Leach tank	
10	Add water		Mix vessel I	agitate
11	Add toluene	T8	Mix vessel I	agitate
12	Add toluene	T28	Mix vessel I	agitate
13	Heat		Mix vessel I	steam/agitate
14	Settle		Mix vessel I	
15	Pump watery emulsion & alkaline leach	Mix vessel I	Emulsion vessel	
16	Add water		Mix vessel I	
17	Heat		Mix vessel I	steam/agitate
18	Settle		Mix vessel I	
19	Pump watery emulsion & alkaline leach	Mix vessel I	Emulsion vessel	
20	Distill until the mixture is dry		Mix vessel I	steam

Table G.2: Dissolving of quinine bisufate

Steps 16 to 20 have to be repeated until the toluene-quinine mixture is emulsion free.

Oxidation of quinine to quinidinone

Step	Operation	Source	Device	Facility
21	Add benzophenone, KOH & NaOH		Mix vessel I	steam, N_2
22	Heat		Mix vessel I	steam
23	Reaction (distillation)		Mix vessel I	steam
24	Cool down		Mix vessel I	cooling water
25	Add cold water		Mix vessel I	
26	Extraction		Mix vessel I	steam/agitate
27	Settle		Mix vessel I	
28	Pump alkaline leach till emulsion or toluene	Mix vessel I	Leach tank	
29	Add water		Mix vessel I	agitate
30	Heat		Mix vessel I	steam/agitate
31	Settle			
32	Pump alkaline leach	Mix vessel I	Leach tank	

Table G.3: Oxidation of quinine to quinidinone.

Sulfuric Acid pre extraction

Step	Operation	Source	Device	Facility
33	Pump contents Mix vessel I	Mix vessel I	Acid vessel	
34	Add water		Acid vessel	agitate
35	Add sulfuric acid		Acid vessel	agitate
36	Heat		Acid vessel	steam
37	Extract		Acid vessel	agitate
38	Settle		Acid vessel	
39	Pump acid extract	Acid vessel	Sulfuric Acid Vessel	

Table G.4: Sulphuric pre extraction.

Extraction with oxalic acid

Step	Operation	Source	Device	Facility
40	Add oxalic acid		Dissolver o.a.	
41	Add warm water		Dissolver o.a.	agitate
(42	Heat if necessary		Dissolver o.a.	steam)
43	Pump oxalic acid	Dissolver o.a.	Acid vessel	agitate
44	Extract		Acid vessel	steam
45	Settle		Acid vessel	

Table G.5: Extraction with oxalic acid.

Meanwhile a second batch of oxalic acid is prepared in the Dissolver o.a.

46	Pump acid extract	Acid vessel	Crystallizer I	
47	Add oxalic acid	Dissolver o.a.	Acid vessel	agitate
48	Extract		Acid vessel	steam/agitate
49	Settle		Acid vessel	
50	Pump acid extract	Acid vessel	Crystallizer I	

Table G.6: Preparation of a second batch of oxalic acid.

Steps 48 to 50 are to be repeated with 200 l and 4 times 100 liter of oxalic acid.

51	Add water		Acid vessel	agitate
52	Add sulfuric acid		Acid vessel	agitate
53	Extract		Acid vessel	steam/agitate
54	Settle		Acid vessel	
55	Pump acid extract	Acid vessel	Crystallizer I	
56	Add NaOH		Acid vessel	agitate
57	Settle		Acid vessel	
58	Pump alkaline leach	Acid vessel	Emulsion vessel	
59	Pump toluene mixture	Acid vessel	Distill	

Table G.7:

Post extraction of the oxalic acid quinidinone extract

Step	Operation	Source	Device	Facility
60	Add toluene	T28	Acid vessel	
61	Pump oxalic acid quinidinone extract	Crystallizer 1	Acid vessel	agitate
62	Heat		Acid vessel	steam
63	Settle		Acid vessel	
64	Pump clear oxalic acid quinidinone extract	Acid vessel	Crystallizer 1	

Table G.8: Post extraction of the oxalic acid quinidinone extract

Crystallization and centrifugation of the quinidinone oxalate

Step	Operation	Source	Device	Facility
65	Add NaOH		Crystallizer 1	
66	Cool		Crystallizer 1	cooling water
67	Pump half contents Crystallizer I	Crystallizer 1	Centrifuge	
68	Stir contents Crystallizer I		Crystallizer 1	agitate
69	Centrifuge in 2 portions		Centrifuge	
70	Collect liquid	Centrifuge	Crystallizer 2	
71	Pulverize kinedinone oxalate Take out of centrifuge		Centrifuge	
72	Store product	Centrifuge	Container	
73	Agitate		Crystallizer 2	agitate
74	Heat		Crystallizer 2	steam/agitate

Table G.9: Crystallization and cetrifugation of the quinidinone extract.

Extraction quinidinone oxalate leach

Step	Operation	Source	Device	Facility
75	Agitate		Acid vessel	agitate
76	Add NaOH		Acid vessel	agitate
77	Pump quinidinone oxalate leach	Crystallizer 2	Acid vessel	
78	Heat		Acid vessel	steam
79	Settle		Acid vessel	
80	Pump alkaline leach	Acid vessel	Leach tank	

Table G.10: Extraction of the quinidinone oxalate leach.

The remainder in the Acid vessel is used to dilute the next batch.

The chemicals used and the formed products are represented in Tables G.11 and G.12.

Used Chemicals	
Chemicals	Quantity
quinine bisulfate	650 kg
Toluene	4000 l
Leach solution	560 l
Filter earth	4 kg
Benzophenone	300 kg
Potassium hydroxide	300 kg
Sodium hydroxide	200 kg
Oxalic acid	150 kg
Diluted sulfuric acid	20 kg

Table G.11: Chemicals used in the quinine process.

Formed Products	
Product	Quantity
quinidinone oxalate	420 kg
Sulphuric acid pre extraction	230 l
benzhydrol/benzofenone	300 kg

Table G.12: Products formed in the quinine process.

Bastiaan VdL ... hove
Nadelen: voorinvest kosten

primaire en secundaire problematiek
- scheduling primair
- hoeveel kost een multiple cell?

- warmtemantel: hoe uit te voeren?
- volume zbe
cond vgl. constructiekosten. (meerdere producten)
- "alle" data voorhanden
- in voor technologie

Pascal VdWijdeven
- conventionele plant voldoet niet
- feed forward control
- separatie niet pijpleiders
- weinig verschil in X-modellen