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DYNAMIC SIMULATION OF A FINE PAPER MILL AND NOVEL METHODOLOGY FOR DYNAMIC OPERABILITY ASSESSMENT

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UNIVERSITÉ DE MONTREAL

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Ce mémoire intitulé:

DYNAMIC SIMULATION OF A FINE PAPER MILL AND NOVEL METHODOLOGY FOR DYNAMIC OPERABILITY ASSESSMENT

présenté par : VIA DOMINGUEZ Dante Alejandro.

en vue de l'obtention du diplôme de : Maîtrise ès sciences appliquées

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DEDICATION

To my wonderful family.

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RÉSUMÉ

L'industrie papetière est très complexe à cause de son haut degré d'intégration. Le procédé conçu pour fonctionner en continu est interrompu par de fréquents cassés du papier, qui sont imprévisibles. Cette perturbation affecte tout le système au travers des réseaux d'eau blanche et de cassés provoquant la variabilité du procédé. Ce qui affecte également la stabilité de la machine à papier en augmentant les probabilités de casses additionnelles.

L'analyse de problèmes aussi complexes requiert l'utilisation d'outils adéquats, comme par exemple la simulation dynamique, qui nous permet d'étudier le comportement d'un procédé réel de manière réaliste.

L'opérabilité dynamique est un autre outil qui nous permet d'évaluer les limitations inhérentes du système pour atteindre des objectifs de commande déterminés.

Les objectifs principaux de ce projet ont été de développer un modèle dynamique pour un procédé de fabrication de papier et de développer un outil d'évaluation d'opérabilité dynamique d'un système.

Dans la première partie du projet, plusieurs logiciels commerciaux de simulation ont été évalués pour déterminer leur capacité à résoudre des simulations dynamiques. Aussi, les conditions pouvant affecter l'exactitude de ce type de simulateurs ont été étudiées

comme les techniques propres de chaque simulateur permettant de minimiser les erreurs de calcul.

La simulation dynamique avait pour buts d'étudier la variabilité du procédé compte tenu des changements survenant dans le procédé et la commande dans le système de gestion de cassés, et de pouvoir l'utiliser comme une plante « virtuelle » pour l'analyse d'opérabilité.

La simulation dynamique du procédé de fabrication du papier a montré que les variables clés dans l'aire de mélange de pâtes, capables de provoquer la variabilité dans d'autres parties du procédé, en particulier à l'entrée de la machine à papier, sont le contenu en fines et les changements dans la proportion des cassés. La simulation dynamique a aussi montré que pour des changements manuels dans les consignes, la fréquence des changements affecte plus la variabilité que la magnitude de ces changements.

Dans la seconde partie de ce projet, une analyse d'opérabilité de la section de mélange des pâtes a été effectuée en utilisant la méthodologie développée par Vinson et Georgakis (2000) pour des systèmes en régime permanant.

Les principales idées de cette méthodologie ont été utilisées pour développer une nouvelle méthodologie pour l'analyse de l'opérabilité dynamique.

La méthodologie proposée combine des nouvelles idées avec des concepts bien établis. Une nouvelle mesure d'opérabilité dynamique (dOM) a été proposée en tenant compte des caractéristiques d'opérabilité inhérentes au procédé et au système de commandes.

Un nouvel indice de performance de commande a été défini, en tenant compte des contributions de la variable contrôlée et manipulée.

Cette méthode est applicable à des nombreux types de procédés incluant des systèmes linéaux et non linéaux, systèmes d'une entrée et d'une sortie et pour des systèmes de plusieurs entrées et sorties sans aucune zéro à partie réelle positive.

L'application de cette nouvelle technique dans le système de gestion des cassés nous permettra le calcul des espaces d'opération requis pour atteindre des niveaux acceptables de variabilité dans la casse d'arrivée.

ABSTRACT

The papermaking industry is very complex due of its high degree of integration. The process, designed for continuous operation, is interrupted by frequent paper breaks, which are unpredictable. This perturbation affects the whole system through the white water and broke networks, causing variability in the process. This affects the paper machine stability and increase the probability of more breaks.

The analysis of complex problems requires adequate tools. One of such tools is the dynamic simulation, which allows us to study the behaviour of a real process in a realistic manner. Dynamic operability is another tool that allows us to evaluate the inherent limitations of the system to achieve control objectives.

The main objectives of this project were to develop a dynamic model for a papermaking process and to develop a tool for evaluating the dynamic operability of a system.

In the first part of the project, several commercial simulation packages were evaluated to determine their capabilities for dynamic simulation. Also, the conditions affecting the accuracy of these simulators were studied, as well as the specific techniques to minimise the calculation errors.

The purposes of the dynamic simulation were to study the process variability due to changes in process and control in the broke management system, and to be used as a 'virtual' plant for the operability analysis.

Dynamic simulation of the papermaking process showed that the key variables in the area of pulp metering and blending, capable to cause variability in other parts of the process, in particular at the entrance of the paper machine, are the fines content and changes in the broke ratio. Dynamic simulation also showed for manual setpoint changes in the broke ratio, that the frequency of these changes rather than their magnitude affects more the variability of the process.

In the second part of this project an operability analysis on the stock proportioning system was performed, using the methodology by Vinson and Georgakis (2000) for steady-state systems. Basic ideas of this approach were used for developing a new framework for dynamic operability assessment. The proposed methodology combines well-established concepts and a few new ideas. A new dynamic operability measure (dOM) was proposed by taking into account the process inherent operability characteristics and the control system. A new control performance index was defined, by taking into consideration the contributions of controlled and manipulated variables.

The applicability of this method covers a wide range of processes, including linear and nonlinear systems, single-input single output systems and for multi-input multi-output systems without RHP transmission zeros.

Applying this new technique on the broke management system would allow determining the required operating spaces to achieve target levels of variability in the headbox.

CONDENSÉ EN FRANÇAIS

Dans l'industrie papetière, le groupe de produits connus comme *papier fins*, comprend tous les papiers blancs destinés à l'écriture et à l'impression, tels le papier bond, l'offset et le papier pour photocopie. La plupart de ces produits ne contient pas de pâte mécanique (wood free), et utilise différentes proportions de pâte de bois feuillus et de résineux pour atteindre un équilibre entre qualité et coût. La pâte de bois feuillus est utilisée pour améliorer la formation du papier et la pâte de bois résineux pour augmenter sa résistance mécanique.

L'élaboration du papier est un processus complexe. Le degré élevé d'intégration augmente la complexité de ces procédés et rend le contrôle plus difficile. De plus, de fréquentes perturbations dans le système interrompent la continuité du procédé. La perturbation, la plus importante du procédé est la casse de feuille de papier. Cet événement est imprévisible et peut se produire n'importe où dans la machine, mais souvent dans la zone de presse et dans la presse de couchage. L'effet de ces casses ne reste pas dans la machine. Cette perturbation se propage partout le système au travers du réseau d'eau blanche et du système de re-circulation de cassés, en occasionnant des variations dans le système.

Il y a une relation directe entre la variabilité du procédé et la stabilité de la machine à papier. Selon Gess et Kanitz (1996), une machine à papier travaille de façon *stable* quand la rétention dans la feuille est constante et quand les propriétés de la pâte ne changent pas de façon significative. Selon Rantala *et al.* (2002), la stabilisation et l'optimisation de la partie humide signifie atteindre un maximum de drainage et de rétention. Ces auteurs ont identifié six variables clés pour la stabilité de la partie humide, à savoir : Consistance, cendres, pH, charge, conductivité et température.

Dans un atelier de papier fin, les plus importantes caractéristiques de qualité à contrôler pour ce type de produit sont tout particulièrement la formation et la porosité. Les variables du procédé qui sont déterminantes pour ces caractéristiques-là sont la consistance, les fines et les cendres.

Pour les papiers fins, en général la proportion de cassés dans la composition de pâtes ne dépasse pas 30% pour la plupart des papiers couchés et 20% pour les papiers non couchés. Idéalement, cette proportion doit être constante et rester à un niveau bas. Cependant, des contraintes reliées à la capacité de stockage de pâte empêchent souvent d'atteindre cet objectif. Le taux de recyclage de pâte cassée est donc contrôlé en fonction du niveau de réservoir de casse. Les variations de ce taux de recyclage cause des changements dans les propriétés de la pâte mixte. Des grands changements de ces propriétés à l'entrée de la machine (caisse d'arrivée) sont associés à l'augmentation de l'instabilité de la machine. La façon de régler le recyclage des cassés peut donc contribuer à l'augmentation de la variabilité du procédé dans la caisse d'arrivée, et en conséquence, affecter la stabilité de la machine à papier.

La simulation de procédés est un outil d'analyse très utilisé depuis quelques décennies pour analyser des systèmes complexes, tel le procédé de fabrication de pâte et papier.

En particulier, la simulation dynamique d'un procédé peut donner des informations cruciales sur le comportement d'un système pendant une période de perturbation et sur les relations de cause à effet, qui sont autrement très difficile à analyser. Un autre outil d'analyse qui peut fournir de l'information sur les limitations propres au système pour atteindre des objectifs de contrôle est l'analyse d'opérabilité. Elle peut donner des informations sur la capacité inhérente du système à répondre à un changement de la consigne de contrôle et pour rejeter une perturbation.

Les objectifs de ce projet ont été définis comme

- étudier plusieurs logiciels de simulation, séquentiels et simultanés pour mieux connaître leurs capacités pour réaliser des simulations dynamiques dans le but de sélectionner un logiciel permettant de développer une simulation dynamique.
- Développer une simulation dynamique d'un atelier de papier fins dans un premier lieu afin d'étudier la variabilité du procédé dans la caisse d'arrivée causée par des changements apportés au procédé et la commande dans le système de gestion de cassés, et aussi pour être utilisé dans l'analyse d'opérabilité.
- étudier les caractéristiques d'opérabilité en régime permanent du système de gestion de cassés et sa capacité de changer entre différentes conditions opérationnelles, et pour rejeter les perturbations.
- développer une méthodologie générale pour évaluer l'opérabilité dynamique des systèmes, qui permet d'évaluer l'effet combiné du processus et du système de contrôle sur l'opérabilité dynamique.

Dans la première partie de ce projet, plusieurs logiciels commerciaux de simulation ont été évalués. On a trouvé que les problèmes de convergence dans les boucles re-circulation sont reliés à l'algorithme de calcul pour les simulateurs séquentiels, car le débit re-circulé est toujours retardé par un pas temps. La meilleure solution pour ce problème c'est la solution itérative de la boucle de re-circulation. Un des simulateurs évalué dispose d'une technique, le réseau débit-pression, qui génère l'itération locale de variables sélectionnées. Un autre aspect dont il faut tenir compte avec ce type de simulateurs, spécialement si la solution itérative n'est pas possible, c'est la sélection très minutieuse de l'ordre de calcul, pour éviter la non convergence. Un pas de temps suffisamment petit, généralement plus petit qu'1 minute, est toujours recommandé pour une simulation dynamique. Pour les simulateurs simultanés, aussi nommés orientés équation, la plupart des problèmes de convergence est reliée à la singularité du problème. Un problème est singulier quand il y a redondance dans la spécification du problème.

Une simulation dynamique d'une usine de papier fin a été développée en utilisant un simulateur simultané, MASSBAL®. La simulation comprend toutes les opérations principales, la section de préparation de la pâte, la section de casses, le circuit d'eaux blanches et l'aire de récupération de fibres, et la machine à papier. Cette machine produit environ 850 t/d et utilise trois types de pâte : la pâte de bois feuillus (HW), produite localement, la pâte de bois résineux (SW) et la pâte cassée ramassée dans la machine à papier et recyclée dans le procédé. La proportion de pâtes vierges (HW et SW) est maintenue constante (85 / 15) et la proportion de pâte cassés additionnée varie entre 10 et 30 %. Différents produits chimiques sont additionnés dans plusieurs endroits du procédé pour améliorer les propriétés mécaniques et optiques du papier. La charge (PCC) est additionnée à la pâte au taux d'environ 15%. La consistance de la pâte diluée à l'entrée de la caisse d'arrivée se situe aux alentours de 0.8%.

La condition de base pour les simulations a été fixée pour une re-circulation de cassés de 10%. Aucune casse dans la machine n'est considérée pour la condition de base.

Pour l'analyse de variabilité, des changements ont été imposés sur plusieurs variables dans la section de gestion de casses. Les variations suivantes ont été considérées:

- Consistance de la pâte HW: 5 % (4.5 – 4.725 %)
- Contenu de fines dans la pâte HW: 20 % (8.0 – 9.6 %)
- Consistance de la pâte cassée diluée: 5 % (4.0 – 4.2 %)
- Proportion de cassés: 50 % (10 –15 %)

L'analyse de variabilité montre clairement que le contenu de fines et la proportion de casses sont deux importantes sources de variabilité dans la caisse d'arrivée.

Des simulations ont aussi montré pour le cas où la re-circulation de cassés est régulée de façon manuelle, que la fréquence de changements de la consigne du contrôleur cause une plus grande variabilité dans le procédé que la magnitude de ces changements. Pour le cas de régulation automatique de la proportion de cassés, les résultats montrent qu'un contrôleur de niveau de réservoir de cassés à haute densité, plus agressif, cause une variabilité plus grande et plus courte dans la caisse d'arrivée, que le même contrôleur calibré de façon plus conservatrice.

Dans la dernière partie de ce projet, plusieurs méthodes ont été appliquées à l'analyse d'opérabilité en régime permanent de la boucle de contrôle du ratio de cassés. La méthode développée par Vinson and Georgakis (2000) a été tout particulièrement utilisée pour évaluer la capacité de cette boucle de contrôle pour répondre à des changements dans la consigne de contrôle. Les résultats montrent que le système à boucle fermé est stable, qu'il y a une interaction forte dans le petit système multidimensionnel considéré pour cette analyse et que le système est un peu surdimensionné pour le rendre plus flexible face à de possibles changements d'opération ou de production.

Finalement, une nouvelle méthodologie pour l'évaluation de l'opérabilité dynamique a été développée. Cette méthodologie est basée sur l'idée de Vinson concernant les espaces opérationnels et introduit quelques nouvelles idées. Un nouvel indice d'opérabilité dynamique a été proposé. Cet indice tient compte explicitement les contributions du procédé et du système de contrôle à l'opérabilité dynamique à boucle fermée. Un nouvel indice de performance de contrôle pour des changements déterministiques dans le procédé a été proposé. Cet indice considère aussi explicitement les contributions de la variable contrôlée et de la variable manipulée. Cette méthode est applicable à plusieurs types de systèmes, incluant le système considéré dans ce projet.

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LIST OF SYMBOLS AND ABBREVIATIONS

CHAPTER 1

CD	cross-direction
MD	machine direction

CHAPTER 2

AIS	available set of inputs
AOS	achievable output space
APC	advanced process control
C&R	controllability and resiliency
CN	condition number
DAEs	differential and algebraic equations
DC	disturbance cost
DCN	disturbance condition number
DCS	distributed control system
DOS	desired output space
EDS	expected disturbance space
IAE	integral absolute error
IDA	input disturbance alignment
ISE	integral squared error
ITAE	integral time-weighted absolute error
ITSE	integral time-weighted squared error
MPC	model predictive control
OCI	output controllability index
RDGA	relative disturbance gain array
RGA	relative gain array
SVD	singular value decomposition

dOI	dynamic operability index
f	funcion f
g	funcion g
t	time
x	state variable
y	controlled variable
y_{sp}	set point
ε	controller error
σ	singular value

Indices

max	maximum
min	minimum

CHAPTER 3

CL	closed loop
MIMO	multi-input multi-output
OL	open loop
SISO	single-input single-output

CHAPTER 4

E	calculation error
F	flowrate
GUI	graphical user interface
t	time
t_s	total simulation time
x	recirculation ratio

Indices

k	iteration number inside each time step

CHAPTER 5

A	ash content
BR	broke ratio
Br	diluted broke
DS	dissolved solids
F	fines
F_1	stream 1 flowrate
HW	hardwood
IMC	internal model control
K_c	controller gain
KIC	consistency controller
K_p	process gain
L	long fibers
LIC	level controller
M	medium-size fibers
PCC	precipitated calcium carbonate
PID	proportional integral derivative controller
PM	paper machine
RVI	relative variability index
SP	setpoint
T	temperature
T_I	controller time constant
VI	variability index
c	consistency
$\hat{y}$	normalized (adimensional) variable
y	variable
y^N	value of y at steady-state
λ	closed loop time constant
τ_p	process time constant

CHAPTER 6

G	steady-state gain matrix
N	Niederlinski index
R	ratio
S	sensitivity function
T	complementary sensitivity function
V	volume
d	disturbance
h_2	level of mixing chest
q	normalized flowrate
r	setpoint
Λ	relative gain array

<u>Indices</u>

i	stream number

APPENDIX A

T_I	controller reset time
Ts	time step
g_F	forward process
g_R	recycle process
k	gain constant
u	manipulated variable
y	controlled variable
γ	factor for disturbance rejection
θ	dead time
λ	closed loop time constant

APPENDIX B

A	area
$AIS(t)$	dynamic available input space
$AIS(t)$	dynamic available input space
$AOS_u(t)$	achievable output space
B	step change in the setpoint or in the disturbance
CV	controlled variable
$DIS_d(t)$	dynamic desired input space
$DOS(t)$	dynamic desired output space
$EDS(t)$	dynamic expected disturbance space
$K_{ij,eff}$	effective gain matrix
MV	manipulated variable
R	ratio, reference value
V	volume
a	normalized area
c	consistency, concentration
d	disturbance
dOM	dynamic operability measure
f_{op}	operable fraction
h	tank level
k	time step
q	normalized flowrate
r	regulatory, normalized ratio
r	setpoint
s	servo
t	time
t*	transient period
t_d	delay time
t_s	settling time

t_{ss},	time to steady-state
u(k)	value of MV at time step k
x	normalized state variable
y(t)	value of CV at time t
α	factors of the CV performance
$\bar{\varepsilon}_u$	average value of the relative error over the transient period
ε_u^*	reference value of ε_u
$\varepsilon_u(k)$	relative error of MV at time step k
ε_y^*	value of ε_y below a selected limit
$\varepsilon_y(t)$	relative error of CV
η	performance
λ_{ij}	relative gain
μ	a function calculating the size of the corresponding space
υ	normalized volume

Indices

A	ash
DS	dissolved solids
I	initial steady-state value of MV
f	final steady-state value of MV
f	fines
i	CV i
j	MV j
u	MV
y	CV

LIST OF APPENDICES

CHAPTER 1: INTRODUCTION

1.1 Problem statement

The term fine paper refers to a broad range of white, uncoated papers for writing and printing, including offset, bond and photocopying. Most of the furnishes use only chemical pulps (wood-free). Generally, hardwood (short fibers) and softwood (long fibers) are used in different proportions, in order to achieve a good relation between product quality and cost.

During the normal operation of a paper machine, it is common to have web breaks in different parts of the machine. Paper breaks are the main source of variability and affect the entire system through the broke and white water network.

The broke pulp collected in the paper machine is sent back to the stock preparation area and mixed with virgin pulp. For fine paper, the amount of broke used in the furnish cannot be too high. Indeed, product quality considerations limit its use to about 30 % in coated grades and up to 20 % in most noncoated grades. Ideally, the broke ratio should be kept constant at a low level. However, this is usually not possible because of inventory constraints. Mill experience tells us that there is a close relationship between the way the broke is managed and the variability of the pulp composition in the headbox. Large and sudden changes in the broke ratio, for instance, are associated with a deterioration of the paper machine stability and, therefore, with an increment of the frequency of paper breaks. Variation in the furnish composition also causes variability in product quality. Thus, a proper design and operation of the pulp blending system is essential for both paper machine stability and acceptable product quality. Nonetheless, it is surprising how this part of the papermaking process is low rated in many mills.

A paper machine is operating in a stable fashion when the retention is constant and the quality of the furnish coming into the system is uniform (Gess and Kanitz, 1996). The main factors affecting the retention are the wet-end chemistry and the fines content in the diluted stock.

According to Rantala *et al.* (2002), the stabilization and optimization of wet end chemistry entails achieving maximum drainage and retention. This is vital for achieving optimal paper quality and paper machine runnability. The authors identified six key variables affecting wet end stability, namely: Consistency, ash, pH, charge, conductivity and temperature. In particular, consistency variations in the short circulation directly impacts on paper quality (MD and CD) and break tendency, and ash variability affects paper quality (strength and porosity), which generates problems in coating and printing.

This work does not intend to solve any specific operating problem, but rather to study steady-state and dynamic overall operability characteristics of the broke management system. Our purpose is to show how they are related to the capability of the control system to reject disturbances, and how changes in process and control in the broke management system affect the variability of key variables, such as consistency, ash and fines content, at the entrance of the forming zone of the paper machine, and the retention. Two analysis tools are used for this purpose, *process simulation* and *operability assessment*. Based on our review of previous works on these subjects, we are also proposing a new general approach to assess the dynamic operability of processes.

1.2 Hypotheses and thesis objectives

An important underlying assumption in this work is that the stability of the paper machine can be affected by the way in which pulp addition is controlled.

The hypotheses of this project are:

- Simulation convergence problems during the transient period can be addressed with an appropriate problem formulation and suitable calculation techniques
- Process variability in the headbox using different process control approaches for the broke management system can be quantified using dynamic process simulation
- The steady state operability analysis by Vinson & Georgakis can be applied to the broke management system of a paper machine to give important insight into process flexibility to achieve control objectives and the inherent capability of the process to reject disturbances.
- Dynamic process operability including control structures can be described using input/output controllability

The objectives of this project are the following:

- To evaluate the capabilities of various sequential and simultaneous simulation packages for dynamic simulation, focusing on their strengths to overcome common problems when developing a dynamic model, with the purpose of selecting an appropriate tool for the operability objectives of this work.

- To develop a dynamic model of a fine paper mill in order to study the process variability in the headbox due to process and control changes in the area of stock proportioning, and to be used in the operability analysis.
- To study the steady-state operability characteristics of broke handling and the ability of the closed loop to move from one operating point to another, and to reject disturbances.
- To develop a general methodology for assessing dynamic operability that can be used to evaluate the combined effect of process dynamics and control system on the operability of processes.

1.3 Methodological approach

The methodology applied in this work, described in detail in **Chapter 3**, consists of four major phases:

- Evaluation of several dynamic simulation packages and the development of the dynamic model of a paper mill.
- Development of the dynamic model of a paper mill and application of this model to the analysis of the impact of process and control changes in a selected sub-system in the stock preparation area, on the variability of key process variables.
- Application of different analysis tools to the steady-state operability analysis and closed loop sensitivity analysis of the selected sub-system.
- Development of a general approach to assess the dynamic operability of processes.

This work is divided as follows: In **Chapter 2** an extensive literature review is given, covering key technical areas of relevance for this research work. **Chapter 3** treats the global methodology used in this work. The evaluation of several dynamic simulation packages and the methodology used to select a simulation tool is given in **Chapter 4**. The strategy used to develop a dynamic simulation is explained **in Chapter 5**, as well as the process variability analysis. In **Chapter 6**, an eclectic methodology for assessing the steady-state of a selected sub-system and the closed-loop sensitivity analysis are presented. Also, a new methodology for the assessment of the dynamic operability is developed in this chapter. In **Chapter 7**, the results are summarized, a few conclusions are drawn and the main contributions of this work are given.

CHAPTER 2: LITERATURE REVIEW

PART I: DYNAMIC SIMULATION

2.1 Process modeling and simulation

Modeling is the mathematical representation of the real world. The 20th century was called the chemical engineering's modeling century (Levenspiel, 2002). Simulation is the imitation of a real process or system (Banks, 1999). It involves a model and experiments made on it to generate an artificial history of the system with the purpose to draw inferences about the operating characteristics of the real system that is represented. Modeling and design are closely related. Engineers use models and simulation by designing new systems to aid in their decision making.

A *process flowsheet* is a collection of icons to represent process units and lines to represent the flow of materials between the units. A *simulation flowsheet*, on the other hand, is a collection of simulation units to represent computer programs (subroutines or models) that *simulate* the process units by solving material and energy balances of the process flowsheet and use stream lines to represent the flow of information from one unit to another. A simulation flowsheet emphasizes information flows (Seider *et al*, 1999). Probably this explains why most simulation programs designed for chemical engineers are process-oriented rather than product oriented.

2.1.1 Steady-state versus dynamic simulation

Steady-state process simulation or *process flowsheeting* is the detailed analysis of process flowsheets by solution of the steady-state material and energy balances (Barton and Pantelides, 1994). The process model can be represented by a system of nonlinear algebraic equations:

$$f(\mathbf{x}) = \mathbf{0} \tag{2.1}$$

where the variables represent the quantities of interest in the system, for example: flow rates, composition, pressure, temperature, heat exchanger duty. The model may also impose linear or nonlinear inequalities that must be satisfied:

$$g(\mathbf{x}) \geq \mathbf{0} \tag{2.2}$$

For example: all temperature and pressure quantities must e positive, dilution rates are specified, concentrations are bonded on a closed interval.

There are three types of problem that can be solved using a flowsheeting program (Shacham *et al.*, 1982): In the *simulation problem,* the process inputs associated with feed streams and the design variables of the units should be specified, and the outputs are unknown. The *design problem* is similar to the simulation problem, except that in this case we want to calculate an input value or equipment parameter from output variables. In the *optimization problem*, some input and design variables may be left unspecified and a cost function is added to the model (**equation 2.1**). Typically, only continuous variables are optimized. Design can be seen as a mathematical programming problem (Westerberg, 2004) which involves the generation of a *superstructure* representing the design space within which are all the design alternatives (*substructure*);

this is the first issue in process synthesis. The second issue is to search, within an optimization framework, among the enormous number (often hundreds to thousands) of alternatives the economically best alternative.

In a *process dynamic simulation* the process model can be represented by a system of nonlinear ordinary differential and algebraic equations (DAEs):

$$\boldsymbol{f}(d\mathbf{x}/dt, \mathbf{x}, t) = \mathbf{0} \tag{2.3}$$

where d**x**/dt represent the derivatives of variables with respect to the independent variable, the time. As with a steady-state process simulation, a dynamic model also includes a number of constraints. The typical calculation is to predict the transient (time dependent) behaviour of a process.

2.2 Simulation tools and main approaches to dynamic simulation

Ponton (1994) defines a *tool* as a software package designed to carry out a well defined although often complex task or set of related tasks and an *environment* as a software system designed to support the use of one or more tools. Tools used in design are process simulators, numerical solvers, and language compilers. Environments include computer operating systems, process simulation packages and modeling systems.

In the early days, dynamic process simulation was performed almost exclusively using high-level programming languages (e.g., FORTRAN, BASIC, Pascal and C) as a tool, but the increasingly power of computers made possible the use of spreadsheet programs and encouraged the development of commercial modular simulation packages (Schroderus *et al.*, 1991). *High-level programming languages* are still in use, they have a number of advantages compared to other methods, including: they are the most flexible simulation environment; they can be used to simulate virtually any type of simulation problem. Despite these advantages, high-level programming languages have some serious disadvantages. Building the simulation of a complex process requires a high degree of programming skills, making the simulation a challenging and time consuming task.

Early 1990s there was a clear trend towards the paradigms of *object-oriented programming*. The application of this approach to the modeling and simulation of dynamic systems made possible the development of flexible general purpose simulation packages supporting hierarchical modeling (*inheritance*), procedures clustered into libraries for reuse (Samphat *et al.*, 2000), and implementation of complex heterogeneous systems using an architecture of the type client-server (Hatnik *et al.*, 2001).

The second group of simulation tools mentioned above, the *spreadsheet programs* have been used since the late 70s, when the first of such programs, VisiCalc, appeared. Spreadsheets are simple and intuitive to use, but clearly they do not have the flexibility to model many practical problems involving dynamic systems. Among the limiting factors for the use of spreadsheets for dynamic simulation we can mention their inefficient use of memory; they do not have convenient facilities to implement a while-loop or a for-loop; complex algorithms are difficult to implement and they are usually slower than commercial simulation packages (Seila, 2003). Perhaps the most serious drawback of spreadsheets is the difficulty of achieving convergence when there are complex interdependencies, or when the calculations depend heavily on physical properties (Julian, 1989).

Most authors distinguish between *sequential modular approach* in which the equations describing each process unit (module) are solved module-by-module in a sequential manner and the *equation-solving approach* in which the entire process is described by a set of differential equations, and the equations are solved simultaneously. However, hybrid systems are also possible. These systems referred to as *simultaneous modular approach*, divide the units in computational loops which are solved together while keeping the overall sequential modular structure. A detailed discussion of these approaches may be found in Westerberg *et al.*, (1979). All these approaches, applied first to process flowsheeting problems, were used to solve dynamic models thereafter. The evolution of steady-state flowsheeting programs and dynamic simulators has been similar in that sense. Some of the flowsheeting packages enhanced their programs with dynamic capabilities. For example, using simple (Euler-type) time-stepping techniques and adding time constants (or capacities) for appropriate units, a steady-state simulator could be applied directly to a dynamic system (Biegler, 1989).

2.2.1 Sequential-modular approach

The most widely used structure for flowsheeting programmes is still the sequential-modular structure. Each unit is represented by a separate mathematical model (unit model) which calculates its outputs given input streams and unit parameters (Perkins, 1979). In sequential simulators a large system is decomposed, or "partitioned" into a set of smaller subsets which can be processed sequentially by "tearing" – a procedure of further decomposition and guessing of a certain subset of variables which are used as initial values to calculate the unknown variables (Westerberg *et al.*, 1979).

The main drawback of this approach is its difficulty to deal effectively with downstream (design) specifications and with recycle streams (of material or information). This is because sequential simulators calculate the outputs of each unit module using known inputs which have to be specified or guessed. As Perkins (1979) points out, there are two approaches to overcome this problem. The first approach uses an *iterative solution*, either letting the user control the iteration of the whole process, or using *control blocks* (**Figure 2.1**) to iterate a number of variables until convergence on the design requirements – implicit iteration.

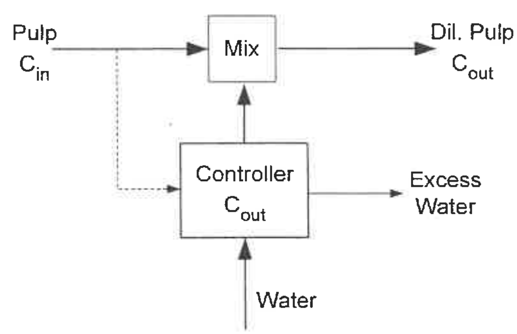


Figure 2.1: Control block to control the outlet consistency of a dilution point
(dashed line: information flow)

Recycle loops require *convergence blocks* or flow pressure networking. Iterations occur to satisfy material, temperature and pressure agreement in a given recycle stream – explicit iteration.

2.2.2 Simultaneous-modular approach (Hybrid systems)

Although most of the effort in the past fifteen to twenty years has been devoted to the simultaneous solution of the entire system, a long way is still to cover to see a simulation package with the power and flexibility of a simultaneous simulator and the obvious advantages of a sequential modular simulator. The rigid (fixed) structure of the unit routines in the sequential modular simulators and their procedural (sequential algorithm) language in general makes the simultaneous solution for the whole process less effective, particularly for design or dynamic simulation (Hernandez and Sargent, 1979).

2.2.3 Equation-based approach

From early 1960's it became apparent that the "modular approach" for process flowsheeting has several limitations when dealing with a process model where the information in the mathematical model does not coincide with the flow of materials in the physical plant, but until mid-1970's most of the effort was oriented to the development of more reliable algorithms to decompose large sparse equation systems and to tear recycle streams. At that time this tendency began to change, leading to the development of the so-called *equation-based* or *equation-oriented*, simultaneous approach. The development of a fully equation-oriented flowsheeting program, FLOWSIM, was begun at the University of Connecticut in 1975 (Shacham *et al.*, 1982).

While the modular organization is typical for sequential simulators, as Sargent (1979) points out, a flowsheeting package does not have to be based on linking subroutines in order to be 'modular' and equation-based simulators can be just as modular in the sense that the numerical solutions procedures (executive) are separated from the plant description (library of unit modules) and hence can be changed at will. In this case the unit modules return the equations describing the unit to the executive which then solves the total set of equations describing the process (Gorczynsky *et al.*, 1979). The unit modules become sets of equations which are introduced explicitly as a type of equation or implicitly as another module. The unit modules can thus be constructed in a building block manner from a relatively small set of equation types, in much the same way as a flowsheet is built-up from unit modules. The essential idea in modular-organized equation-based simulators is to have each model (module) contributing its equations only and not a solution of them (Westerberg, 1998). Examples of this type of flowsheet packages are QUASILIN®, SPEED-UP® and MASSBAL®.

2.3 Steps in model building

Model building involves several steps. Several authors (Banks, 1999; Law, 2000; Carson, 2003) have given general guidelines for a simulation project. A systematic procedure for building a model from first principles has been given by Marquardt (1996), and Hangos and Cameron (2001). The phases and steps differ something from one author to another, but they generally include the following:

1. *Problem formulation and settings of objectives*. Three important overall considerations are:
   - Model boundary and scope,
   - Level of detail,
   - Project scope

2. *Overall project plan* - time estimates and project timelines.
3. *Conceptual model and assumptions.* This phase involves the decision-making on how to represent each operation unit (set of equations or modules required) and a list of all assumptions (e.g., a reservoir may be considered 'perfect mixed').
4. *Data collection, pre-treatment and analysis.* Data sources include databases, manual records, automatic data collection systems, samples, laboratory analysis, and verbal information. Data pre-treatment may include filtering to remove 'noise', averaging, elimination of trends, and elimination of gross-errors (data reconciliation).
5. *Model building.* The conceptual model constructed in Phase 3 is coded into a computer recognizable form, an operational model.
6. *Model Verification and Validation. Verification* deals with building the model *right*. It involves the *inspection* of the model to verify whether the transformation from a flowchart form into an executable computer program has been done correctly, and the process of finding and removing programming errors (debugging). Thus, it answers to the question "Does it work correctly?" Verification seeks to show that the computer program performs as expected and intended. *Validation*, on the other hand deals with building the *right* model. It aims to answer the question "Does the model adequately represent the real-world system?" Through validation, we try to determine whether the simplifications and omissions of detail that we have knowingly and deliberately made in our model, have introduced unacceptably large errors in the results. Several excellent references are Balci (1997), Sargent (1999), Anagnostopoulos (2002), and Yuan *et al.* (2003).

7. *Experimentation, analysis and reporting* - This phase involves: Design of scenarios to be simulated, decisions concerning the number and length of runs, analysis of results and documentation.

2.4 Main Applications of dynamic simulation

Typically, dynamic flowsheet simulation packages are presented in the literature as a tool used throughout the life cycle of a plant, from conceptual design through the operational analysis (Goldfarb, 1995), but dynamic simulation is also gaining importance in process design as a means of verifying the controllability and disturbance resiliency (these terms are defined in section 2.8) of a potential process (Seider *et. al.*, 1999) and for development of advanced process control (APC) systems and operational optimization. So, Ye *et al.* (2000) report a graphical user interface that combines a dynamic simulator and a distributed control system (DCS) that creates a virtual plant in the computer. This system has been used for training operators and to analyze and tune the APC controllers.

In industrial practice, however, most of the applications have dealt with *operation* or *retrofitting*. Laganier (1996) lists several reasons why we have not been able to fully exploit the potential capabilities of this tool. The first and probably the mayor reason is the difficulty to achieve a satisfying profit-to-cost ratio with the commercial software currently available. A second difficulty lies in the user-friendliness and robustness – or lack of them. In effect, building a complex process model requires a lot of practice with a specific software, and the model might not seem robust enough to be modified by anyone else, but only by the model builder, unless the user knows really well the simulation package. This makes a model, in general, less useful for the final user. As Barton (1992) points out, the large investment required to build a dynamic model can be justified only if it becomes a knowledge base on which activities throughout the entire lifetime of a process can be based.

Typically, traditional applications of dynamic simulation are *off-line*. Biegler *et al.* (2002) enumerate a list of such applications:

- design to avoid undesirable transients for chemical processes during process startups and shutdowns,
- design of distributed (dependent on spatial position) unit operations such as reactors,
- design and dynamic operation of batch processes,
- evaluation of control schemes under abnormal operations.

2.4.1 Applications in the pulp and paper industry

Applications of dynamic simulation reported in the literature include:

Rounsley (1983) used the simulation package SLAM (Simulation Language for Alternate approaches to Modeling) in combination with the programming language FORTRAN to evaluate the broke handling system of a new paper machine. Croteau and Roche (1987) developed a dynamic simulation of an integrated newsprint mill using PAPDYN, to study the broke handling and the white water management in order to reduce fiber losses and to avoid broke tank overflows. Bussière *et al.* (1992) used the dynamic version of PAPMOD, simulator developed at Paprican, to investigate the cause of variations in the properties in ultra-high yield pulp used as a furnish for a newsprint machine. Koskinen and Ritala (1993) discuss the use of digital signal processors (DSP) in the evaluation of control models and in the detection of process and sensor faults. The simulation environment used for this purpose was MATLAB/SIMULINK, and multivariate analysis (MVA) was used to analyze the difference between the true outputs and the simulated outputs. Jones and Koepke (1994) used MAPPS, a sequential modular simulator with dynamic capabilities to develop more robust control schemes for the wet end of a paper machine. Orccotoma *et al.* (1997) used SPEEDUP to study the dynamics of pulp components in newsprint mill as a function of paper breaks, changes in the broke ratio and changes in fines content in the inlet pulp stream. Shirt (1997) used IDEAS focusing on the wet end chemistry for a fine-paper machine. Niemenmaa *et al.* (1998) developed a dynamic model of a board machine for grade change control by combining standard unit operation models provided by APMS model libraries with new modules developed from first principles. A completely new paper machine model library was developed for APMS. Bonhivers (1999) developed a dynamic simulation using CADSIM plus PAPDYN to study the effects of paper breaks on the white water inventories and the paper machine operation, and to evaluate the disturbance rejection capacity of the control system. Kokko *et al.* (1999) used the simulation tool APMS to investigate the functionality of new process and control configurations in the stock preparation of a fine paper mill. Airikka *et al.* (1999), using the same simulator studied the effect of process variables on the basis weight and the ash content dynamics. Houle *et al.* (1999) studied different scenarios with the main objective to reduce fresh water consumption in an integrated newsprint mill; they used the CADSIM plus PAPDYN platform. Khanbaghi *et al.* (2000) developed a nonlinear model of a pressure screen for control purposes. This model was based on piping network theory and the dynamic version of Bernoulli's equation. Since the obtained model had unknown parameters, it was necessary to combine steady-state and dynamic estimation methods to identify the parameters. Simulation results were used to validate the model against a data set which wasn't used for estimation. Wilson and Balderud (2000) developed models at different degrees of complexity of a five layer paper-board machine using IDEAS and SIMULINK; they highlight the difficulties in validating a large dynamic model. Haag and Wilson (2001) report their experience building a large-scale board machine model using IDEAS and SIMULINK. Eddy *et al.* (2001) developed a dynamic simulation of newsprint paper machine wet end, using IDEAS to study the effect of grade changes on key parameters. Balderud *et al.* (2001) also used IDEAS to model at high level two board machines, for machine re-design and the development of new paper board grades in one case, and for control and optimization studies in the other case. They found that the simulation speed decreases considerably by hydraulic calculations, so for the required time step of 1 second, they could achieve simulations speeds of only 3 to 5 times faster than real time. Cho *et al.* (2001) applied mathematical modeling using the platform MATLAB/SIMULINK to study the filler retention in paper for a pilot paper machine at the Centre Spécialisé en Pâtes et Papiers (CSPP), CEGEP de Trois-Rivières. Lapièrre and Wasik (2002) created a module in CadSim Plus that peforms optimization by annealing using a modified simplex method; this module can be implanted in any

CadSim Plus model. Masudy (2003) used CadSim Plus to develop a high-fidelity dynamic simulation of a pulp mill from the digesters through the drying machines and the steam plant, in order to evaluate mill upgrade alternatives. Dabros *et al.* (2004) applied simulation-based optimization, using the platform WinGEMS plus Visual Basic to study broke recirculation strategies for an integrated newsprint machine. Inspired on the famous Tennessee Eastman challenge problem, Castro and Doyle (2004) present a complete benchmark problem of a pulping process (for both the fiber line and the chemical recovery areas).

2.5 Trends in process modeling and simulation

Marquardt (1996) has given a comprehensive review of the state of the art and trends in computer-aided modeling and simulation. He identified two mayor lines of development:

- General modeling languages, with the object-oriented model representation as underlying philosophy
- Integration of these languages in knowledge based modeling tools

The *object-oriented simulation*, with its object-hierarchical structure and its embedded model and simulation algorithm into the object (**Figure 2.2**), is still one of the main trends in the current development of new simulators. But, combining this procedure with the networking technology called *open architecture* is having a profound impact in how we work. This approach allows splitting very large and complex models in autonomous subsystems (objects), which can be simulated individually and worked up by separate team members using LAN's, WAN's, as well as satellite networks. Separately built objects can then be put together using a master program. The PTOLOMY® platform (Hatnik *et al.*, 2001) allows this type of modeling and simulation.

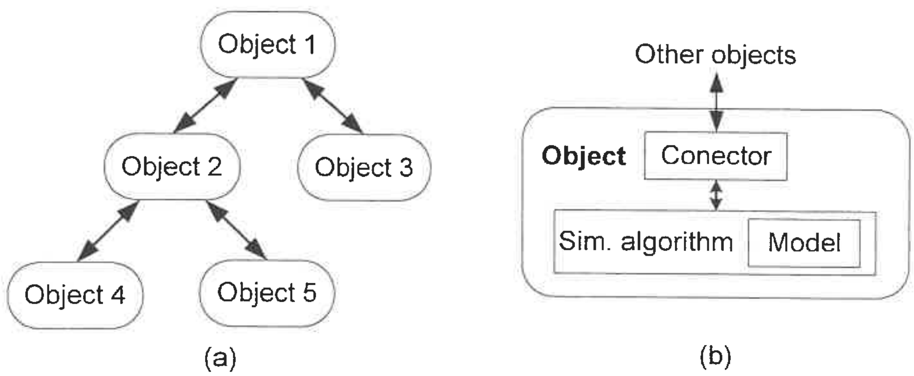


Figure 2.2: Object-hierarchy (a) and model building (b)

Scharwaechter *et al.* (2002) describe a prototypical simulation framework – CHEOPS® for the integration of different dynamic simulation tools. This approach has been applied to the modeling/simulation of a continuous process consisting of a reactor and a sequence of four distillation columns. In one case, for example, the reactor has been modeled by an equation-oriented modeling environment such as gPROMS®. An equation-oriented distillation model with detailed tray hydraulics was written in a generic modeling language such as Modelica, and a DAE solver was applied to simultaneously solve the reactor model and the model of the first distillation column, considering that these two units are in a cycle. The resulting modules are then linked with the controller module in e.g. MATLAB®/SIMULINK® and the rest of the plant model in e.g. HYSYS®. The obvious advantage of this approach is its high flexibility.

Other field of intense research at present is the *on-line* dynamic process optimization that can be considered as a natural extension of the dynamic simulation (Biegler *et al.*, 2002). Specific tasks in this area include:

- nonlinear model predictive control (NMPC) requiring the solution of a dynamic optimization problem with a nonlinear dynamic process model,
- system identification with nonlinear process models to identify the states and unmeasured inputs of the process, given measured inputs and outputs,
- estimation tasks related to identification including gross error detection, data reconciliation and model parameter estimation.

Perhaps the most spectacular example of new applications of dynamic simulation is the process simulation via the Web. In a recent publication, Gu *et al.* (2003) reported the use of the interactive Internet simulation (iiSIM®) system that according to the authors allows mill engineers to troubleshoot process problems and train new technical hires via the Internet. This system uses WinGEMS® as simulator interface.

2.6 Critique of sequential modular and the simultaneous approach

Sequential modular simulators are still the dominant type of simulators on the market. They have obvious advantages, but also some limitations.

Advantages:

- User-friendly program - easy for the users to understand and learn.
- Much smaller computer memory requirements. Only those equations involving one unit operation need to be solved simultaneously.

- Large number of existing unit operation models that calculate outputs given inputs are available in libraries. This simplifies the model building.
- Very robust (in comparison to equation oriented simulators). This characteristic facilitates making changes to the model.

Limitations:

- The fundamental limitation of sequential modular flowsheet simulators is that the pre-coded models (modules) are fixed.
- Difficult to converge highly integrated processes - i.e., many recycle streams.
- Design calculations much more difficult to set up and converge than simulation calculations.
- Computationally expensive, especially for models involving hydraulic calculations. For this reason, many dynamic simulations have to be limited to mass and energy balances.
- May converge badly posed problems - e.g., redundant specifications.

Simultaneous (equation-oriented) simulators, on the other hand have also their strengths and weaknesses.

Advantages:

- Much more efficient than sequential simulators solving complex models, involving recycles and design specifications.
- The artificial distinction between simulation and design specification sets is removed.

- The primary advantage of this approach is: it is much easier to extend the model library and modify existing models. In particular, this capability is very useful for dynamic simulation or flowsheet optimization.
- The diagnosis of certain modeling error (e.g., badly posed problems) is easier, because an equation-oriented simulator can analyze the entire equation system for problems such as singularity.
- More powerful programming capabilities.

Problems:

- Equation management is complex.
- Large computer storage required (not a serious problem with current computers).
- Numerical problems include obtaining derivatives and singularity.
- Models are highly sensitive to initial values.
- The more serious disadvantage of this approach is: the general purpose nonlinear equation solvers are not as robust and reliable as the sequential modular approach.

Part II: Operability Analysis

2.7 Process design and operation

Prior to the extended use of computers in the process of designing, process synthesis, the first stage of process design, was based essentially on "rules of thumb" (*heuristics*), gained in the industrial practice. Heuristics are still in use, but they are frequently organized into *expert systems* (Seider *et al.* 1999). The use of flowsheeting packages to screen design alternatives, characteristic of the first generation of synthesis tools, allowed engineers to *simulate* complex processes and get insight of the new process. The second generation was characterized by the application of optimization techniques in decision making with the unrealistic goal to replace the engineer by a machine. The third generation of tools is aimed to the development of techniques for the synthesis of flexible processes (Morari, 1983).

The need to integrate plant operation aspects (including process dynamics and control) into the earliest stages of a process design was realized for many years. So, Ziegler and Nichols (1943) six decades ago in an often cited paper emphasized the close interaction between process and control: "…it is important to realize that controller and process form a unit. A poor controller is often able to perform acceptably on a process which is easily controlled. The finest controller made, when applied to a miserably designed process, may not deliver the desired performance." However it was not until recently, when suitable tools and techniques were available, that the activities of process and control structure design could be integrated. Several authors (Zhu et al., 1996; Gál *et al.*, 1998; Lewin *et al.*, 2002; Meeuse and Tousain, 2002) stressed the importance of the integration of design and control. Some authors, notably Vu *et al.* (1997), Schweiger and Floudas (1997) and Bansal *et al.* (2000) have discussed two approaches to perform the integration of process design and control. In the first, interactions between design and control are considered but the steady-state process design and the control system are optimized *sequentially*. In the second approach, the process design and the control system are optimized *simultaneously* which allows the identification of more economical configurations. The development of rigorous, high-fidelity dynamic models is prerequisite for the successful application of these approaches.

Farschman *et al.* (1998) showed that one can develop stable, responsive control schemes for processes without having detailed dynamic models of them. All one needs are the dynamic material and energy balances based only on the inputs and outputs to the process. This seems to explain what control practitioners have observed many times in a plant; when people have installed PID controllers onto processes, and tuned them, they worked; without any model. However, if we are addressing the operability of a new plant, we will need accurate models, not only for the process being designed but also for expected disturbances. This of course poses another problem, because at early stages of the process design the required data are not usually readily available.

2.8 Controllability and dynamic operability of processes

The controllability theory for finite dimensional linear systems was introduced by Kalman (1960); he introduced the concepts of *controllability* and *observability* which play an important role in the control of multivariable systems. For any lineal system, described by the equations

$$\begin{aligned} \dot{\mathbf{x}} &= \mathbf{Ax} + \mathbf{Bu} \\ \mathbf{y} &= \mathbf{Cx} + \mathbf{Du} \end{aligned} \tag{2.4}$$

the system is said to be controllable if a control vector $\mathbf{u}(t)$ exists that will transfer the system from any initial state $\mathbf{x}(t_0)$ to some final state $\mathbf{x}(t)$ in a finite time interval. A system is said to be observable if at time t_0, the system state $\mathbf{x}(t_0)$ can be exactly determined from observation of the output $\mathbf{y}(t)$, (Roland, 2001). An important consequence of this definition is that the controllability can be used as a measure for the ability to use a system's external input to manipulate its internal state. On the other hand, observability is a measure for how well internal states of a system can be inferred by knowledge of its external outputs.

Since Kalmans's milestone-work a large amount of work has been done on the fields of process design and control, and on the interactions between design and control. However there is no general agreement on how the operating characteristics of a process should be characterized, and how the process controllability can be measured. Many terms and controllability measures have been introduced in the literature in an attempt to capture the close relationship between the inherent process characteristics and the operating characteristics. Operational requirements applied for chemical processes include: operability, controllability, flexibility, switchability, availability, reliability, maintainability and resiliency (see e.g. Perkins and Walsh, 1996; Van Schijndel and Pistikopoulos (1999) for an extensive overview). Some of these terms are used as synonymous, or with just slightly nuances in the meaning. Meeuse and Grievink (2000) reserve the term operability for the ability to cope with all these operational requirements. So operational requirements like controllability and switchability are subsets of operability. In the rest of this section and in the next we are going to review some of these definitions and controllability indices.

Morari (1983) in a breakthrough work introduced the term *resiliency.* This property of the process has a steady-state or static and a dynamic aspect. "The *static resiliency* refers to the ability of a plant to handle different feedstocks, product specifications, operating conditions, etc." On the other hand, the *dynamic resiliency* "describes the ability of a controlled process to move quickly and smoothly from one operating condition to another and to deal effectively with disturbances." It is important to note that in this framework, no control structure has been assumed. Thus, the resiliency measures the inherent dynamic operability of a process.

Skogestad and Wolff (1992), and Skogestad and Postlethwaite (1996) understand the process controllability similarly to the previously defined dynamic resiliency: "Controllability is the ability to achieve a desired performance within various limitations on process operations, despite of external disturbances and uncertainty in design parameters, by using available input and manipulated variables."

Lin *et al.* (1994) defined *structural controllability* as follows.

1) A process is structurally controllable if a disturbance does not propagate into other parts of the process.
2) Structural controllability is good if an undesirable disturbance does not propagate.

Structural controllability depends only on the process structure. The structural controllability framework was also used by Zhu *et al.* (1996) in their *hierarchical design approach* for the integration of process and control.

Weitz and Lewin (1996) gave following definitions. *Controllability* can be defined as the ease with which a continuous plant can be held at a specific steady state. An associated concept is *switchability*, which measures the ease with which the process can be moved from one desired stationary point to another. Similarly, *resiliency* measures the degree to which a processing system can meet its design objectives despite external disturbances and uncertainties in design parameters. From these definitions one can conclude, that the controllability and resiliency measures are merely diagnostic tools within the design procedure. Lewin (1999) has also suggested two approaches to ensure that chemical plants meet design specifications: (i) controllability and resiliency (C&R) screening methods early in the design process and (ii) integrated design and control to optimize and integrate the design of the process and its operation.

More recently (Vinson, 2000; Vinson and Georgakis, 2000) defined the *operability* of a process in these terms: "A process is operable if the available set of inputs is capable of satisfying the desired steady-state and dynamic performance requirements defined at the design stage, in the presence of a set of anticipated disturbances, without violating any process constraints." Uztürk and Georgakis (2002) formulated a *dynamic operability* framework that aims to quantify the inherent properties of the process. Here, a measure similar to settling time is used to quantify the dynamic performance.

Although the methods for calculating the *dynamic controllability*, *dynamic resiliency* and *dynamic operability* are different, these terms are used in general to designate essentially the same inherent characteristics of the process which determine its ability to meet design specifications and to change from one operating condition to another.

Meeuse and Grievink (2000) point out that the operational requirements have an effect on different time scales. For example, one of the main operational requirements in the short time scale is the production of products that meet specifications despite disturbances. This requirement has a steady-state and a dynamic aspect and is commonly called *controllability*. On longer time scales on the other hand, processes are required to respond fast in an economic way to changing market demands. This results in two operational requirements:

(a) Production at different operating points. This is a static property and is generally called *flexibility*, and

(b) Economic switching between operating points (including startup and shutdown operations). This is a dynamic property and is called *switchability*.

2.9 Performance assessment

There is a close relationship between process controllability and performance under closed-loop conditions, even though this relation is not always clearly defined. In fact, controllability assessment usually needs a performance criterion as benchmark. Qin (1998) makes the difference between *stochastic performance monitoring*, concerned with the assessment of the output variance due to unmeasured, stochastic disturbances (white noise) and the more traditional *deterministic performance monitoring*, such as step changes in setpoint or disturbance variables, settling time, and the stability margin of the control system.

Among the deterministic performance monitoring criteria that can be used for controllability studies we can include (Ogunnaike, 1994): The *minimum rise time* and the *minimum settling time*. There are also *time-integral* performance criteria, such as the

Integral Absolute Error (IAE) and the Integral Squared Error (ISE). These performance indices are based on the controller error, $\varepsilon = y_{sp} - y$, where y_{sp} is the set point and y is the controlled variable.

Harris (1989) proposed the use of closed-loop data to evaluate and diagnose controller performance using *minimum variance control*, (MVC), (Åstrom, 1967). The MVC is feedback control which achieves minimum output variance. Important properties of the MVC include: the closed-loop dynamics using MVC is always first-order plus dead time, no matter what the process dynamics is, and all process poles and zeros are cancelled by the MVC. This is why the MVC is very sensitive to process changes (Qin, 1998). Qin (1998) gives a comprehensive overview on the status at that time of control performance monitoring using minimum variance principles, and a brief tutorial on performance assessment is given as well. Although there is no other way to exactly achieve minimum variance than minimum variance control, several factors make the use of this approach inappropriate. Such factors include: negligible dead time, low order process and multivariable interaction. Thus, a trade-off should be made between these and the deterministic performance assessment methods.

2.10 Controllability and dynamic resilience (operability) measurements

Controllability evaluation methods may be classified into three by the model used in the evaluation procedure, steady-state model-based, linear dynamic model based, and nonlinear dynamic model-based ones (Lee *et al.* 2001).

Georgakis *et al.* (2001) made a broad classification of the different approaches to the operability analysis into two categories as linear and nonlinear model-based methods, depending upon the system structure. Considering that many of the controllability measurements were developed assuming steady-state conditions, and some others take explicitly the dynamics into account, one could add two sub-categories to each category. Noticeably, many of the proposed controllability and resiliency measures are calculated within an optimization framework.

2.10.1 Linear systems

The controllability analysis relies on a continuous-time state space model (**equation 2.4**) or input/output models in the transform domain:

$$\mathbf{y(s) = G(s)u(s) + G_d(s)d(s)} \tag{2.5}$$

where **G**(s) and $\mathbf{G}_d$(d) are referred to, respectively, as process and disturbance *matrix transform functions*.

2.10.1.1 Steady-state controllability indices

One of the first measures of process controllability is the *Relative Gain Array* (RGA), introduced by Bristol (1966). RGA is a measure of the process interactions in multi-input, multi-output control problems. The RGA has been used in process control design to find pairings between controlled and manipulated variables that minimize the interaction when the control loop is closed. As Luyben and Luyben (1997) point out, the problem with pairings to avoid interaction is that interaction is not necessarily a bad thing. Therefore, the use of the RGA in deciding how to pair variables is not an effective tool for process control applications. Conversely, the RGA is useful for avoiding poor pairings. The main strength of the RGA analysis is indubitably its simplicity, and it has been widely used to design multi-loop control structures. The usefulness of the RGA is based on its relation to other fundamental closed-loop system properties such as stability, robustness, failure tolerance, performance (Grosdidier, Morari and Holt, 1985; Yu and Luyben, 1987; Skogestad and Morari, 1987). The effect of model uncertainty on the RGA analysis has been studied by Chen and Seborg (2002). Processes with RGA coefficients close to unity are relatively insensitive to uncertainties in the process model, and vice versa. Detailed discussions and many practical applications of the RGA can be found in a monograph by McAvoy (1983) and in the textbook by Shinskey (1996).

Various measures have been suggested to quantifying the effect disturbances on achievable performance:

- RDGA - Relative disturbance gain array (Stanley *et al.*, 1985)
- IDA - Input disturbance alignment (Cao and Rossiter, 1998).

Both indices allow the analysis of only one disturbance at a time.

A geometric approach, based on operating spaces was proposed (Vinson, 2000; Vinson and Georgakis, 2000) to calculate the *Output Controllability Index* (OCI) which aims at quantifying the effect of limited range of the inputs on achieving the performance objectives of the process. Since no control structure is assumed, this index quantifies the inherent operability of the process.

A useful tool to analyze the stability of a closed-loop system with integral action is the *Niederlinski index* (Ogunnaike, 1994; Luyben and Luyben, 1997). It utilizes only the steady-state gains of the process, (**G**(s) in **equation 2.5**). For a 2x2 system the method is a necessary but not sufficient condition for stability; for higher dimensional systems, it provides only sufficient conditions.

2.10.1.2 Dynamic operability indices

The original RGA analysis was based exclusively on steady-state information; hence it does not consider the dynamic behaviour of the process when dealing with disturbances or set point changes. Thus, many researchers have proposed dynamic versions of the RGA (DRGA) (Bristol, 1978, McAvoy, 1983, Jensen *et al.*, 1986). Recently, McAvoy *et al.* (2003) proposed another approach to the DRGA, based on a proportional optimal controller. This new approach requires a less detailed feedback controller design than other approaches. They also give examples where the traditional RGA gives the wrong pairings and an inaccurate indication of the amount of interaction.

Singular values. The N singular values σ_i of a real N x N matrix **A** are defined as the square root of the eigenvalues of the matrix formed by multiplying the original matrix by its transpose.

$$\sigma_{i[\mathbf{A}]} = \sqrt{\lambda_{i[\mathbf{A}^T\mathbf{A}]}} \qquad (2.6)$$

The matrix **G**(s) in **equation (2.5)** is transformed by *singular value decomposition* (SVD) into the product of two rotational matrices and a diagonal matrix of singular values. The minimum and maximum singular values (σ_{min} and σ_{max}, respectively) both provide information regarding the impact of manipulated variable constraints on the controllability of the process (Lewin, 1996). The *condition number* (CN), defined as the ratio $\sigma_{max} / \sigma_{min}$, provides an indication of process ill conditioning, that is, processes in which either the output variables are not independent or the input variables are not independent. Such processes are significantly more difficult to control (Morari and Zafiriou, 1989). RGA and CN can be also used to assess the *robustness*, measured as plant sensitivity to input or output uncertainty (Skogestad and Havre, 1996).

The *resiliency* of a process is measured in terms of the size of the *minimum singular value* of the process steady-state gain matrix (Morari, 1983). Mathematically, a resilient process is one that attains a large minimum singular value for the steady-state gain matrix (i.e., at zero frequency). Processes with large minimum singular values are less susceptible to manipulated variable saturation than are processes with small minimum singular values. Further, it has also been shown that processes with large minimum singular values are more *robust* (or insensitive) to process/model mismatch than those with smaller minimum singular values (Johnston and Barton, 1984; Grosdidier *et al.*, 1985; Koung and MacGregor, 1992).

Similar to the steady-state case, there are a number of measures in the literature that aim to quantify the effect of disturbances on the dynamic controllability of linear systems:

- DCN - Disturbance condition number (Skogestad and Morari, 1989)
- DC - Disturbance cost (Lewin, 1996).

The DC is the only disturbance rejection index that can handle multiple disturbances.

Zheng and Mahajanam (1999) introduced a controllability index based on the cost associated with dynamic controllability. The basic idea is to minimize the additional surge capacity required for a given flowsheet to meet dynamically all the objectives and constraints under the expected disturbances. This concept has been used by Zhen *et al.* (1999) to synthesize an optimal plantwide control system.

Lee *et al.* (2001) used a procedure based on relative order analysis and *structural decomposition* to evaluate controllability and to select design alternatives. This procedure involves the identification of pathways of disturbances in the process based on structural information only. To this end, graph theory is usually used.

Uztürk and Georgakis (2002) extended the operability framework of Vinson and Georgakis (2000) and defined a dynamic Operability Index (dOI) as a fraction of the operating ranges that can be achieved within the desired response time given the available input ranges. The dynamic performance was calculated using a *minimum-time optimal controller* (Zadeh and Whalen, 1962). Subramanian *et al.* (2001) expanded this concept to nonsquare systems (more inputs than outputs).

Useful tools in the controllability assessment are also the 'classical' stability analysis methods, such as the different *stability criteria* (Routh, Bode, Niquist), (Ogunnaike, 1994; Luyben and Luyben, 1997). In particular, the gain and phase margins on Bode and Niquist plots provide an indication of the *robustness* of a feedback system. That is, gain and phase margins quantify the amount of uncertainty that can be tolerated.

2.10.2 Nonlinear Systems

The process model usually is represented by the following state-space representation:

$$\begin{aligned}\dot{\mathbf{x}} &= \mathbf{F}(\mathbf{x},\mathbf{u},\mathbf{d})\\ \mathbf{y} &= \mathbf{G}(\mathbf{x},\mathbf{u},\mathbf{d})\end{aligned} \tag{2.7}$$

where **F** and **G** are functions relating the vectors of states, **x**, outputs, **y**, inputs, **u** and disturbances, **d**.

2.10.2.1 Steady-state controllability indices

The concept of flexibility index was introduced by Swaney and Grossmann (1985a) for quantifying the steady-state operability of nonlinear processes. It is defined as the maximum normalized uncertainty in its parameters that a process can tolerate without violating any constraints.

The method suggested by Vinson (2000) and Vinson and Georgakis (2000, 2001) is not limited to linear process models, since the operating spaces can also be calculated by **equation 2.8**. The nonlinear Output Controllability Index (OCI) is defined similarly to the linear case.

2.10.2.2 Dynamic operability indices

Bahri et al. (1997) formulated an optimization-based approach using dynamic MINL programming to assess the operability of a plant in the presence of disturbances. The basic idea was to move the nominal operating point to a 'secure' area, so that the sensitivity to disturbances was minimized. They defined the objective function in terms of economic factors and calculated the difference between optimum point and back-off point, which quantifies the savings obtained by decreasing the process variability.

Vu *et al.* (1997) focused on two operability issues, *operability* and *switchability* of a mini integrated plant using a nonlinear programming framework. To calculate the best trajectories of the control variables and the profiles of the state variables were calculated including the Integral Squared Error (ISE) as one of the constraints. Schweiger and Floudas (1998) also utilized the ISE as a weighted constraint to the optimization problem, and varied the weighting values to generate a set of trade-off solutions between economic and controllability objectives. The traditional choice for a controllability measure is the ISE.

Ekawati and Bahri (2001) incorporated the Output Controllability Index (OCI) (Vinson, 2000) within the dynamic operability framework for regulatory cases. They also provided a new controllability index, the *General Integral Absolute Error* (GIAE), which involves the whole outputs and time space and takes into account the interaction between variables.

The constrained optimization-based approaches developed by Uztürk and Georgakis (2002) for linear squared systems and the extension to nonsquared systems by Subramanian *et al.* (2001) have been also applied to nonlinear systems.

More recently, a similar approach to the one used by Georgakis and coworkers (Vinson and Georgakis, 2000; Subramanian and Georgakis, 2001), was developed by Cheng and

Yu (2003) to study the trade-off between steady-state economics and dynamic controllability of recycle plants is analyzed for ternary systems. First, they calculated the optimal operating region on steady-state basis, based on the *minimal total annual cost* (TAC) and introduced the concept of *reachability*, defined as the reachable production rate as the manipulated variables vary. Then, for dynamic controllability assessment, based on reachability, he proposed the *production-rate handling capability* as controllability measure. They found that optimally designed recycle plants are in general operable.

2.11 Applications in the pulp and paper industry

Most of the applications of controllability studies are referred to the chemical industry. The list of applications in the pulp and paper industry is rather sparse.

Al-Awami and Sidrak (1998) produced a typical work where several techniques were combined to evaluate the operability of a process. They addressed process sensitivity and interaction analysis for Kamyr digesters using RGA, singular value decomposition (SVD) and condition number (CN) to improve the ill-conditioned system. The Niederlinski's stability measure was used to assess the closed-loop stability.

Soehartanto and Beteau (1999) used an analysis based on asymptotically stability to select the appropriate control strategy for a pulp and paper wastewater treatment system.

The traditional production management strategy in paper manufacturing is based on a volume-intensive approach. This approach is no longer appropriate, and production has to be controlled by an approach that considers inventory performance along the full length of the supply chains. Control theory has been applied to study product chain dynamics. Kleinedam *et al.* (2000) used this approach to study different scenarios with respect to controllability and stability, which are prerequisites for effective chain management.

Khanbaghi *et al.* (2000) performed a controllability analysis of a nonlinear model of a pressure screen to determine the degree of coupling. To this purpose, the calculated the RGA for the linearized steady-state model.

Orccotoma et al. (2001) used the controllability analysis proposed by Skogestad (1994, 1996) to determine the maximum allowable variability of the pulp furnish to the process. Their results showed that the output variables, the basis weight and the first-pass retention, may be maintained within the interval of ± 1% of their nominal values, if the maximum variability in the consistency and fines content of the thick-stock is kept lower than ± 1% and ± 2%, respectively.

Lama *et al.* (2003) also used Skogestad' s method to the selection of variables in the short loop of a paper machine, and proposed an alternative method based not on the selection of controlled variables, but rather on the selection of manipulated variables.

Hauge et al. (2002) performed controllability studies and developed a nonlinear physical based model in order stabilize the wet end of a paper machine and design a model predictive control (MPC) system. Their results indicated that that in order to track setpoint changes, to obtain offset free control, and to reject disturbances, it is necessary to be able to influence some of the measured disturbances either manually or automatically.

2.12 Critique of controllability and dynamic operability assessment methods

The use of controllability indices to judge the operability of a process has some limitations. These limitations include:

- it is difficult to link the controllability index and the closed-loop performance,
- the majority of indices are based on a linear steady-state model,
- some of these indices require square systems,
- each controllability index reflects only one aspect of the process operability. Thus, more than one technique is usually needed to draw satisfactory conclusions. The problem is that the combined effect of different indices is difficult to analyze and requires experience.
- Finally, some of these methods (e.g. RGA) are applicable only to multi input / multi output (MIMO) systems.

Some authors have suggested alternative approaches that try to overcome these limitations. For example, Meeuse and Grievink (2000) using a generic model of a closed-loop where the controller is a multivariable internal model controller (Garcia and Morari, 1982), identified the controllability limiting phenomena, instead of using controllability indices. These limiting phenomena are:

- Disturbance sensitivity (= open-loop disturbance sensitivity). It determines the required plant capacity.
- Poorly measurable outputs (measurability). The importance of measurability is obvious since control depends critically on available measurements.
- Non-invertibility of the process. Morari (1983) identified four properties of the plants that limit the inversion of the plant model: time delays, right half plane zeros, constraints on the input variables and model uncertainty.
- Input effectiveness (= closed-loop disturbance sensitivity). It determines the available plant capacity.

An alternative approach to controllability and dynamic operability diagnosis relies on closed-loop simulations using rigorous dynamic process models (Weitz and Lewin, 1996). However, this is not practical in the first stages of process design (Morari, 1983; Weitz and Lewin, 1996) for two reasons: (a) it is both time and resource consuming and may require unavailable data; and (b) any result is biased by the control structure adopted and will compromise the objectivity of the diagnosis.

When dealing with nonlinear systems the main limitation of controllability and dynamic operability measurements involving an optimization framework is the computational complexity. Because of this complexity many application are limited to small case-studies.

Most of the controllability analysis tools address two issues: (i) The control configuration, i.e., how manipulated and controlled variables should be paired; and

(ii) How the stability of the overall system is affected by properties inherent to the process. Few researchers (Downs and Ogunnaike, 1994; Zheng and Mahajanam, 1999) have addressed explicitly the effects of product variability (product purity) specifications on process controllability. The impact of operability and performance on process variability has also received little attention.

2.13 Selected gaps in the body of knowledge

There are certainly a large number of gaps in the body of knowledge; some of them were listed above. In this work, we want in particular to address the following:

- Several authors (Nikoukaran and Paul, 1999; Franch and Carvallo, 2003) have discussed the selection of a simulation software package in a general manner, but there is no publication about specific (calculation algorithm related) problems when using a sequential or simultaneous simulator for building a dynamic simulation, and how these problems can be avoided or, at least, how their impact on the simulation convergence can be minimized.
- Some authors, notably Orccotoma (1997), Bonhivers (1999) and Dabros (2002) have studied certain aspects of broke recirculation and process variability, focusing more on the control of inventories. The effect of different control approaches and operating regimes of the broke management system on the process variability in the headbox has been little investigated.
- There is also a little amount of operability studies applied to the pulp and paper industry, in general, and to the broke system, in particular. These works

addressed the short loop of a paper machine (Orccotoma, 1997; Lama et al., 2003) and the wastewater treatment system (Soehartanto and Beteau, 1999). On the other hand, each operability measure describes only one aspect of the process operability.

- Both process and control system determines how well a process can operate. However, it is difficult to link process operability and control performance with the available operability and performance indices (Morari, 1983; Meeuse and Grievink (2000).

CHAPTER 3: OVERALL METHODOLOGICAL APPROACH

In **Figure 3.1** the methodological approach used in this project is depicted. This project was divided in four major phases and each phase is composed of several steps. Activities include:

3.1 Evaluation of dynamic simulators

- Characterize the calculation error associated with the sequential algorithm. Identify the main factors for this error and investigate ways to minimize it.
- Investigate strategies to overcome common problems when building a dynamic simulation with sequential and simultaneous simulators.

3.2 Development of a dynamic simulation

- For both the steady-state and dynamic model, perform a systematic verification (debugging) along the entire model building process
- Validate this simulation informally against available data used in previous simulation (1999)
- Set base case operating conditions
- Select a few key process variables to characterize the process variability
- Define a variability metric
- Design a few scenarios with the purpose to show the effect of process and control changes on the process variability

3.3 Assessment of the steady-state operability and the closed-loop sensitivity

- Select a sub-system from stock preparation area and develop a linear model for this subsystem
- Investigate the control structure (input-output pairing) and the closed-loop interactions
- Evaluate the closed-loop stability for the linear subsystem using the Niederlinski method
- Apply the operability analysis framework developed by Vinson and Georgakis (2000) using the steady-state simulation (nonlinear model) to analyze the input-output controllability of the selected subsystem
- Analyze the closed-loop sensitivity analysis

3.4 Dynamic Operability Assessment

1. Define a new dynamic operability framework, its requirements, conditions, limitations and applicability
2. Define a suitable control performance index that can be incorporated in this operability framework
3. Define a new dynamic operability measure
4. Investigate the properties of this operability index for a simple SISO system
5. Expand this approach to MIMO systems

Specific aspects of each phase are discussed in the following chapters.

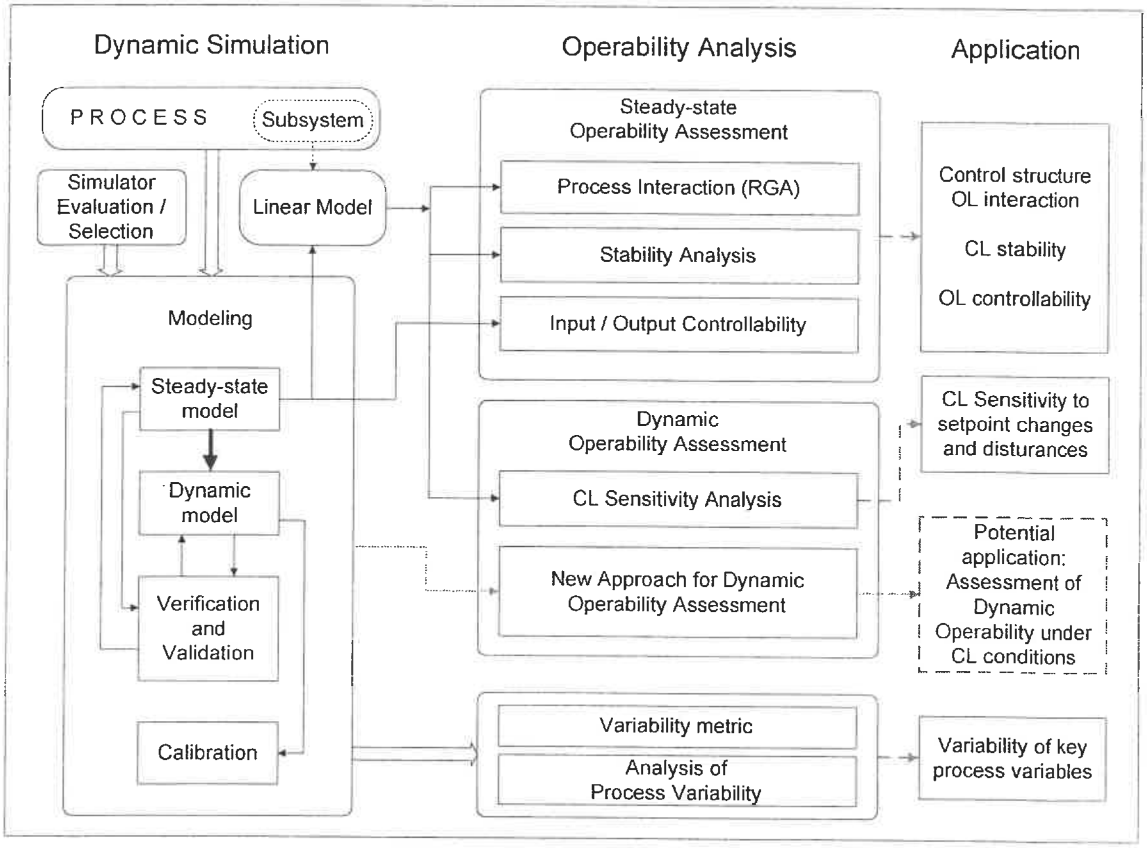


Figure 3.1: Overall methodological approach

(OL = Open loop, CL = closed loop)

(Dotted arrows indicate potential applicability to the dynamic operability assessment of the broke management system, considered in this work)

CHAPTER 4: SIMULATOR SELECTION FOR DYNAMIC SIMULATION

4.1 Introduction

Appendix A1 lists the main dynamic simulation packages currently used in the pulp and paper industry. **Appendix A2** discusses common problems when developing a dynamic model with sequential and simultaneous simulators, and shows practical ways to solve them. Three simulation packages were evaluated and the emphasis of this work was put on how to get the most benefit out of each type of simulator. Specific techniques to avoid convergence problems and minimize calculation errors in transient periods are highlighted in each simulator. Knowledge of these techniques is essential in order to build an accurate dynamic simulation. It is shown that sequential simulators require in most cases small time steps (not higher than 0.5 min) and the use of an iteration algorithm for recycle loops, in order to avoid numerical instability. For simultaneous simulators, on the other hand, a variable time step was found to be best.

4.2 Main criteria for the selection of the simulation tool

One of the major decisions in the development of a dynamic simulation is to select the simulation tool. Schroderus *et al.*, (1991) have given guidelines for comparing and selecting the right tool for the intended objective. Basically, the methodology for choosing software packages compares user requirements and package capabilities. More systematic techniques based upon scoring of simulation packages according to a number of criteria, have been discussed by Nikoukaran and Paul (1999). A different approach was suggested by Franch and Carvallo (2003). The authors used the ISO/IEC quality standards (the families of 9126 and 14598 are related to software product quality and evaluation) to develop a six-step methodology for building structured quality models. These quality models relate the domain of application and the standardized quality requirements.

What Lorenz (1999) has written with regard to the modelling languages for differential and algebraic equations (DAEs) is also applicable for simulation packages. There is no absolute "best" choice among the simulators and the simulation practioner must select carefully the one with the characteristics to address a particular problem. Lagnier (1996) has mentioned three points between them trade-off should be made when selecting a dynamic simulator tool:

- *Capabilities.* This includes data reconciliation and optimization capabilities, parameter estimation, flexibility (the possibility to develop user models or to change existing library models), availability of different numerical methods.
- *User-friendliness.* Included in this set are the possibility to develop customized interfaces and the tools provided with the software to access and display information.
- *Cost.*

The existing commercial simulation packages comply differently to these characteristics, but in general there is still the need to develop or improve following areas:

- mechanisms provided by the software to define and to handle complex sequences and logical decisions (e.g. batch operation);

- capabilities to model continuous and discrete processes in the same model (some numerical methods become unstable when simulating e.g. start-ups and shut downs);
- capabilities to model stochastic uncertainties (e.g., random disturbances);
- hierarchical modeling - it is highly convenient for complex models;
- connectivity – simulation programs should be able to take advantage of networking and to interface with some other programs for specific tasks (e.g., design of advanced process control configurations, optimization, output data analysis), as well as connection to DCS systems;
- integrated data reconciliation (filtering, gross error detection).

4.3 Evaluation of commercial simulation packages

A great deal of work has been done by the author to evaluate the capabilities for dynamic simulation of several commercial simulation packages used in the pulp and paper industry. **Tables 4.1** and **4.2** summarize the main characteristics of these software packages. The traditional method of comparing user requirements and simulator's capabilities was used in this work.

Since one of our main requirements to the dynamic simulation packages was the accuracy, our effort was focused on understanding how errors -sometimes very large in magnitude- may occur for a certain process configuration or for certain process conditions, and how they can be minimized. This concerns in particular the sequential simulators. To evaluate the behavior of these simulators in the transient period of a dynamic simulation, a simple process model was used (**Figure 4.1**). A step change on the outlet flow from the tank was imposed to simulate a process disturbance and the calculation error around the recycle loop was calculated as relative error between the flowrates F4 and F1.

Table 4.3 clearly shows how mass balance errors appear in a recycle loop when a sequential algorithm is used *and* there is only one iteration per time step. A step change has been imposed in the process outlet stream, at t = 100 min. Two minutes later the controller reacts, then all streams around the recycle start to change and we get the first error. The reason for this error is a one-step delay in the recycled stream (F2) in the mass balance calculation of the mixer. This delay has nothing to do with transport delay; it is simply a numeric delay in an algebraic loop. As this calculation pattern is repeated at each time step, the error can be magnified by other factors, such as the calculation order and controller aggressiveness. **Figure 4.2** shows the effect of switching the position of key units (Mixer and Splitter) in the calculation order. Simulator "A" becomes unstable, whereas Simulator "B" can still manage this change. The different integration methods used by these simulators account for this difference. Simulator "B" uses a more stable integration method. However, this integration method becomes less efficient if the controller is made more aggressive. This type of problems can be solved if the mass balance calculation of the recycle loop is made iteratively until certain criterion of convergence has been reached (**Figures 4.3** and **4.4**). In contrast to Simulator "B", Simulator "A" has this feature and can solve this kind of problems if we include pressure in the model (**Appendix A2**). Larger time steps also affect both, the simulation accuracy and the numerical stability.

Also, it is important to know which the requirements of each simulator are in order to achieve the desired accuracy and what the limitations are. For instance, the package IDEAS® allows building a fairly realistic dynamic model, but this may require specifications data for valves and pipes that are not available, and the cost of this realism is a significant drop in the execution speed. Wilson and Balderud (2000) have reported that the simulation speed of a large-scale paper machine model was only 2 to 3 times faster than real time which was too slow for the indented controller design studies. The hydraulic calculations are responsible for this slowness.

In the equation-based simulator MASSBAL®, almost all problems leading to unconverged results were related to *singularity*, that is, redundant specification. This problem can be avoided with a careful selection of variables and the proper definition of relationships. However, this can be a difficult task in large models and may require some trial and error.

Three aspects led us to prefer the simultaneous approach over the sequential algorithm:

a) *Accuracy*. Although the accuracy of sequential simulators (**Table 4.1**) may by sufficient for most practical problems, our investigations indicate that the accuracy of this type of simulators is more sensitive to changes in process and simulator parameters. For instance, a wrong selection of the calculation order combined with an aggressively tuned controller may result in large mass balance errors and big oscillations.

b) *Flexibility*. This feature is usually related to the programming facilities of the simulation package and its capability to allow the user to make changes to the model and the way modules are specified. In general, equation-based simulators show a higher flexibility and have no problems to solve design (downstream specification) problems.

c) *Reliability*. Sequential simulators are known for being more robust that their simultaneous counterparts and, therefore, more reliable. However, they have a feature that can weak seriously this reliability, especially in complex models. Sequential simulators make the model building easier by calculating automatically the degree of freedom and telling the user which variables must be specified. This feature may lead to wrong results by converging badly posed problems. This is also the case when the calculation order is selected incorrectly. The manual of one of the evaluated sequential simulators recommends changing the "optimized" calculation order in a large model following our experience to improve convergence or to avoid convergence problems.

It is fair to mention that the problems affecting the accuracy, flexibility and reliability of sequential simulators can be managed to some degree and, therefore, realistic, accurate models can be developed with this type of simulators (**Appendix A2**). CadSim Plus®, with its pressure-flow network facility, which enables local iterations, has an advantage over WinGems® in that sense. However, this may require making changes to our problem formulation. Still, design problems are easier calculated with a simultaneous simulator.

Although Simulink® shows the highest marks with respect to these characteristics, it has the serious disadvantage of making the model building a very complex task. Since no library of pre-coded operating units is available, the user must program their own modules. Moreover, it will be necessary to program a pressure-flow network platform where these modules can be connected to each other, in order to perform mass and energy balance calculations. Based on these considerations, the simulation package MASSBAL® was chosen in this work to develop the dynamic simulation of a papermaking process.

Table 4.1: Main features of commercial simulation packages

MAIN FEATURES / SOLVER / ACCURACY		WinGEMS (WG) / CadSim Plus (CS)	MASSBAL	IDEAS	MATLAB / SIMULINK
▪ Calculation Algorithm		Sequential	Simultaneous	Hybrid	Simultaneous
▪ Time step		Fixed	Fixed and variable	Fixed	Fixed and variable
▪ Integration solver		WG: Euler method CS: Mass balance approximation	Adaptive Runge-Kutta Euler Trapezoidal	Euler method	Several methods available
▪ Solver limitations		Convergence problems if improper calculation order was selected. Since WG does not iterate, it can have difficulties to solve design problems	Complex models can be difficult to converge, if the right set of specifications was not selected	Mixing of flow and pressure objects can originate convergence problems	Not detected
▪ Pressure-flow network		WG: No CS: Yes	Yes	Yes	No
▪ Ability to handle large networks		Yes, but they need good guessed values to converge	Thousands of objects can be included; start file required	Hierarchical modeling capability, but speed is a limiting factor	Hierarchical modeling capability makes it possible
▪ Interconnectivity		Excel: real time data exchange; easier in WG	Excel Add-in Simulink: MB blockset (both only for s-s simulation)	Excel: real time data exchange	Excel Add-in Matlab and Simulink are perfectly linked for data exchange
▪ Overall Simulation Accuracy (Rel. Error)	S-S Dyna-mics	10^{-5} - 10^{-6} % 10^{-3} % (transient period)	10^{-11} % avg. 10^{-10} %; max. 10^{-3} %	10^{-13} % Up to ~ 0.3 % (transient period)	10^{-16} % 10^{-12} %

Table 4.2: General features of commercial simulation packages

GENERAL FEATURES	WinGEMS (WG) / CadSim Plus (CS)	MASSBAL	IDEAS	MATLAB / SIMULINK
▪ User friendliness	Easy to learn/use; WG very intuitive	Requires some experience	Requires training and some experience	Requires some knowledge of process control
▪ Flexibility	Good	Good	Very good	High
▪ GUI	Very good CS: Closer to real P&ID	Good	Very good	Process control oriented
▪ Program outlet quality	Very good	Good	Excellent	Excellent
▪ Applicability	Pulp & Paper Industry	Chemical Industry Pulp & Paper Industry	Chemical Industry Pulp & Paper Industry	General purpose Control system simulation
▪ Main applications	Process design Process optimization	Troubleshooting Training		Process Control Optimization

Table 4.3: Calculation error between F1 and F4 after a step change in the tank outlet flowrate

Time (min)	Tank outlet stream (m3/min)	F1 (kg/min)	F2 (kg/min)	F3 (kg/min)	F4 (kg/min)	|error| (%)
100	10	9983	2495.8	12479	9983	0
101	12	9983	2495.8	12479	9983	0
102	12	10043	2576.8	12539	10031	0.12
103	12	10123	2526.2	12631	10105	0.18

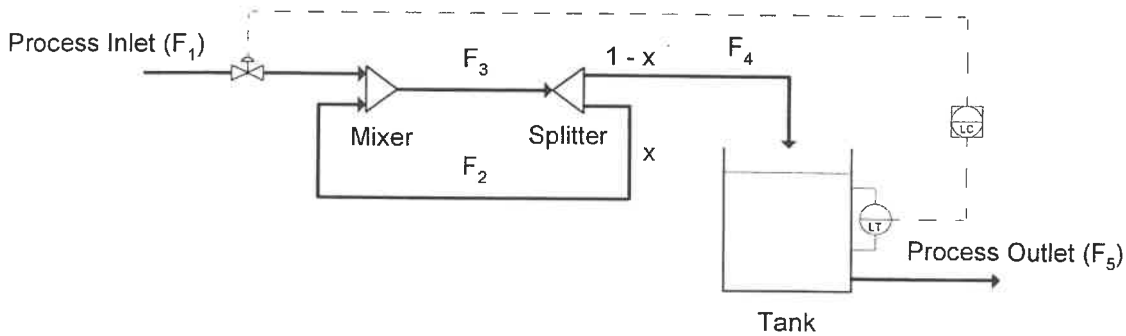


Figure 4.1: Process flowsheet investigated

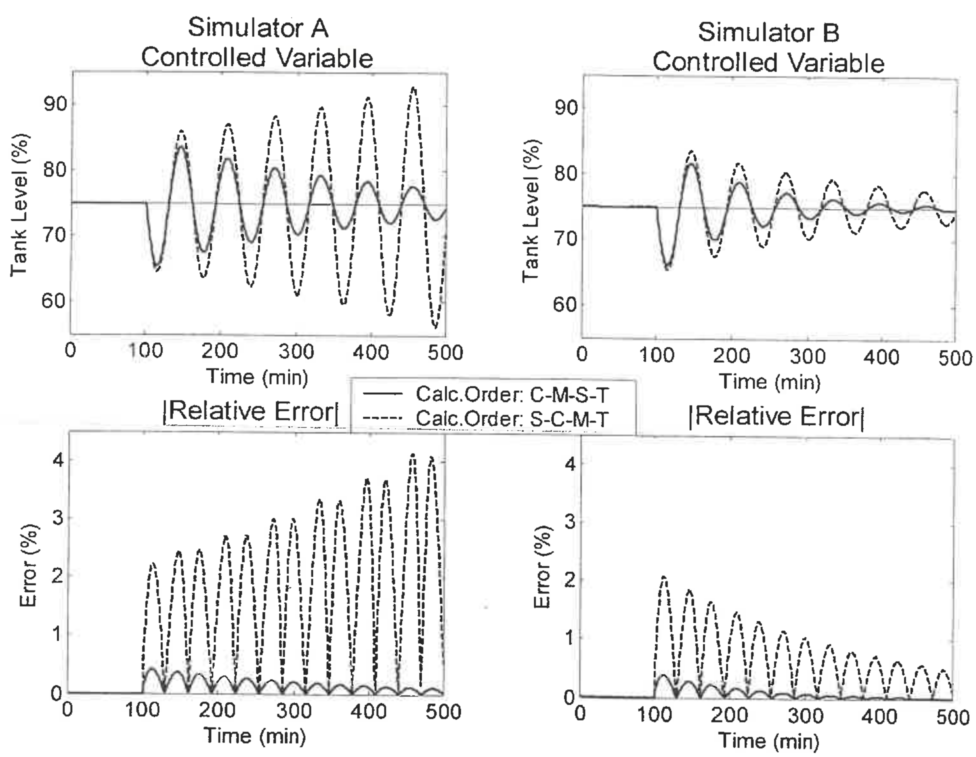


Figure 4.2: Effect of the calculation order on the dynamic response and the error around the recycle loop for two sequential simulators, when there is no iteration

(C-M-S-T: Controller-Mixer-Splitter-Tank;

x = 0.20; Disturbance = 20%; Time step = 1 min; Kc = 40 L/min/Vol-%, τ_I = 2 min;

left: Simulator "A", right: Simulator "B")

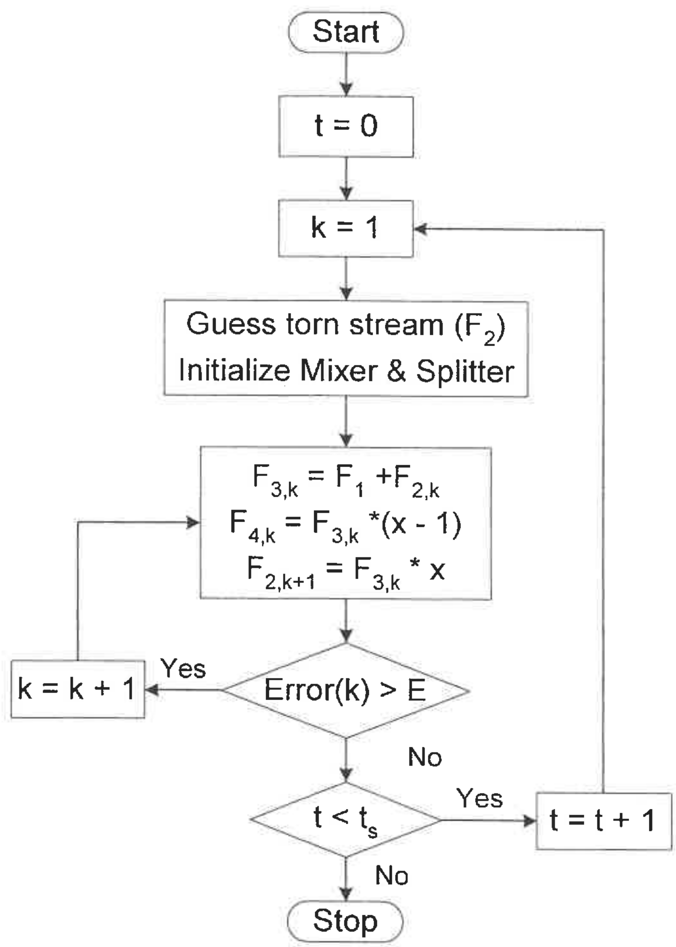


Figure 4.3: "Convergence block" inserted in a sequential calculation algorithm to iteratively solve the recycle loop

(E = convergence criterion [relative error between F_1 and F_4],

k = iteration number inside each time step,

x = recirculation ratio, t_s = total simulation time)

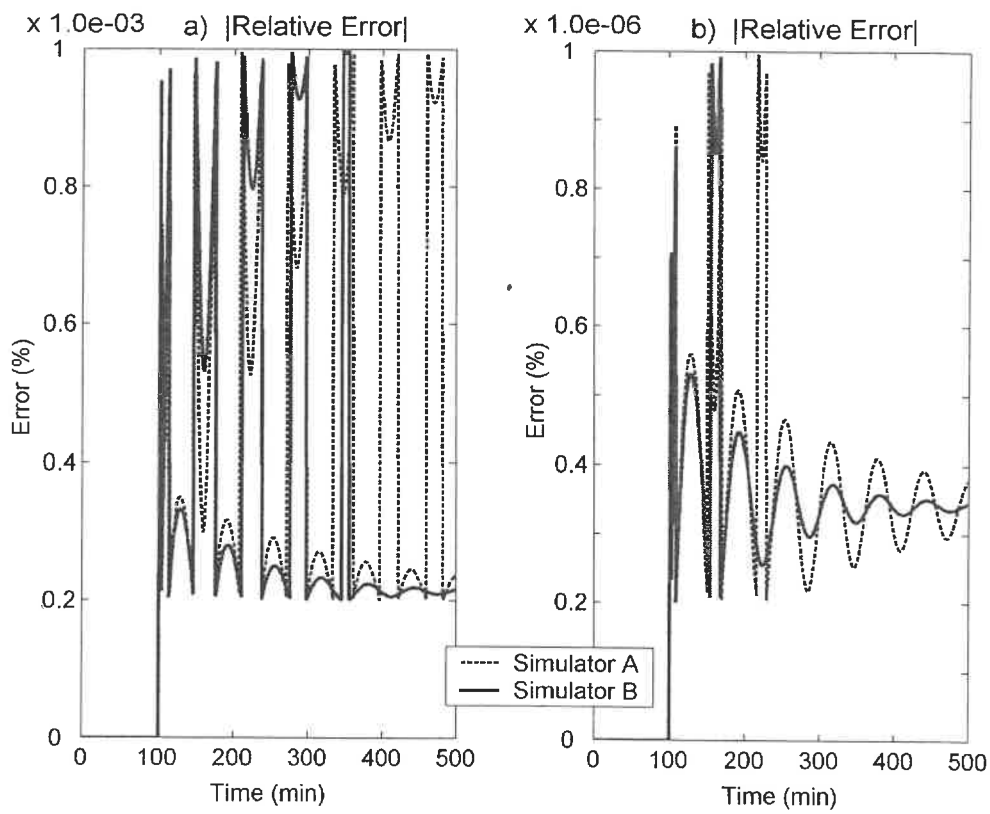


Figure 4.4: Error around the recycle loop obtained with the iterative solution of the recycle loop

a) Convergence criterion: $E = 10^{-3}$ %
b) Convergence criterion: $E = 10^{-6}$ %

CHAPTER 5: DYNAMIC SIMULATION OF A PAPER MILL

5.1 Process description

A dynamic simulation of the paper machine No 8 (PM 8), Domtar-Windsor, has been developed using the equation-based simulator MASSBAL. **Figure 5.1** shows the scope of this simulation. The two paper machines at the mill, PM 7 and PM 8, produce similar grades of wood-free fine paper and can share if needed both white water and broke. For the purpose of this work, we will consider them as completely separated systems. A production rate of 850 t / d for PM8 has been considered.

Furnish pulp is composed of virgin pulp and broke. Two types of virgin pulp are used, namely hardwood pulp, produced locally and softwood pulp, purchased in bales and then repulped. The required good formation and strength are given by the hardwood and softwood fibers, respectively. The relationship between hardwood and softwood is kept constant as 85 to 15, and their consistencies are controlled to 4.5 and 4.2 %, respectively. Broke, produced during breaks of the sheet in different parts of the paper machine is collected in several tanks located under the paper machine, diluted with clear white water to a consistency of 2.7 to 3.0 % and sent to two storage tanks; from here the diluted broke is sent through a decker to a big high density broke storage tank, where broke is stored at about 10 to 11% consistency. Before used in the pulp furnish, broke is diluted in three dilution points with cloudy white water, stored in two intermediate tanks and goes through a screen to remove impurities and destroy fiber flocks. Finally, the diluted broke has a consistency of about 4.0 %. Mixing of the three pulp sources is made in a small "mixing box", just before the mixing tank. The addition of broke is variable and depends basically upon the level in the high-density broke tank.

Chemicals are added to the furnish stock at different points of the process to improve the mechanical and optical properties of the paper. These chemicals include fillers, internal size and retention agents, and wet-strength products. About 15% filler (PCC) is added just before the pressure screen in the short circulation. Diluted furnish stock is provided to the headbox at a consistency of about 0.8 %

5.2 Main assumptions

The main assumptions made to build this model are as follows:

- The broke and white water system of PM7 and PM8 are completely separated.
- Only mass and energy balances are considered. The effects of pressure and momentum on the slow process dynamics considered here are neglected.
- Heat losses between 0.5 and 4 % were assumed for the reservoirs, considering the drop of temperature between inlet and outlet and the flowrates.
- The effect of refiners on the fiber fractionation is negligible, since only light to moderate refining is applied.
- The separation units (cleaners and screens, and also the forming zone) can be 'modeled' with constant fractionation factors.
- There is a perfect mixing in all reservoirs. All tanks are assumed to have a cylindrical geometry.
- No transport delay is considered.

Six stream types were defined and it is assumed that the pulp and white water streams are composed of seven components:

Streams	Components (in kg/min)
Main Stream	Water
Softwood	Steam
Broke	Long fibers
White Water	Medium size fibers
Steam	Fines
Chemicals (only for mass balance)	Ash
	Dissolved solids

The term "main stream" is referred to the main pulp stream, which starts in the bleached pulp high density storage tank and ends at the entrance of the headbox, after mixing with other pulp streams and chemicals, and dilution with white water in several points across the process.

Ash is assumed to be composed exclusively by PCC (filler), and the total dissolved solids are composed by organic (mainly cationic starch) and inorganic dissolved matter. Fines are small (76 micro-meters diameter) cellulosic materials that are small enough to pass through a forming fabric. The relationships used to calculate the fiber fractions and other derived variables are given in **Appendix A4, Table A4.1**.

5.3 Simulation development

The main characteristics of the simulator used to build this simulation are described in **Appendix A3**. For the purpose of model building, the selected process was divided in five major areas, namely: the stock preparation area, with the pulp blending system as core process; the broke handling area; the white water and fibre recovery system; the approach system, where pulp cleaning and screening are the main operations; and the paper machine.

Building a dynamic simulation comprises several steps. The first step always consists in building the steady-state model. Expanding this model to dynamics basically consists in superimposing the control system onto the steady-sate model and adding logical relationships to simulate the operating conditions. We followed the following strategy:

1. The whole process was divided as mentioned above. This allowed us to identify 'clusters' of units which can be built together and saved provisionally in separated files. Guessed values were used to initialize each 'cluster'. Afterwards, the 'clusters' were put together and connected in the main file. This procedure requires making auxiliary mass and energy calculations and proved more useful in the initial stages of the process modeling, say in the first half of the modeling. As the model is getting more complex and more recycle streams are closed, the 'cluster'-approach becomes less practical.

2. The importance of having good initial conditions is essential for success in a MASSBAL simulation. Therefore, it is imperative to build the model step by step, adding no more than two or three units at each step. The usual practice is to use the converged outputs of one step as initial values for the next step.

3. A systematic process of debugging (Verification) was carried out from the beginning, because waiting until the model has been built is too risky. It could be too late for finding programming errors, and the model may never work correctly.

4. The last step in the model building was calibrating it. This essentially means making changes to process parameters (basically fractionation factors and heat losses), and fine tune the controller parameters. Also, the specifications for the relation between manipulated variables and the controller output may need to be adjusted, in order to obtain the desired model outputs.

5.3.1 Steady-state simulation

The main operating units from the stock preparation system through the paper machine were included in the model. A complete list of these units is given in **Appendix A4, Table A4.2**. This table also shows the specifications, relationships between variables and specific hypothesis for each unit. This model is composed of 392 internal units, 820 internal streams, 5286 parameters and 6835 dependent stream variables.

5.3.2 Dynamic simulation

The model is composed of 421 internal units, 339 ordinary differential equations and 5085 algebraic equations, and the number of specified parameters and dependent stream variables equals 6852 and 7192, respectively. A variable simulation time step was chosen, and the convergence criterion was fixed to 0.1 %, the integration accuracy by default. The integration method used was the adaptive Runge-Kutta. The average error is in the order of 10^{-11} % and the maximum error around 10^{-3} %. The simulation lasted 3.7 min for the base case (simulation time = 480 min, no breaks) and is about 130 times faster than real time, running on a Pentium® 4, 1.60GHz. In general, this model shows a good robustness for most changes made on the model, but there are a few cases where we might have convergence problems (**Appendix A3**).

5.3.2.1. Control system

The main objectives of the control system in the papermaking process are: (1) to provide the required amount of furnish pulp to the paper machine, (2) to keep targeted concentrations of fibrous material and chemicals, and (3) to regulate the inventories.

Table A4.3, Appendix A4, shows the dimensions and residence time of each level-controlled tank considered in this simulation. The model includes 18 control loops for level control and 12 loops for consistency control, as well as the basis weight control loop. PI controllers have been used in all control loops.

5.3.2.2. Controller tuning

Controllers in each control loop were tuned using the internal model control (IMC) based tuning method. The relationships used to calculate the controller gain K_c and the reset time T_I, are:

$$K_c = \frac{2}{K_p \lambda}; \quad T_I = 2\lambda \tag{5.1.}$$

for level controllers, and

$$K_c = \frac{\tau_p}{K_p \lambda}; \quad T_I = \tau_p \tag{5.2}$$

for consistency controllers. In both cases, K_p represents the process gain, τ_p is the process time constant and λ is the closed loop time constant.

The calculated values of K_c and T_I have to be converted to the corresponding units used by MASSBAL®'s PID controller. The gain units are (Controller Output % / Controlled Variable %), and the Reset Ratio is just the inverse of T_I. The resulting controller parameters are given in **Table A4.4** and **Table A4.5 (Appendix A4)**, for level and consistency controllers, respectively.

5.3.3 Model validation

Available real data from 1999 were used to validate the steady-state model. These data are composed of average steady-state values of flowrates, consistencies, temperatures, and laboratory measurements of pulp components. Laboratory analysis of fiber fractions were performed at different points along the process, from the stock preparation area through the paper machine. Appropriate values of fractionation factors and heat losses were selected to fit the simulated outputs of each unit to real data. After the process model was completed, when needed, small changes were yet made to the fractionation factors to adjust the outputs. For most of the streams a difference of less 10% between simulated and real data was achieved. An informal validation of the dynamic model was also performed, using a qualitative/graphical method. Step changes were induced for several variables (model inputs), and the response of the model were observed for a number of variables (model outputs) across the process. The sense and size of the changes indicate that the dynamic model reflects reasonably well the real process.

5.3.4 Base case

In fine paper mills, paper quality and broke inventory control limit the amount of broke that can be added to the furnish to a relatively narrow range. Some grades should not exceed 20 %. In general, the broke fraction in the pulp furnish is less than 30 %. Ideally, the amount of broke should be kept as constant and low as possible, so that paper machine stability and paper quality are not affected. Web breaks in the paper machine, however, prevent of achieving this objective. In this work, we shall consider the target range of broke ratio from 10 to 30 %, and the nominal operating point corresponding to the base case has been fixed at the lowest level, that is, 10 % broke ratio. No breaks are assumed for the base case, but a constant trimming of 4 % to the couch pit is considered.

5.3.4.1. Distribution of fibre fractions and other pulp components

Figure 5.2 shows how the fibre composition changes from the pulp storage tanks through the headbox. Clearly, there is a trend for the fines content to increase, from the mixing chest trough the headbox. The separation units and the dilution of pulp with white water, rich in fines, cause this trend.

Figure 5.3 shows the variation of three important variables (ash, total dissolved solids and temperature) along the paper making process, from the stock preparation area through the headbox. The higher ash content in the machine chest with respect to the mixing chest (**Figure 5.3a**) is due to the addition of white water after the mixing chest to control the consistency. White water from the white water chest (about 63 % ash content) is used for this purpose. Notably, broke pulp has a higher content of total dissolved solids, DS (**Figure 5.3b**). These DS are mostly composed of cationic starch and other organic compounds added to the pulp furnish in the approach system, and are recirculated with the broke. Vacuum thickening of broke causes this increment of DS. Heat looses are compensated by direct steaming of white water in the clear white water reservoir and in the silo. Although there is an important temperature difference between the storage tank of hardwood, softwood and broke (**Figure 5.3c**), the temperature differences between the mixing chest, machine chest and the headbox are not significant.

5.4 Case study: Effect of process and control changes on the process variability

5.4.1 Introduction

Fine paper includes all those grades with special requirements for printing. The main requirements for this type of paper are a good formation, low porosity and uniform basis weight. Thus, the constant feed of thick stock with homogeneous properties is a pre-requisite for achieving a good product quality. The key pulp properties that affect the quality of fine paper include the following: consistency, ash and fines content. Consistency and the ash content affect specially the formation, basis weight and paper opacity, whereas the fines content in the feed pulp to the headbox affect the drainability and retention.

This study addresses the problem of process variability of these key pulp properties at the headbox, due to changes in process and control in the broke management area. These two aspects are considered in detail in the following sub-sections.

A simple Variability Index (VI) was used, which is defined by:

$$VI = 100\left(\frac{y - y^N}{y^N}\right) = 100(\hat{y} - 1) \qquad (5.3)$$

where $\hat{y}$ is the normalized (adimensional) variable y, and y^N is its value at steady-state. In order to compare the effect of changes of different magnitude and for different variables, the Relative Variability Index (RVI) has been defined by

$$RVI = \frac{\hat{y}_i - 1}{\hat{y}_j - 1} \qquad (5.4)$$

This index measures the effect of a change in the variable y_j on the variable y_i.

5.4.2 Effect of process changes during normal operation (No paper breaks)

The pulp blending system (**Figure 5.4**) has been chosen to perform a series of dynamic simulations. Step changes in a few selected variables have been performed and the dynamic responses of some pulp properties have been recorded. The purpose of this analysis is to identify key variables that potentially can cause the variability of pulp properties and components at the entrance to the paper machine. This variability can affect severely the paper machine stability and the paper properties, increasing at the same time the probability of more web breaks. Keeping adequate conditions in the broke management system is, therefore, imperative.

Following step changes on four variables have been performed:

- Hardwood pulp consistency (HW-c): 5 % (4.5 – 4.725 %)
- Fines content in the Hardwood pulp (HW-F): 20 % (8.0 – 9.6 %)
- Diluted broke consistency (Br-c): 5 % (4.0 -4.2 %)
- Broke ratio (BR): 50 % (10 -15 %)

5.4.3 Disturbance rejection during web breaks

Paper breaks of 30 minutes duration are considered. Once a web break has occurred in the paper machine, there are basically two alternatives to control the addition of the collected broke, manual control, still practiced in many mills, and the automatic control. The main control objective is to keep the proportion of broke in the pulp furnish and the inventories within specified ranges.

Manual control. Two scenarios are considered (**Figure 5.8**):

i) In the first scenario (1S), we let he broke ratio increase from its initial value at steady-state to the final value (base case) in one step, and go back to its initial value.

ii) In the second scenario (4S), the broke ratio is required to make four steps to go the lowest to the highest value, and vice versa.

Automatic control. The control configuration of the pulp proportioning system is depicted in **Figure 5.5**. Here, the high density broke tank level is cascaded with the broke ratio controller. That is, the output of this level controller becomes the setpoint for the broke ratio controller. This ratio is adjusted by changing the diluted broke flowrate. Thus, this flowrate is the only manipulated variable of theses two control loops.

5.4.4 Results and discussions

Figures 5.6 and **5.7** clearly show that changes in the broke ratio and the fines content of the hardwood pulp are two important sources of variability in the headbox. Specially, fines seem to have the largest potential for creating upsets in the paper machine.

Figure 5.9 shows a rather unexpected result. When manual adjustment is used to reject a disturbance (increase of the broke storage tank level due to one break), a single large increment in the broke ratio appear to have less impact on the process variability than four sequential shorter increments of the broke ratio. Obviously, the frequency of changes rather than the magnitude of the change of the broke ratio cause more upsets in the process.

Figure 5.10 shows the variation of the broke ratio for four values of the controller gain, and in **Figure 5.11** one can see that the more aggressively a controller has been tuned (faster response), the larger is the variability in the process. But, we also have to consider that the more sluggish the controller tuning is, the more persistent is the process variability. Although a conservative tuning is more advisable, a trade-off has to be made between reduction of process variability and longer periods of variability.

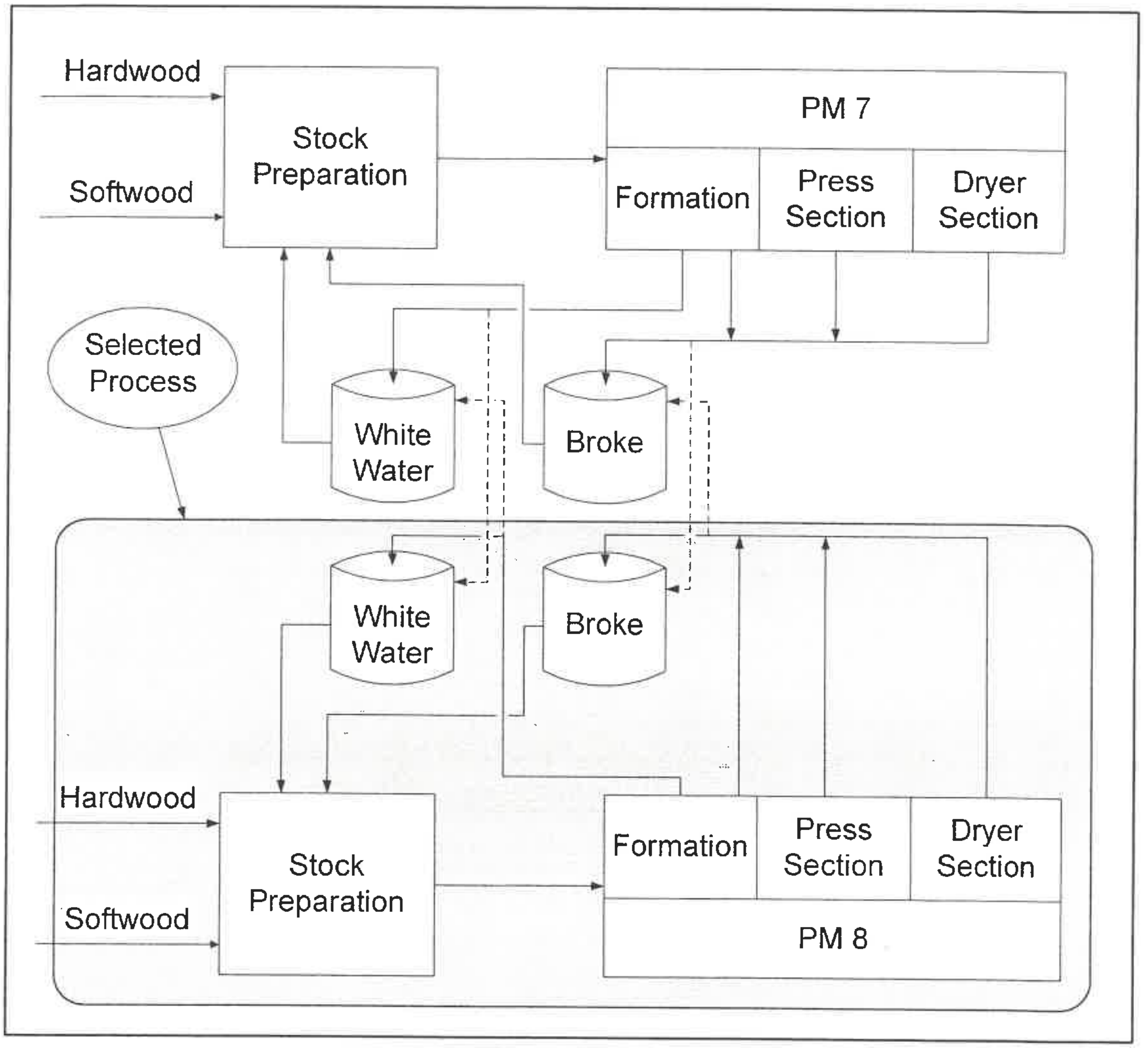


Figure 5.1: Scope of the dynamic simulation

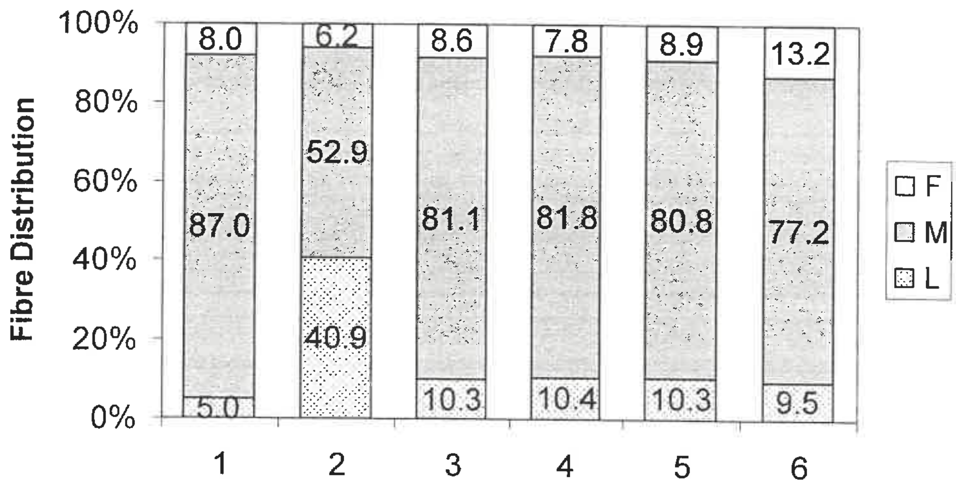


Figure 5.2: Fibrous material distribution across the papermaking process (Base case)

(F = Fines, M = Medium-size fibers, L = Long fibers)

1 = Hardwood storage tank

2 = Repulped softwood storage tank

3 = High density broke storage tank

4 = Mixing chest

5 = Machine chest

6 = Head box

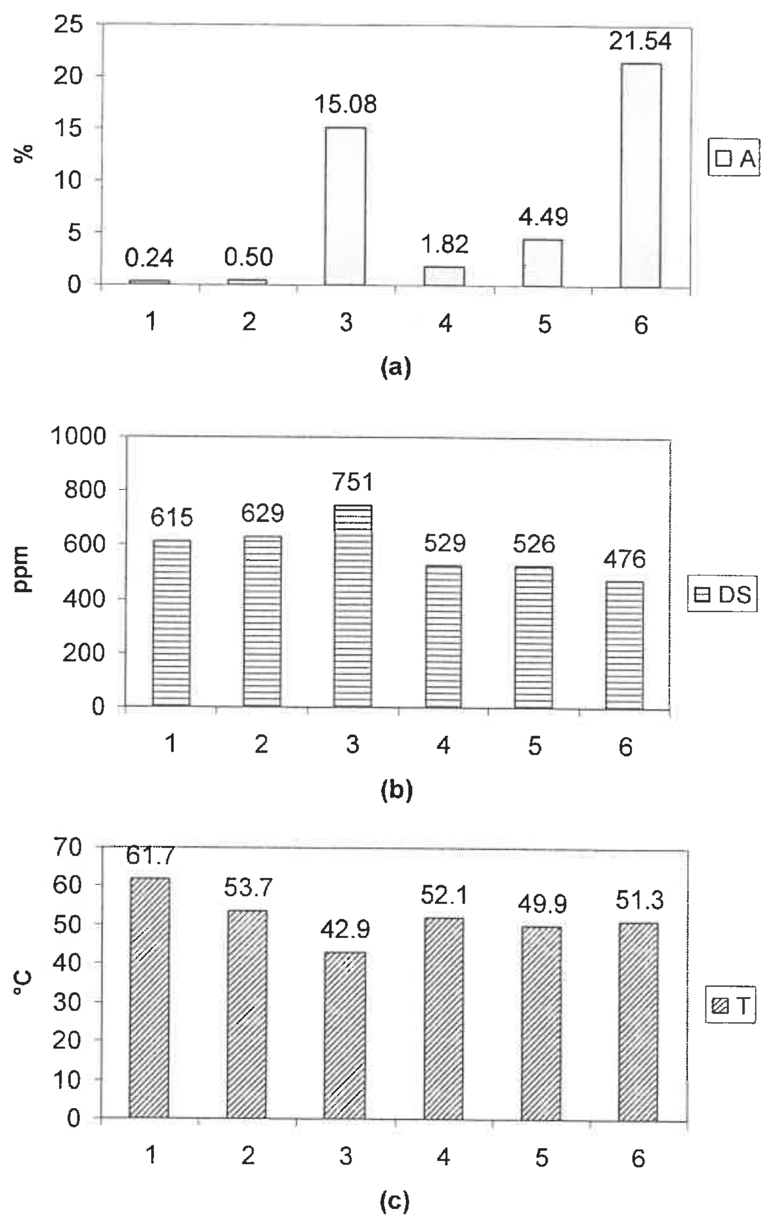


Figure 5.3: Distribution of important variables across the papermaking process (Base case)

(A = Ash, DS = Dissolved Solids, T = Temperature)

1 = Hardwood storage tank
2 = Repulped softwood storage tank
3 = High density broke storage tank
4 = Mixing chest
5 = Machine chest
6 = Head box

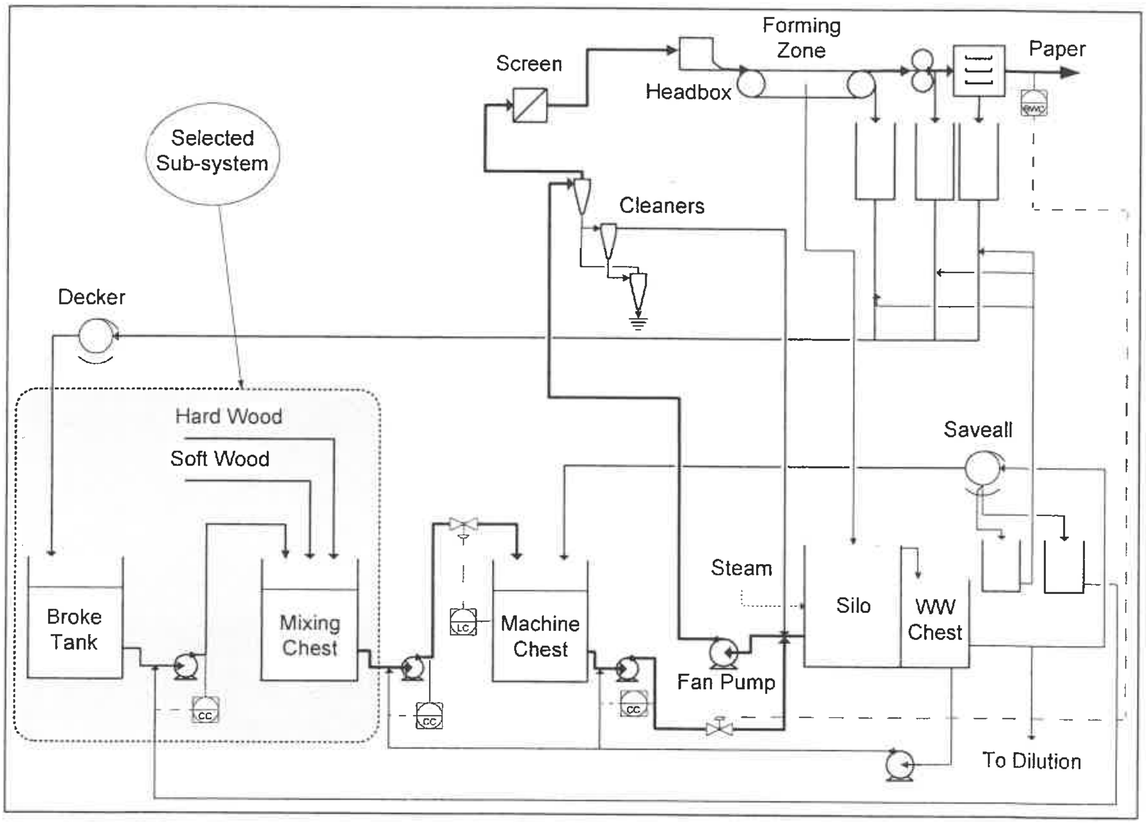


Figure 5.4: Simplified paper mill flowsheet showing selected area for variability and operability analysis

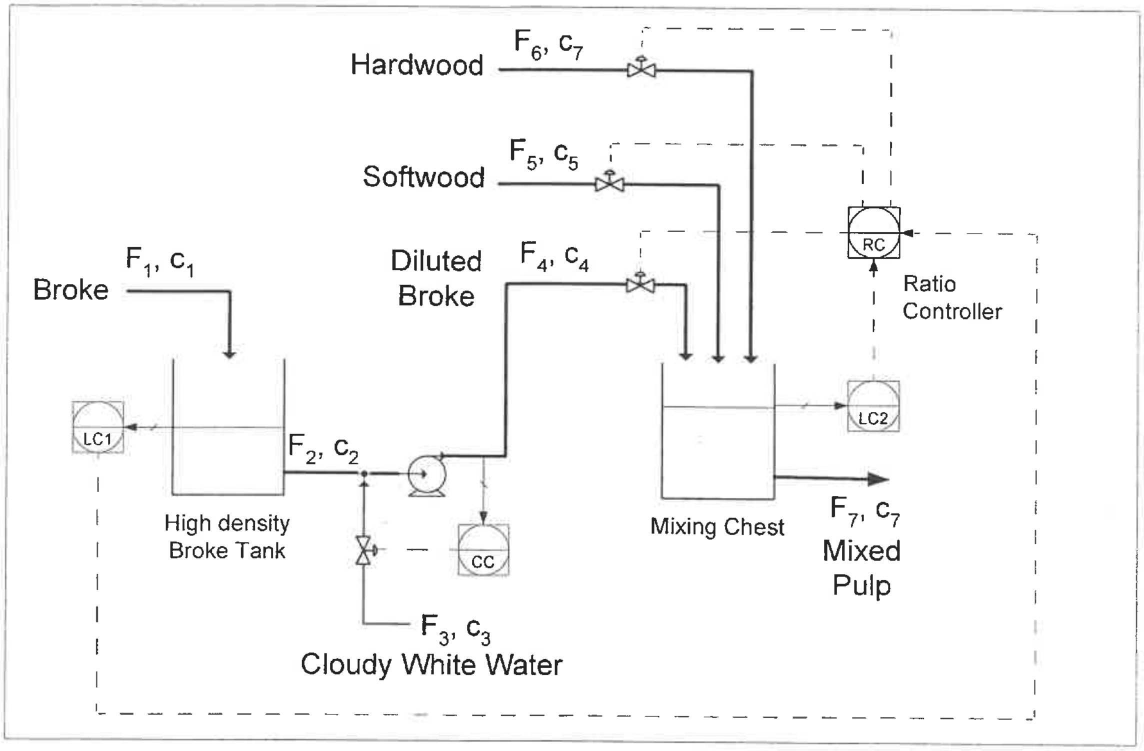
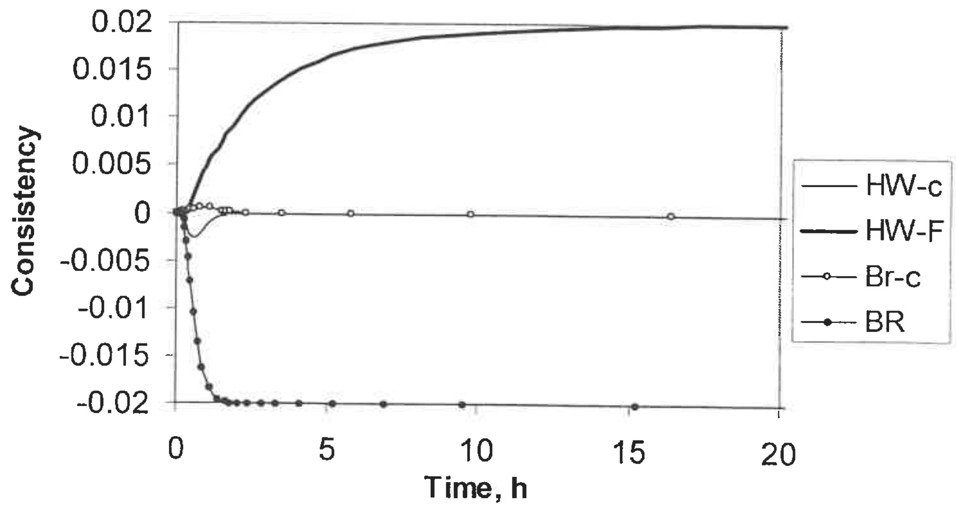
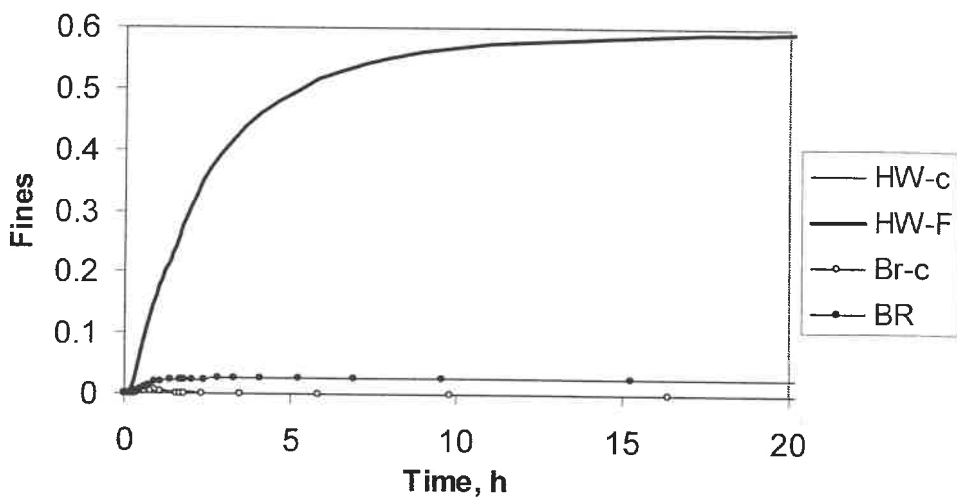


Figure 5.5: Control configuration of the pulp proportioning system



(a)



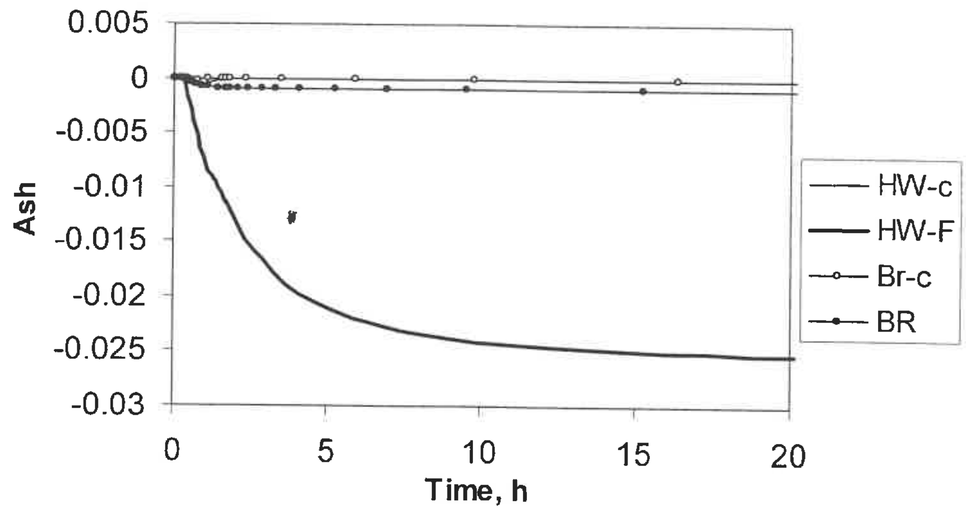
(b)

Figure 5.6: Relative variability (RVI) of consistency and fines content in the headbox for one step change perturbations

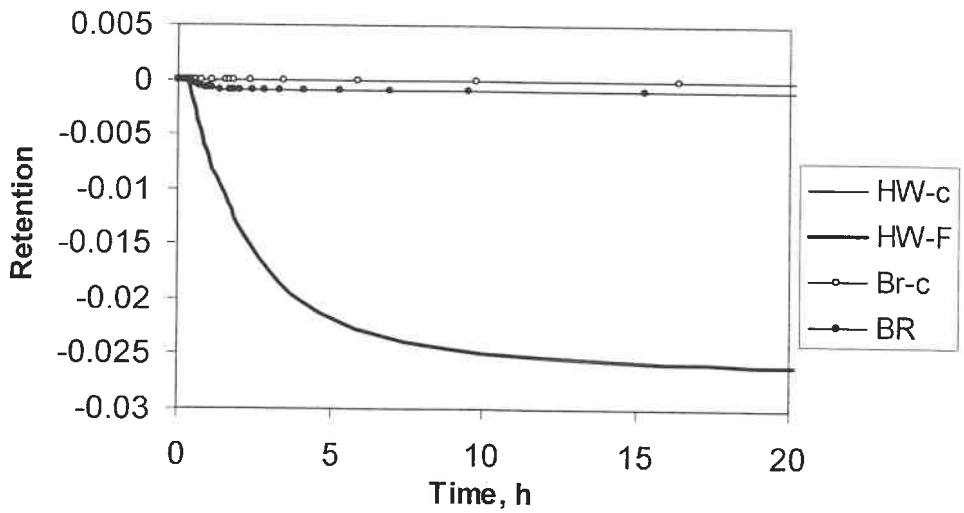
Disturbances: Consistency and fines content of the hardwood stream (HW-c and HW-F), diluted broke consistency (Br-c) and broke ratio (BR), in terms of normalized values

(No paper breaks)

(a) Consistency in the headbox, (b) Fines content in the headbox



(a)



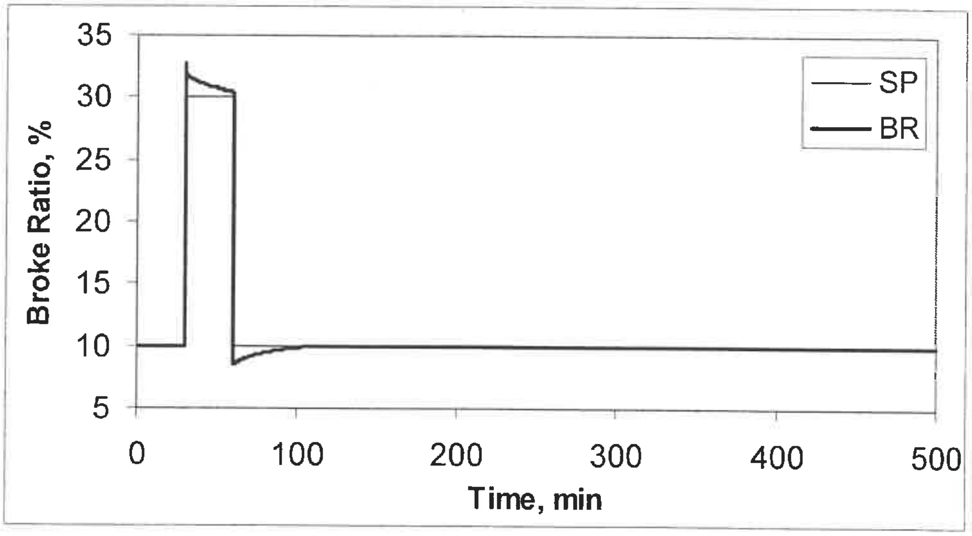
(b)

Figure 5.7: Relative variability (RVI) of ash content in the headbox and retention for one step change perturbations

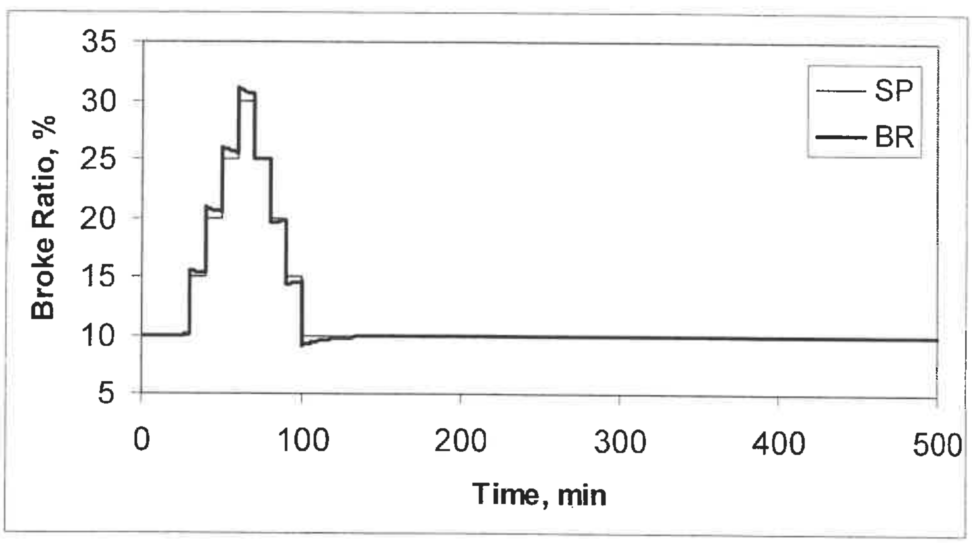
Disturbances: Consistency and fines content of the hardwood stream (HW-c and HW-F), diluted broke consistency (Br-c) and broke ratio (BR), in terms of normalized values

(No paper breaks)

(a) Ash content in the headbox, (b) First-pass retention



(a)



(b)

Figure 5.8: Manual adjustment of the broke ratio

Break duration = 30 min

(a) one step (1S), and (b) four steps (4S)

(SP = Setpoint, BR = Broke ratio)

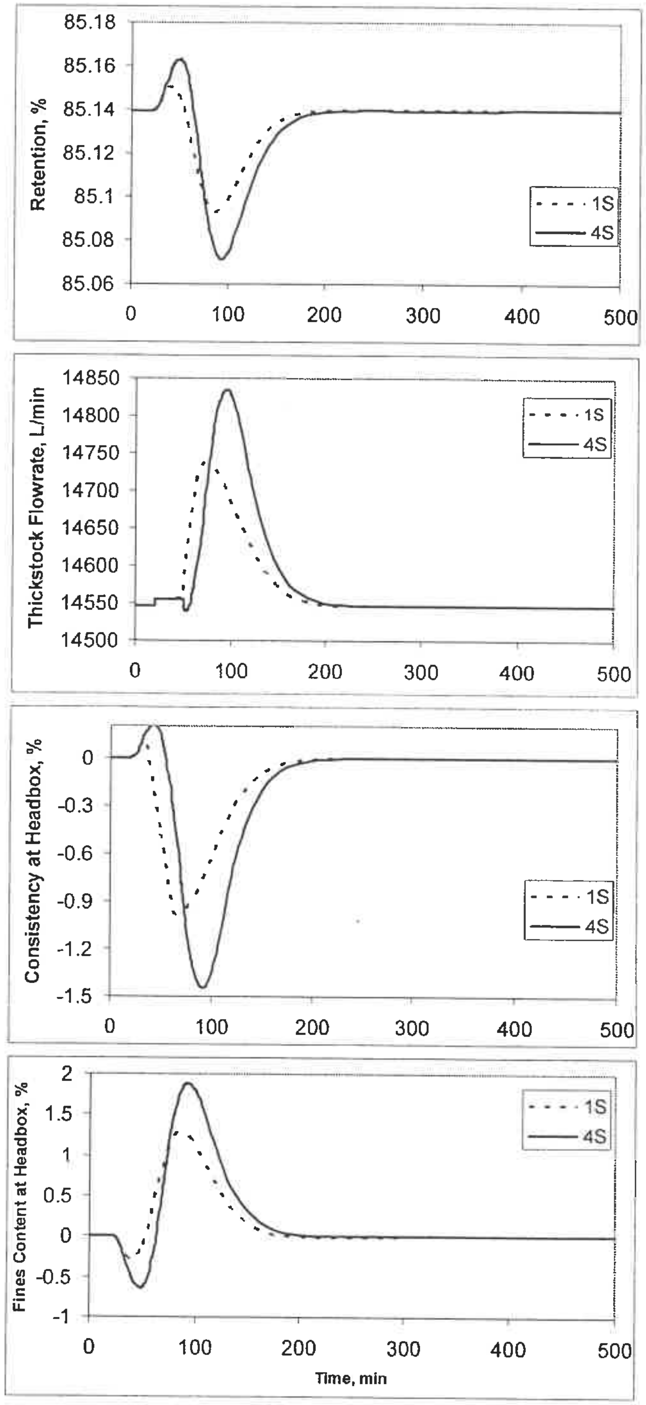


Figure 5.9: Variability after manual adjustment of broke ratio (1S = 1 step, 4S = 4 steps)

Variability Index (VI) was used for consistency and fines content at headbox

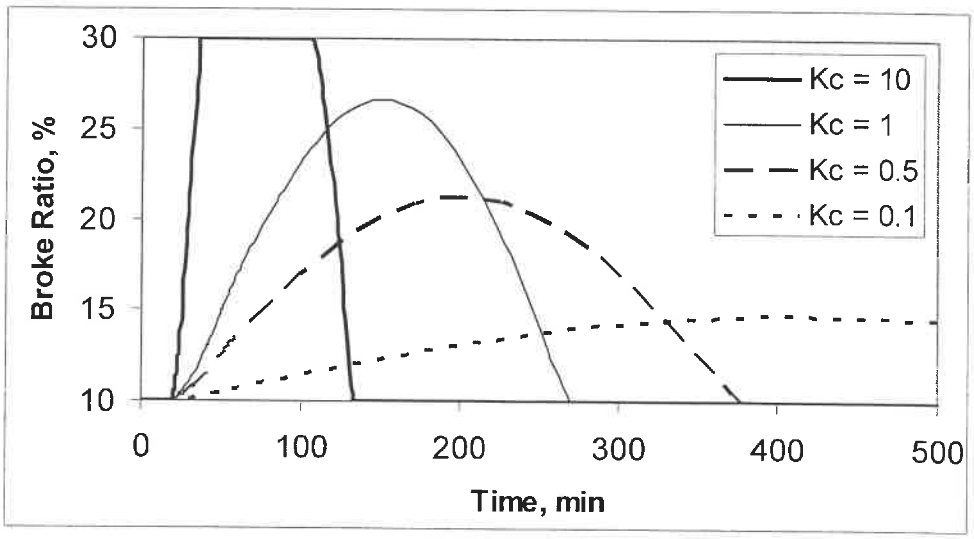


Figure 5.10: Variation of the broke ratio as a function of the broke tank level controller gain

(τ_I = 10 min in all cases)

Break duration = 30 min

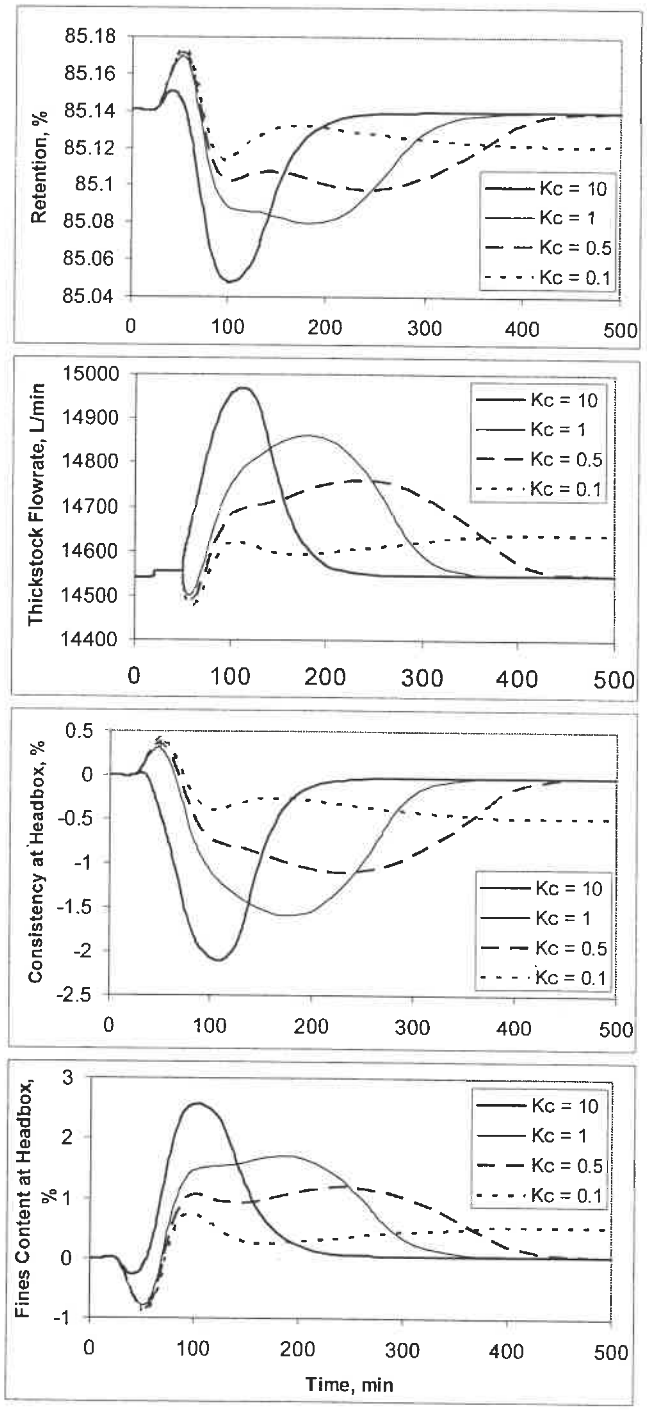


Figure 5.11: Effect of the broke tank level controller tuning on the process variability

Variability Index (VI) was used for consistency and fines content at headbox.

CHAPTER 6: STEADY-STATE OPERABILITY ASSESSMENT OF THE BROKE MANAGEMENT SYSTEM AND DEVELOPMENT OF A NEW APPROACH FOR DYNAMIC OPERABILITY ASSESSMENT

6.1 Introduction

As stated in the hypotheses, the methodology by Vinson and Georgakis (2000) for input-output controllability can be applied to the broke management system and can give important insight about the flexibility of the system and its capacity to reject disturbances. The complexity of real systems, however, makes it necessary the use of eclectic methodologies for operability assessment. The combined use of several analysis tools can capture the different aspects of the process operability.

In this work, some operability analysis was performed on the selected subsystem (**Figure 5.4**). In particular, two standard tools were used, the relative gain array (RGA) and the Niederlinsly criterion for closed-loop stability. Both methods require only steady-state information. Thus, a simplified linearized model for the selected sub-system was developed. In particular, the RGA gives information about the recommended input-output pairing, in order to minimize the multiloop interaction. An input-output controllability analysis for steady-state conditions was performed, in order to detect possible limitations to the process controllability due to input constraints. The sensitivity of the key control loop to track setpoint changes and to reject disturbances is determined, as well.

The results are given in the following sub-sections, and the methodology for assessing input-output controllability developed by Vinson and Georgakis (2000) is briefly explained in **Appendix B1**.

In **Appendix B3** a new approach for the assessment of the dynamic operability of processes is developed. This approach is based on the controllability concepts proposed by Vinson and Georgakis (2000, 2001) for the steady-state case. The operating spaces are redefined for the dynamic case and a new dynamic Operability Measure (*dOM*) is proposed. This operability index is based on the idea that the operability of a process under closed-loop conditions is dictated by both, the process dynamics and the closed-loop characteristics. The first component of this index, called Operable Fraction (f_{op}) measures the achievable operating spaces by taking into account only the process dynamics. Since there are no control structures, f_{op} measures the inherent ability of the process to track setpoint changes and to reject disturbances. The second component of *dOM* is given by the control performance. It is assumed that both, controlled and manipulated variables contribute to the global performance of the control system. A new performance index is proposed for deterministic changes in the process. This index was defined by combining classical performance indices.

The methodology for dynamic operability analysis has been developed in detail for a single-input single-output (SISO) linear system. An extension to more general multi-dimensional linear systems is also proposed and an example of application is given for a 2x2 distillation control problem.

6.2 Steady-state operability analysis of the broke management system

6.2.1 Problem statement

In the previous chapter, dynamic simulation of a fine mill has shown that process and control changes in the area of pulp proportioning may have a great impact on the variability of key variables, which determine in a large extent the paper machine stability. From the analyzed variables in the broke management area, changes in two variables, the broke ratio and the fines content in the hardwood feed pulp appear to have a significantly impact on the downstream variability. Since we are assuming perfect mixing in all tanks, variations in the pulp stream consistencies are damped out quite well by the reservoirs. On the other hand, the fines content in the broke management area is not a controlled variable and is caused externally, in the pulp mill. Thus, the broke ratio remains as the only controlled variable that potentially can upset the paper machine stability.

6.2.2 Subsystem model

The selected subsystem to perform operability analysis is the pulp proportioning system, depicted in **Figure 5.5**. Assuming isothermal conditions, the nonlinear model for this system is given in **Tables B2.1** to **B2.4 (Appendix B2)**. By dividing the physical variables by reference values, one can define dimensionless variables (**Table B2.5**). The model in terms of normalized variables is given in **Tables B2.6** to **B2.8**.

The selected controlled (y_i) and manipulated (u_i) variables for the simplified model are $\mathbf{y} = [c_4\ h_2\ R_1\ \mathrm{R}_2]^{\mathrm{T}}$ and $\mathbf{u} = [F_3\ F_4\ F_5\ F_6]^{\mathrm{T}}$.

where c_4 is the diluted broke consistency, h_2 is the level of the mixing chest, and R_1 and R_2 are the Hardwood/Softwood ratio and the broke ratio, respectively. F_i is the flowrate of stream i. All other variables are assumed to be constant.

The linearized process model relating inputs to outputs, in terms of normalized variables, results in:

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} = \begin{bmatrix} -0.905 & 0 & 0 & 0 \\ \dfrac{16.21}{s} & \dfrac{16.21}{s} & \dfrac{16.21}{s} & \dfrac{16.21}{s} \\ 0 & 0 & -51.27 & 9.69 \\ -0.799 & 0.814 & -0.221 & -0.237 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} \tag{6.1}$$

6.2.3 Results and discussions

For the subsystem model (**Eq. 6.1**), the relative gain array RGA can be calculated as

$$\Lambda = \begin{array}{c} \begin{array}{cccc} F_3 & F_4 & F_5 & F_6 \end{array} \\ \begin{bmatrix} 1.00 & 0 & 0 & 0 \\ 0 & 0.22 & 0.13 & 0.65 \\ 0 & 0 & 0.84 & 0.16 \\ 0 & 0.78 & 0.03 & 0.19 \end{bmatrix} \end{array} \begin{array}{c} \\ c_4 \\ h_2 \\ R_1 \\ R_2 \end{array} \tag{6.2}$$

Hence, the RGA method suggests the following pairing: $\{F_3 - c_4\}$, $\{F_6 - h_2\}$, $\{F_5 - R_1\}$ and $\{F_4 - R_2\}$. In effect, this corresponds to the industrial practice. The high density broke tank level (h_1) is usually controlled by manipulating the broke ratio (R_2). Thus, the flowrate F_4 (diluted broke) becomes the manipulated variable for both h_1 and R_2. This suggests a cascade control configuration. Since most of the elements of the RGA are lying in the range [0, 1], this also tells us that there is a high degree of interaction between the control loops.

The closed-loop stability of a multiloop system can be evaluated using the Niederlinski index N. A system of n loops will be unstable if following condition holds:

$$N = \frac{|\mathbf{G}(0)|}{\prod_{i=1}^{n} g_{ii}(0)} < 0 \tag{6.3}$$

where $\mathbf{G}(0)$ is the steady-state gain matrix and g_{ii} are the diagonal elements. This condition is necessary and sufficient only for 2x2 systems; for higher dimensional systems, it provides only a sufficient condition. For the system considered here it results $N = 5.26$. Thus, the system is structurally stable, and the stability will depend upon the controller parameters.

Figure 6.1 shows the servo output controllability index (*s–OCI*) for the broke ratio controller, using the steady-state (nonlinear) model developed in the previous chapter. The value of 1 for s-OCI indicates that the process is operable at steady-state and there are no limitations to the desired outputs due input constraints. In fact, one can see that the system is somewhat over designed, in order to make the process flexible in face to paper grade changes, for instance. The available inputs allow the addition of broke up to approximately 42 % of the pulp furnish. This, certainly, was expected for an existing plant.

6.3 Closed-loop sensitivity

The key control loop in the subsystem is the broke ratio control loop, where the controlled variable is the broke ratio, R_2, the manipulated variable is the diluted broke flowrate, F_4, and the process gain is $K_p = 0.14$. It is, therefore, important to know the capability of this control loop to move from one operating condition to another and its capability to reject disturbances is. An analysis in the frequency domain can answer this question.

For a single-input-single-output (SISO) system (**Figure B3.1**, **Appendix B3**), the transfer function relating the set-point (r) and disturbance input (d) is given by

$$y(s) = \frac{g_p(s)g_c(s)}{1+g_p(s)g_c(s)}r(s) + \frac{g_d(s)}{1+g_p(s)g_c(s)}d(s) \tag{6.4}$$

the *sensitivity function* for the closed-loop is defined (Burns, 2001) by

$$S(s) = \left.\frac{y}{d}\right|_{r=0} = \frac{1}{1+g_p(s)g_c(s)} \tag{6.5}$$

and the *complementary sensitivity function* is defined by

$$T(s) = 1 - S(s) = \frac{g_p(s)g_c(s)}{1+g_p(s)g_c(s)} \tag{6.6}$$

A necessary and sufficient condition for having a perfect set-point tracking and disturbance rejection is:

$$T(j\omega) = 1 \text{ and } S(j\omega) = 0 \tag{6.7}$$

Figure 6.2 shows that the capacity to reject disturbances is improved with increasing speed of response (lower values of lambda), but this sensitivity to disturbances decreases continuously for any controller tuning up to around 0.5 rad/min (disturbance period = 2min). For higher frequencies the sensitivity remains constant, but the control system is less capable to reject disturbances. This type of system is known as "high-pass filter", that is, low-frequency disturbances are effectively filtered whereas high-frequency disturbances pass directly to the output. The capacity to track a set-point change behaves in a similar way. That is, for low frequencies (up to 0.1 rad/min or periods of set-point changes > 10 min) there is a good set-point tracking. For higher frequencies, the set-point error becomes smaller with increasing speed of response.

Time delay not only affects the performance of a control system, but it also clearly affects its capacity to reject disturbances and to track set-point changes (**Figure 6.3**). As expected, the disturbance rejection is more affected at high frequencies and the negative effect on the set-point tracking only appears at frequencies higher than 0.1 rad/min.

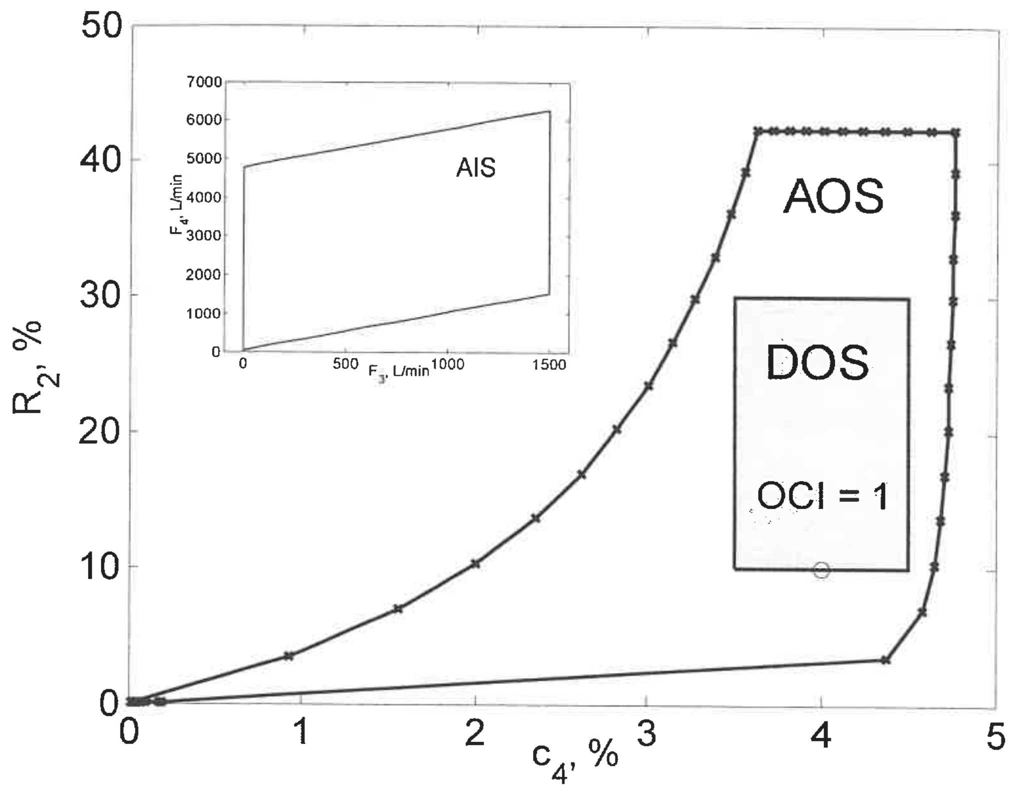


Figure 6.1: Output operability for set point changes in the broke ratio and the diluted broke consistency

R_2 = broke ratio, c_4 = diluted broke consistency;

F_3 = white water flowrate, F_4 = diluted broke flowrate

AIS = Available Input Space,

DOS = Desired Output Space,

AOS = Achievable Output Space

OCI = Output Controllability Index

o = Base case

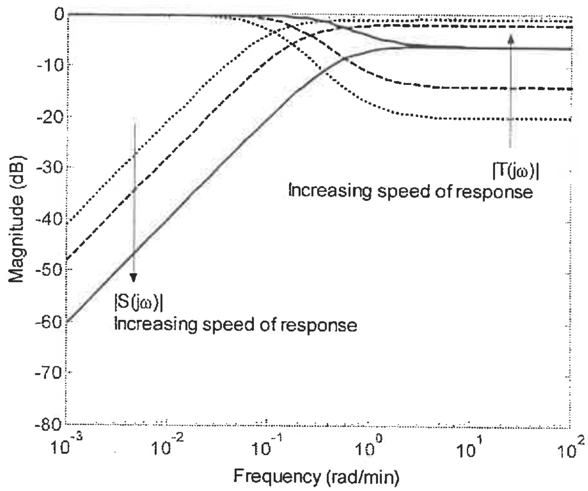


Figure 6.2: Sensitivity (S) and complementary sensitivity (T) functions for the broke ratio controller

PI controller (Solid lines: λ = 2min, dashed lines: λ = 5min, dotted lines: λ = 10min)

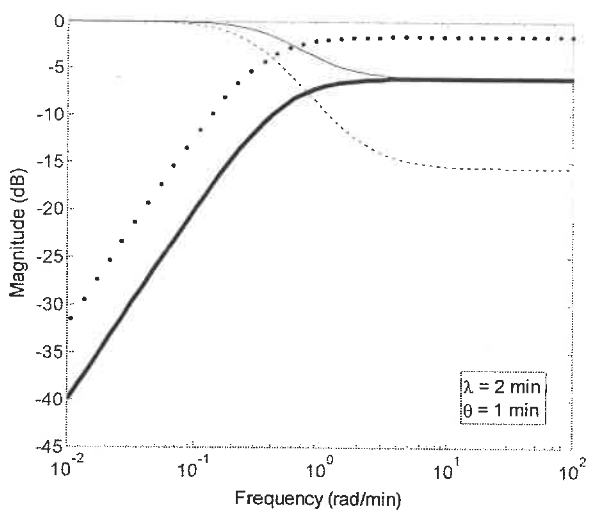


Figure 6.3: Effect of time delay (θ) on the sensitivity and complementary sensitivity functions

Thick lines: sensitivity functions; thin lines: complementary sensitivity functions

Solid lines: No delay; dotted lines: process plus time delay

CHAPTER 7: CONCLUSIONS AND RECOMMENDATIONS

7.1 Conclusions

Chapter 4 addresses the evaluation of several dynamic simulation packages for dynamic simulation and selection of a simulation tool to develop a dynamic model. It has been shown that a one-step delay is generated in the recycle stream at each iteration when a sequential simulator is used to solve a recycle loop. This may cause for some process configurations an oscillating response and a big calculation error. The magnitude of the error can be minimized by using an iterative solution of the recycle. The calculation order must be carefully chosen if iteration is not possible due to simulator software limitations. The Euler backward difference integration method used by one of the analyzed sequential simulators showed a higher robustness than the mass balance approximation used by the other sequential simulator. Convergence problems with an equation-based simulator are mainly related with redundant specification (singularity) and the integration method used.

Chapter 5 deals with the development of a dynamic simulation of a fine paper mill by using an equation-based simulator. This simulation was used to analyze the dynamics of pulp components across the process and the process variability in the headbox due to changes in process and control in the area of pulp furnish preparation. Changes in the fines content in this area, as well as changes in the broke ratio have been identified to be important sources of variability upstream of the headbox. If changes of the broke ratio are made manually, it was found that the frequency of change has a larger impact on the process variability than the magnitude of each change. If automatic control is applied to the broke management, more aggressively tuned controllers have a detrimental effect on the paper machine stability.

In **Chapter 6** several operability analysis tools, including Vinson's (1998, 2000) input-output controllability approach, were applied to analyze the steady-state operability characteristics of the broke management system. The results show that the control loops in the pulp proportioning system are highly interactive, and the existing process was over designed to allow a flexible operation. A sensitivity analysis of the broke ratio control loop was also performed to analyze the capability of the closed-loop to reject disturbances and to follow changes in the setpoint. This analysis shows that a more aggressive controller tuning of the broke ratio controller results in a higher sensitivity of the control system to reject disturbances and to move between different operating points. Time delay affects this sensitivity.

Vinson's approach was extended to dynamic systems. A new approach for the assessment of the dynamic operability was developed. New control performance and dynamic operability indices have been proposed. The operability index, called dynamic Operability Measure (*dOM*), explicitly takes into account the closed-loop performance in addition to the inherent capability of the process to move between operating points and to reject disturbances. It reflects, therefore, the combined contribution of the process and the control system. This approach was tested with a simple SISO system. The applicability to multidimensional systems was illustrated with a control design problem for a 2x2 system.

7.2 Contributions to knowledge

The achieved results contribute to a better understanding of the key factors that affect the accuracy of dynamic process simulators. Using dynamic simulation of a fine paper mill the key variables that contribute to process variability in the headbox and to paper machine instability were identified. Furthermore, a general methodology for assessing the dynamic operability of processes has been developed.

Specific contributions include:

- The main factor affecting the convergence in the transient period when using commercial sequential dynamic simulators has been found to be the calculation algorithm. This problem is particularly critical when there are recycles in the simulated process, and it can be avoided by using iterative solution. Other measure that helps to minimize convergence problems is the selection of a small time step (0.5 min or less). Numerical instability problems can be overcome by selecting a controller time constant to time step ratio not smaller than 2.5. When using a simultaneous simulator, a variable time step reduces significantly the simulation time and the best available integration method for the specific problem should be selected in order to avoid numerical instability. In general, the Euler method is not recommended for large models. Good initial values are always required to achieve converged results.

- Using the mill-wide dynamic simulation of a fine paper mill, two process and control changes, in the pulp blending area have been identified to be the most important sources of variability in the paper machine headbox. These key variables are the fines content and changes in the broke ratio. It was found that a conservative tuning of the broke level controller causes less variability in the paper machine headbox, but at the cost of longer periods of variability. Also, the dynamic simulation has shown that frequent changes in the broke ratio has a more detrimental effect on the process variability than the magnitude of these changes.
- Several steady-state operability analysis methods show that the pulp proportioning system contains highly interactive control loops, the system is closed-loop stable and the process was designed to allow flexible operation. Although the desired broke ratio for fine paper usually does not exceed 30%, the input-output controllability analysis on steady-state basis shows that the maximum amount of broke that can be added to the pulp furnish is about 42%. Furthermore, the sensitivity analysis in the frequency domain shows that the capability of the broke ratio control loop to reject disturbances and to track setpoint changes is improved with increasing speed of response and decreasing frequency of disturbances and setpoint changes. For any controller tuning, the sensitivity to disturbances continuously decreases up to around 0.5 rad/min, or a disturbance period of 2 min. For periods of setpoint changes smaller than 10 min, or frequencies higher than 0.1 rad/min, the setpoint error becomes larger.

- A new general approach for assessing dynamic operability has been developed. This includes a new control performance index for deterministic problems and a new dynamic operability measure. It has been shown that the proposed operability measure effectively captures different aspects of the dynamic operability of processes, such as input constraints, time delay and control structure. On the other hand, the control performance index also includes the contribution of the manipulated variable to the overall closed-loop performance.

Some implications of the proposed dynamic operability assessment include its applicability to design and retrofit problems. A relatively simple example of screening of control design alternatives for a distillation column has been shown. In greenfield design, disturbances are never fully accounted for in dynamic process simulation and operability analysis. In this case, the simultaneous design of process and control system seeks to maximize *dOM*.

In retrofit problems, many real process data exist, and true disturbances can be represented. Usually, however, not all disturbances are known (measured). Since model mismatches are of concern in this case, a more detailed analysis is required. For example, criteria of fitness must be defined, and data pre-treatment and reconciliation need to be performed.

7.3 Recommendations for future work

It is recommended the application of the proposed dynamic operability framework to the broke management system with the purpose of evaluating the required operating ranges for a target variability in the headbox.

The wide applicability of this new approach for dynamic operability was stressed but, there are several aspects that need to be addressed. These include the following:

- Effect of model incertitude on the operability measure.
- Procedure of application for non-square systems
- Implementation within an optimization framework
- Application to real systems (requirements on process data, on-line applicability).

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APPENDICES

APPENDIX A: PROCESS SIMULATION

APPENDIX A1

DYNAMIC SIMULATORS FOR THE PULP AND PAPER INDUSTRY

Among the simulation packages aimed to the pulp and paper industry, we can include: WinGEMS® by Pacsim Inc., CadSim Plus® by Aurel Systems Inc. and IDEAS® by IDEAS Simulation Inc. built on top of the environment Extent® (Krahl, 2001) by ImagingThat! Both WinGEMS and CadSim Plus are sequential simulators, specifically designed for the pulp and paper industry, and the main difference between them is that CadSim Plus allows the user to *pressure-flow network* selected streams in order to promote convergence by local iteration. IDEAS is a hybrid general-purpose simulation package that allows hierarchical modeling and has an optional component library intended for the pulp and paper industry.

Another simulation package with some library components for the pulp and paper industry is the dynamic equation-based simulator MASSBAL3® (integrated with the steady-state simulator MASSBAL2®), initially by Open Models Inc., integrated later into HYSYS® by Hyprotec Ltd., now owned by Aspen Tech Inc.

The first three simulation packages are currently the most used in North America for dynamic simulation in this industrial sector. In Europe, especially in Scandinavia, there are other tools in use, these include: APMS® (Advanced Paper Mill Simulator), a WindowsNT® based dynamic simulator built upon the environment APROS® (Advanced PROcess Simulator), and the simulation tool Dymola, intended for large systems and based on the object-oriented, general-purpose modeling language Modelica. A Modelica component library was implemented with pulp and paper process modules.

APPENDIX A2

EVALUATION OF CRITICAL FACTORS FOR DYNAMIC SIMULATION

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Abstract

There are a number of common problems that can be encountered when building a dynamic simulation. These problems can severely affect the simulation accuracy and even prevent convergence. This paper is aimed at the novice practitioner. It evaluates two sequential simulators widely used in the pulp and paper industry, as well as one general purpose simultaneous simulator, focusing on available techniques to overcome convergence problems and to improve accuracy.

Keywords: DYNAMIC SIMULATION; SEQUENTIAL AND SIMULTANEOUS SIMULATORS; CONTROLLER TUNING; TRANSIENT RESPONSE; CONVERGENCE

1. Introduction

Limitations in computer power and storage capabilities in the past two decades restricted the use of simulation software packages to steady-state applications, namely retro-fitting and design tasks [1]. This situation has changed, and today dynamic simulation has become an important tool to analyze complex systems and is increasingly used in industry and in universities. A literature search on the applications of dynamic simulation shows that researchers now feel more confident about performing "large-scale" dynamic simulations [1,4,8]. Another reason for this interest in dynamic simulation is the growing awareness of the tight relationship between process design and control.

There are three basic approaches to solve flowsheeting systems: *the sequential modular approach*, in which the equations describing each process unit (module) are solved module-by-module in a sequential manner, the *simultaneous* or *equation-based approach*, in which the entire process is described by a set of differential equations and the equations are solved simultaneously, and finally the *simultaneous modular approach*, which combines sequential and simultaneous calculations methods. The latter type of simulator, which will not be considered in this paper, is sometimes called a *hybrid* simulator. Several authors [5,11,12,13,14] have described the features and techniques of the different approaches, enumerating their advantages and disadvantages, and emphasizing specific characteristics.

1.1. *Evaluated simulators*

The main requirement for a dynamic simulator is accuracy, and therefore the user must be aware of the factors that may limit accuracy in the simulator, which can in turn prevent convergence.

This paper consists of a comparative evaluation of the capabilities of several commercial simulation packages to perform an accurate dynamic simulation. The main purpose of this work is to help the novice practitioner build an accurate dynamic simulation by highlighting the strengths of each simulator, although it is not our intention to recommend which simulator is best. Practical hints are very useful in the first stages of a dynamic simulation, since this activity can be challenging and time-consuming, especially when a lack of expertise may lead to inaccurate results.

For obvious reasons, the evaluated simulators are not explicitly identified. Their major characteristics are summarized in **Table A2.1**.

2. **Effect of time step and controller tuning**

The evaluated sequential simulators use PID controllers based on discrete time (digital) models [9]. In these types of controllers, continuous time is replaced by a constant sample time (time step), Δt. Hence, the simulation time step and controller tuning need to be treated together.

Although any tuning method can be used to tune controllers in the model, in order to prevent cycling the Lambda tuning method or internal model control (IMC) based tuning are recommended. In these methods, a unique parameter, Lambda (λ), which is the time constant of a closed loop, needs to be selected [2]. The IMC-based PID tuning can be based on either setpoint tracking or disturbance rejection. In the next two examples, the second procedure is used.

2.1. *Process with a large time constant*

A typical example of this case is the level control of a surge vessel, depicted inside the box in **Figure A2.1** (i.e., disregarding the consistency control and recycle). This is an integrating, non-stable process characterized by the following transfer function

$$G_p(s) = \frac{K_p e^{-\theta s}}{s} = \frac{e^{-\theta s}}{As} \qquad \text{(A2.1)}$$

where A is the cross-sectional area of the tank and θ the dead time. For the sake of simplicity, neglecting the dead time and using an IMC filter of the form

$$f(s) = \frac{\gamma s + 1}{(\lambda s + 1)^2} \qquad \text{(A2.2)}$$

where γ is selected to achieve good disturbance rejection, a PI controller results with following parameters

$$K_c = \frac{2}{K_p \lambda}; \quad T_I = 2\lambda \qquad \text{(A2.3)}$$

where K_c and T_I are the controller gain and the integral time, respectively.

For a tank with a total capacity of 200 m^3 and setting the controlled level to 75%, the residence time and mixing time constants are, respectively:

$T_R = 20$ min

$\tau_{tank} = 15$ min

To ensure good mixing, it is recommended to select a value of $\lambda \geq \tau_{tank}$. Experiments were performed using two values of λ around τ_{tank}. The corresponding controller parameters for a PI controller are shown in **Table A2.2**.

The following operating conditions are considered.

Inlet stream:

Consistency: $c_i = 4$ %

Temperature: $T_i = 20$ °C

Outlet stream:

Initial flowrate: $F_o = 10$ m^3/min

Disturbance: $\Delta F_o = 5\%$ @ t = 100 min

Figures A2.2 through **A2.5** show the dynamic responses of the controlled variable (tank level) to a step change consisting of a 5% increment in the outlet flowrate, using each simulator. If a sequential simulator has local iteration capability, it should be used in order to prevent the unstable, oscillating responses that may occur even with simple models, such as those obtained in **Figure A2.2**. The oscillations can be eliminated using smaller time steps, but the oscillating behavior is amplified for decreasing values of Lambda ($\lambda \leq 10$ min). For this reason, when using Simulator A, the user is advised to enable local iteration when it is suitable to promote convergence in a dynamic simulation. From **Figures A2.3**, **A2.4,** and **A2.5**, we can see that the response time of the closed loop depends on the value of λ, i.e., smaller values of λ cause a faster response of the closed loop, and vice versa. Another important result is that, for the same value of Lambda, the responses of the controlled variable are almost the same, no matter which time step was selected (Simulators A and C). On the contrary, Simulator B shows a rather strange effect of the time step, characterized by different settling times for different values of the time step; it seems that the integral time is changing according to the time step. Simulator B uses a strongly stable method to approximate an integral, but as the controller becomes moderately aggressive, the stability of this method is dependent on the size of the simulation time step (Ts). Thus, in this case the simulation did not converge for λ = 10 min and Ts = 1 min. On the other hand, when using the simultaneous simulator C, no difference was found between the two tested integration methods: the A-Stable Euler method, which uses the backward approximation of a derivative and is not affected by the size of the time step, and the adaptive Runge-Kutta method.

Notably, there is a difference in the magnitude of the response for Simulator A (ten times larger) compared to the other two simulators. This is obviously an effect of the iterative calculation method. However, a determination of which of these transient responses better reflects a real process can only be made by comparing the simulated values with real data.

2.2. *Process with a small time constant*

One of most important control loops from the pulp mill through to the final point of dilution ahead of the paper machine is the consistency control. Consistency controllers are typically located at the outlet stream of a vessel tank, which is intended to damp out fast consistency variability. White water of low consistency is used to dilute the pulp (**Figure A2.1**). The main objective of the consistency control is to minimize process variability at the headbox, where a variability of 1% in the mean is considered high, 0.5% is good, and below 0.3% is excellent [10]. Consistency control loops are comparatively fast processes with small time constants (usually τ = 3 to 5 s), which are almost entirely determined by the consistency transmitter internal damping features, and characterized by a function that is first order with respect to time delay transfer:

$$G_p(s) = \frac{K_p e^{-\theta s}}{\tau s + 1} \qquad \text{(A2.4)}$$

where the dead time θ should be no longer than 3 seconds at the maximum demand flow. Neglecting again the effect of time delay and using an IMC filter of the form

$$f(s) = \frac{1}{(\lambda s + 1)} \qquad \text{(A2.5)}$$

controller gain and integral time of the PI controller are given by

$$K_c = \frac{\tau}{K_p \lambda}; \quad T_I = \tau \tag{A2.6}$$

When tuning a real process, the parameter λ should always be based on the dead time θ, keeping the relation $\lambda \geq \theta$ to avoid resonance. When θ is ignored, we can choose much larger values of λ. So, if $\lambda = 30$ s, the controller gain becomes:

Kc = 0.286 m^3/min/Cons-%

For the same tank characteristics and keeping the same initial conditions in the inlet stream, additional data to run the simulations are given as follows (no recycle stream is considered yet).

Inlet stream:

Disturbance: $\Delta c_o = 2.5$ % @ t = 50 min

White water stream:

Consistency: $c_{ww} = 0.02$ %

Temperature: $T_{ww} = 20$ °C

Outlet stream:

Flowrate: $F_o = 500$ t o.d. /d

Consistency: $c_o = 3.5$ %

Simulation runs were performed for several combinations of integral time and time step (**Figures A2.6, A2.7** and **A2.8**). Once again, the same trends as with the level controller are observed. With sequential simulators, it is better to choose smaller values for T_I and Ts for faster processes, but it is important to keep in mind some limitations. A value of T_I / Ts equal to or greater than 2.5 must be maintained with Simulator A in order to avoid numerical instability. With Simulator B, this value must be increased up to at least 12 for Ts = 1 s, in order to obtain converged results. On the other hand, with a simultaneous simulator, the size of the time step with respect to the integral time is not a significant issue.

3. **Effect of integration method**

If several integration methods are available, such as in Simulator C, it is important to select the right method for a given problem. In general, the Euler method takes shorter time steps and therefore yields smoother results than the Runge-Kutta method, but as this type of simulator treats the time and time step as variables like any other, it may fail to detect an event if this event falls too close to a significant nonlinearity (i.e., a changing variable). To illustrate this, two consecutive disturbances have been performed in the studied process (**Figure A2.1**). First, we let increase the inlet consistency by 2.5% and then a sudden increment of 2% in the white water pressure was simulated. **Figure A2.9** shows a nonconverged time step when using the Euler method. Another drawback of this method is that the size of the time step might be so small for a given accuracy as to render the simulation time impractically long. Moreover, this method might also become numerically unstable for strongly stiff problems. Stiff problems are those in which some dynamic effect with a short characteristic time remains present to a small degree within the process while the dominant dynamic effects have a long characteristic time. For example, a very small tank in one part of the process may have reached an effective steady state, while elsewhere composition changes in a large tank continue to occur.

4. **Recycle systems**

4.1. *The calculation order in sequential simulators*

The calculations in this type of simulator are usually performed in the same order as the material flows through the flowsheet. With a simulator capable of performing local iteration, such as Simulator A, the calculation order is not an important issue, since the selected variables are iterated until convergence before they are passed to the next units. With Simulator B, the user is advised to carefully select the calculation order when dealing with recycle systems. Even a simple process like the one represented in **Figure A2.1** needs some analysis to determine the correct calculation order. Simulator B requires the tank (Tk) outlet flowrate to be specified, and given that the second input to block M2, the dilution point, is calculated by the consistency controller, this unit is completely specified, and its output is used as input to the Splitter unit (S). Since the process outlet flowrate has been fixed, there remains only one output (the recycle stream) for unit S to be calculated. The recycle stream and the inlet flowrate, externally determined by the level controller, are the two inputs that the mixer M1 requires. Therefore, M2 must precede M1 in the calculation order in order to avoid fast and increasing oscillations in the recycle flowrate (**Figure A2.10, I**). This leads to two alternative calculation orders:

Tk → M2 → S → M1 or M2 → S → M1 → Tk

In the first alternative, the recycle stream is initialized with 'zero'. From the previous analysis it is clear that, with Simulator B, the recycle flowrate cannot be kept constant after a disturbance has entered the system (**Figure A2.10, II**).

4.2. *Initial conditions*

Initial conditions are critical to obtain good results and convergence in any simulation, regardless of the type of simulator used. The initial steady-state conditions are those that exist before introducing any perturbation to the system or changes to any controller set point. With Simulators A and C, appropriate initial values can be determined after one run to steady state. With Simulator B, it is more difficult to eliminate the initial steady-state error, and an iterative procedure is required to determine the initial conditions. **Figure A2.10, II** shows that an initial 'jump' still occurs after three passes.

4.3. *"Snowball effect"*

Another important phenomenon related to recycle systems is the so-called "snowball effect", studied extensively by Luyben [6]. Even though this is a steady-state phenomenon, it may cause undesirable results in a dynamic simulation. It is characterized by an unbounded increment in the flowrates of a recycle loop (**Figure**

A2.10, I). In our example, this effect was induced by changing the level controller mode from "on" to "perfect control" in Simulator C. According to Luyben [7], "the fundamental reason for the occurrence of snowballing in recycle systems is the large changes in composition that some control structures produce when disturbances occur". However, our observation is that this phenomenon is rather generated by the one-step delay that appears in the calculation algorithm of sequential simulators, when there is only one pass through the model, i.e., one iteration at each time step. That is why the same phenomenon is not observed with Simulators A (with iteration) and C. Again according to Luyben, a useful heuristic rule to overcome snowballing problems is to control the flow of a stream somewhere in the loop.

4.4. *Dynamic effect of recycle*

Finally, we will briefly discuss the dynamic effect of recycle. The corresponding input-output relationship to the block diagram in **Figure A2.11** is

$$y(s) = \frac{g_F(s)g_1(s)}{1 - g_F(s)g_R(s)} u(s) \tag{A2.7}$$

where the input u and the output y are inlet and outlet consistency, respectively. Assuming that the tank can be represented by a first-order process, the mixing processes M1 and M2 are instantaneous, and neglecting the dynamic effect of the recycle, it can be shown that

$$y(s) = \frac{\left(\dfrac{k_1 k_2}{1 - k_2 k_R}\right)}{\left(\dfrac{\tau}{1 - k_2 k_R}\right)s + 1} u(s) \tag{A2.8}$$

where k_1, k_2 and k_R are the gain constants of the mixing processes M1 and M2, and the recycle process, respectively, and τ is the time constant of the tank. **Figure A2.12** shows how the response becomes highly dependent on the recycle gain as its value approaches k_R=1. Fortunately, most of the recycle loops in pulp and paper making processes have a gain much less than this value, and therefore the recycle process can be completely ignored when tuning the consistency controller [3].

5. Conclusions and recommendations

- Both sequential and simultaneous simulators are capable of yielding good results for dynamic simulation, provided they are set up properly and used to their full capacity.
- For the sequential modular simulators which were examined in this study, properly adjusting the simulation time step (Ts) to a small enough value (Ts $\leq$ 0.5 min in most cases) and using iteration at each time increment for recycle loops are the best measures to avoid convergence problems and to enhance accuracy. The reset time, T_I, should be chosen as a function of Ts, keeping a ratio of $T_I/Ts \geq 2.5$, in order to avoid numerical instability.
- If the sequential simulator cannot perform an iterative solution of recycle loops, the calculation order should be carefully chosen in order to avoid nonconvergence.
- When using a simultaneous simulator, a variable time step is preferable (the simulation time decreases dramatically), and to avoid convergence and stiffness problems, the best available integration method for a particular problem should be used. The Euler method is not recommended for large models.
- In all cases, it is recommended to adjust the simulation time step and controller parameters to the values that best fit the real process data. There is always a tradeoff between simulation accuracy and simulation run time.
- Finally, the importance of good initial values in both types of simulators is critical for convergence.

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Table A2.1: Major characteristics of analyzed simulators

Simulator	Calculation Algorithm	Integration Solver	Iteration	Time Step
A	Sequential	Mass balance approximation, but several methods available in its library	Yes	Fixed
B	Sequential	Euler backward difference	No	Fixed
C	Simultaneous	Adaptive Runge-Kutta Euler Trapezoidal	No	Fixed and variable

Table A2.2: Level controller tuning

λ (min)	Kc (m^3/min/Vol-%)	T_I (min)
20	2	40
10	4	20

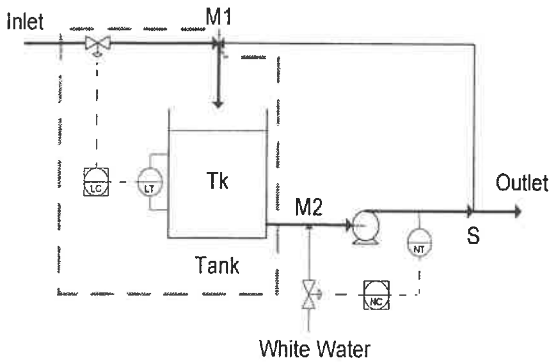

Figure A2.1: Level controlled surge vessel (inside box) and consistency control loop

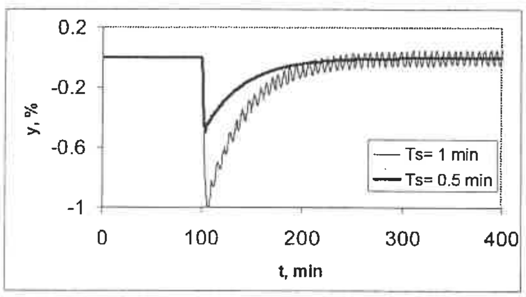

Figure A2.2: Response to 5% step change in the outlet flowrate, as a function of Ts - Simulator A, no iteration

(Ts: Time step; λ = 20 min)

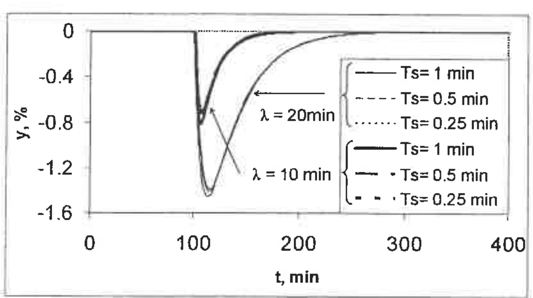

Figure A2.3: Response to 5% step change in the outlet flowrate, as a function of λ and Ts - Simulator A, with iteration

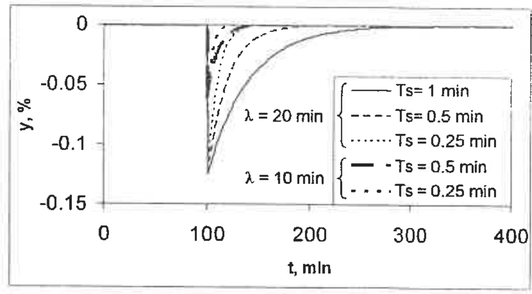

Figure A2.4: Response to 5% step change in the outlet flowrate, as a function of λ and Ts - Simulator B

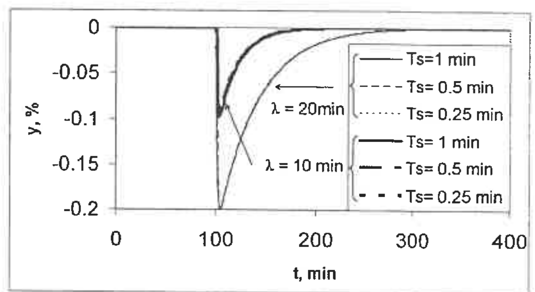

Figure A2.5: Response to 5% step change in the outlet flowrate, as a function of λ and Ts - Simulator C

(Integration method : Euler)

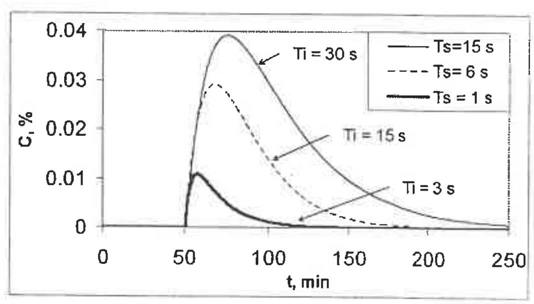

Figure A2.6: Response to 2.5% step change in the inlet consistency, as a function of TI and Ts - Simulator A, with iteration

(T_I: Integral time; λ = 30 s)

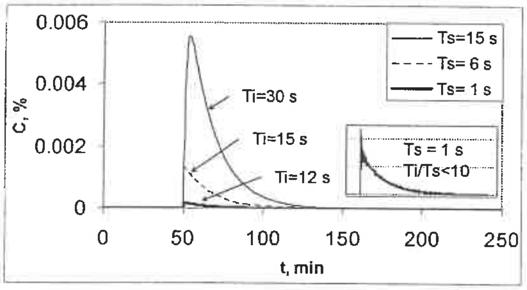

Figure A2.7: Response to 2.5% step change in the inlet consistency, as a function of TI and Ts - Simulator B

(λ = 30 s)

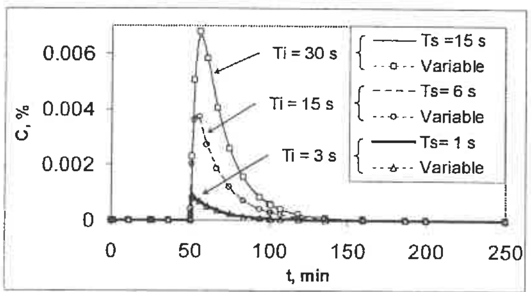

Figure A2.8: Response to 2.5% step change in the inlet consistency, as a function of TI and Ts - Simulator C

(λ = 30 s; Integration method: Runge-Kutta)

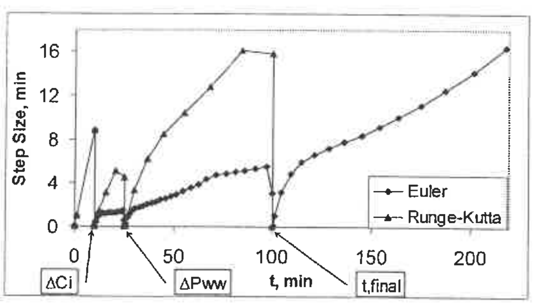

Figure A2.9: Effect of integration method on convergence - Simulator C

(Time step: Variable;
ΔCinlet = 2.5% @ t=10 min;
ΔPwhite water = 2% @ t=25 min)

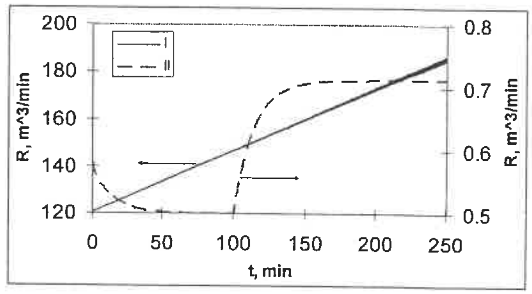

Figure A2.10: Effect of recycle and calculation order (CO) - Simulator B

(I: "Snowball effect" for perfect controlled tank, CO = M1-Tk-M2-S;
II: Recycle flowrate (R) using PI level control, CO = Tk-M2-S-M1)

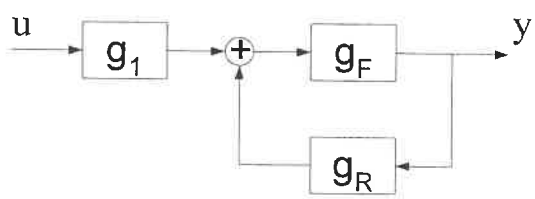

Figure A2.11: Block diagram of analyzed process

(g_1: transfer function of first mixing point;
g_F: forward process (tank + dilution point),
g_R: recycle process)

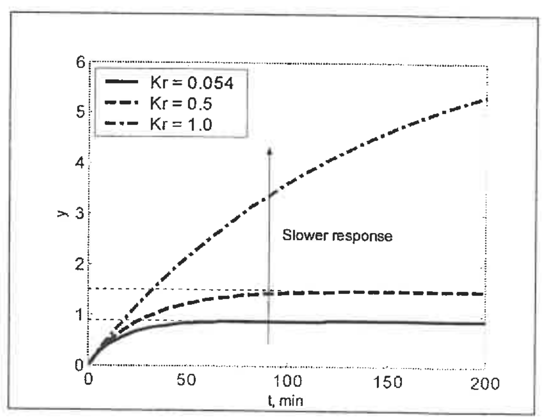

Figure A2.12: Effect of recycle gain on response to a step change in the input variable

APPENDIX A3

SIMULATOR CHARACTERISTICS

A simultaneous modular simulator, MASSBAL 3.8.1 has been used to build both the steady-state (MASSBAL 2) and the dynamic simulation (MASSBAL 3). MASSBAL 2 is a software program used to calculate the steady-state heat and mass balances of industrial processes. MASSBAL 3 is an extension of MASSBAL 2 and is intended to perform simulations that contain some or all of following dynamic features:

- unit operations with holdup,
- process controllers,
- time-dependent specifications on feeds, unit operating parameters, or process conditions.

MASSBAL uses a companion program, MB-Trend, which can be called from within the Graphical Flowsheeting Tool (GFT) to generate graphs of any selected variable in the model as function of time.

A dynamic simulation requires initial conditions, which are in force at the starting point of the simulation. The initial conditions replace the differential equations one-for-one. If algebraic equations are present, a starting solution must be performed to find consistent values that satisfy the algebraic equations as well as the initial conditions. The solution of the starting conditions resembles a steady-state simulation (though the initial conditions do not necessarily imply a steady state).

As the simulation proceeds, a numerical integration technique discretizes the differential equations with respect to time so that they are approximated by algebraic equations for the new values of the variables. This method allows MASSBAL 3 to use the same simultaneous equation-solving techniques as MASSBAL 2.

The default integration method used by MASSBAL 3 to solve the dynamic problem is a strongly A-stable, adaptive Runge-Kutta method. The letter A states for absolutely. Numerical integration methods are named A-Stable if their stability -which describes how the difference between the calculation and the function being approximated changes as the computation proceeds- is not affected by the size of the time step in a dynamic simulation. MASSBAL 3 has the option of using either a fixed time step (specified by the user) or a variable time step. The variable time step is automatically adjusted to maintain an integration accuracy condition that can be specified by the user.

At each time step, two stage solutions are performed at intermediate points across the time step, combining the discretized differential equations with the algebraic equations that describe the process model. Each stage is solved using the Newton-Raphson method in exactly the same way that MASSBAL 2 solves a steady-state problem. Usually, the number of iterations required for each stage is small because extrapolation of variables from the previous two time points gives a good initial guess for the stage calculation. The stage solutions are combined in a weighted average with the previous time point to generate the solution for the full time step.

An approximate solution is also computed which does not require more equation-solving iterations and therefore requires relatively little computational effort. It is compared with the solution generated by the integration method to obtain error estimates for the variables. The largest error is then compared with the accuracy criterion in order to adjust the time step up or down. MASSBAL 3 will declare a step to have failed if the accuracy criterion used for step size adjustment is exceeded by more than a certain margin. This margin essentially defines an accuracy criterion for step size acceptance. In the event of failure, MASSBAL 3 will automatically backtrack to the last successful time point and take a smaller step which is more likely to give acceptable accuracy.

Once a step size for the next time interval has been determined, MASSBAL 3 checks if

(a) any events have been missed in the step just taken, and

(b) if (on the basis of linear extrapolation) any events are likely to be encountered in the next step.

Case (b) can be suppressed by a user option, though this is not normally recommended. If condition (a) or (b) is encountered, then MASSBAL 3 goes into *event-location mode*, which means that the time step specification equation is replaced by the event condition equation. The time step is then treated as an unknown, which is solved for simultaneously with the process variables by the equation-solver at the new time step.

MASSBAL was not designed specifically for the pulp and paper industry and has a number of general modules commonly used in the chemical industry for building an accurate steady-state simulation. The high accuracy and reliability are certainly their main advantages, compared to a sequential simulator. However, this powerful simulator also has some limitations. So, it has a rather small library of pre-coded modules, which does not allow building a quite realistic dynamic model. Among its limitations we can mention the following: MASSBAL 3 is not capable to model transport delay, nor plug flow, and its programming capabilities are not the best. Another drawback of this simulator is that, during a dynamic simulation, it generates a very large file (fairly above 100 MB for a model of several hundreds of units), called DYN file, which can eventually cause problems when transferring data from one computer to another.

Model *robustness* is concerned with the ability to make changes to unit parameters or to the model. The simulation should still give converged results after these changes. Thus, model robustness is closely related to the simulator flexibility, which in turn depends on a high degree on the calculation algorithm used by the simulator. Unfortunately, MASSBAL® has a few limitations to this ability. They include the following:

- Perhaps the most important limitation is related to the ability to control temperatures. Two different stream types (for instance, a pulp and a steam stream) can not be added directly in a MASSBAL model; firstly, one stream has to be converted to the other stream type. In the case of adding steam to a reservoir, in order to compensate for heat losses, the steam stream is first converted to the corresponding stream (pulp or water). This is done by equating the enthalpies of both, steam and pulp/water streams. This works well when the desired temperature is specified with a "set" specification (steady-state), but if we try to control the outlet temperature with a PI controller, the model does not converge and gives wildly changing values of flowrates and temperatures. For this reason, temperature in this simulation is not a controlled, but a specified variable.

Less serious limitations to the robustness are related to numerical instability for certain conditions. Usually, a solution can be found for these problems, which include:

- A few tanks (e.g., the Silo) in a paper mill operate normally by overflowing. When trying to simulate this, the Overflow option for the unit DYNTANK (dynamic Tank) causes numerical problems (numerically singular) when solving the Starting state for cases of two or more tanks in series. This is because the outlets are initially *not* assumed to be overflowing. Since this problem happens at the Starting conditions, the simulation exits with a fail message. To overcome this problem, we have no option, but to make the dynamic tank unit a perfect controlled tank, that is, a steady-state unit.

- Numerical instability also happens when a variable hits a limit, typically a "zero" specification for a unit outlet flowrate or a controller outlet. This is the case when discontinuities, e.g., a paper break, are simulated. The solution to this problem is to chose a small value, but greater than zero (e.g. 10^{-3}) for that variable.

APPENDIX A4

DOCUMENTATION – SIMULATION MASSBAL EN RÉGIME PERMANENT ET DYNAMIQUE

DOMTAR – WINDSOR
MACHINE À PAPIER No 8

Logiciel	:	MASSBAL 3.8
Unités d'ingénierie	:	SI
Temps base de débit	:	min

Table A4.1: Définition de courants

Nom / Type	Composant			Variable			Relations
	Nom	Classe	Unité	Nom	Classe	Unité	
1. MAIN 2. SOFTWOOD 3. BROKE 4. WATER	WATER	Liquid	kg/min	TEMPERATURE		°C	
	LAR	Insoluble	kg/min	VOLUME		L/kg	
	MED	Insoluble	kg/min	H		kJ/kg	
	FIN	Insoluble	kg/min	DUTY		kJ/s	
	ASH	Insoluble	kg/min	VFLOW		L/min	
	DISOL	Soluble	kg/min	TOTALSOLN		kg/min	
PAPER				TOTALINSOLUBLES		kg/min	
				TOTALSOLIDS		kg/min	
				PCSOLIDS		%	
				TONNAGE		o.d. t /d	
				CONSISTENCY		%	
				TOTALSOLUBLES		kg/min	
				FLOW		kg/min	
				TOTFIB	Linear	kg/min	TOTFIB = LAR + MED + FIN + 0.000
				L%	Ratio	%	L% = LAR / TOTFIB * 100
				M%	Ratio	%	M% = MED / TOTFIB * 100
				F%	Ratio	%	F% = FIN / TOTFIB * 100
				DS_PPM	Ratio	ppm	DS_PPM = DISOL/TOTALSOLN * 1.000E+06
				ASH%	Ratio	%	ASH% = ASH / TOTALINSOLUBLES * 100
				HDEBIT	Product	kJ/min	HDEBIT = FLOW * H *1.667E-2

Nom / Type	Composant			Variable			Relations
	Nom	Classe	Unité	Nom	Classe	Unité	
5. CHEMICAL PROCESS	FIN ASH DISOL	Insoluble Insoluble Soluble	kg/min kg/min kg/min	TEMPERATURE VOLUME H VFLOW TOTALSOLN TOTALINSOLUBLES TOTALSOLUBLES FLOW DEBIT_T/D	Product	°C L/kg kJ/kg L/min kg/min kg/min kg/min kg/min t/d	DEBIT_T/D = FLOW * 1.440
6. STEAM FLUID	WATER STEAM	Liquid Vapour	kg/min kg/min	TEMPERATURE PRESSURE VOLUME H S VFLOW TOTALVAP TOTALSOLN QUALITY TS FLOW		°C kPa L/kg kJ/kg kJ/kg.°C kg/min kg/min kg/min % °C kg/min	

Table A4.2: Liste de spécifications, relations et hypothèses

Les variables contrôlés (VC) et manipulées (MV) sont soulignés (*italique*)

Unité	Entrée	Sortie	Spécifications / Consigne	Relations	Hypothèses / Commentaires
812-001 (ADDER) (Pompe)	*IN1 : Eau blanche trouble* (MV) IN2 : Du réservoir de pâte blanche	OUT : Au cuvier de mélange	*OUT CONSISTENCY* (VC) = 5.5	IN1 VFLOW / KIC 2270 OUTPUT = 50	- Contrôleur KIC 2270 : VC = Var. Contrôlée VM = Var. Manipulée
812-045 (ADDER) (Pompe)	IN1 : Eau blanche de la machine (VM) IN2 : Pâte de la colonne de mélange 812-037	OUT : Vers les tamis	*OUT CONSISTENCY* (VC) = 3.9	IN1 VFLOW / KIC 2433 OUTPUT = 50	- Contrôleur KIC 2433 : VC = Var. Contrôlée VM = Var. Manipulée
812-049 (ADDER) (Pompe)	IN1 : De la colonne de mélange 812-038 *IN2 : Eau blanche de la machine* (VM)	OUT: Au silo	*OUT CONSISTENCY* (VC) = 3.5	IN1 VFLOW / KIC 2270 OUTPUT = 50	- Contrôleur KIC 2433: VC = Var. Contrôlée VM = Var. Manipulée

Unité	Entrée	Sortie	Spécifications / Consigne	Relations	Hypothèses / Commentaires
812-113 (ADDER) (Pompe)	IN1 : Du tamis 3e stade IN2 : Eau blanche trouble	OUT : Au ramasse pâte	OUT VFLOW = 15000		
812-142 (ADDER) (Pompe)	*IN1 : Eau blanche trouble* (VM) IN2 : Casses	OUT: Casse diluée vers l'épaississeur	OUT VFLOW = 1000 *OUT CONSISTENCY* (VC) = 2.52	IN1 VFLOW / KIC 2270 OUTPUT = 20	- Contrôleur KIC 2335: VC = Var. Contrôlée VM = Var. Manipulée
812-147 (ADDER) (Pompe)	*IN1: Eau blanche trouble* (VM) IN2 : Casses	OUT: Casse diluée vers l'épaississeur	OUT VFLOW = 1000 *OUT CONSISTENCY* (VC) = 2.52	IN1 VFLOW / KIC 2270 OUTPUT = 20	- Contrôleur KIC 2339 : VC = Var. Contrôlée VM = Var. Manipulée
812-157 (ADDER) (Pompe)	*IN1: Eau blanche trouble* (VM) IN2 : Casses (du cuvier)	OUT : Vers le tamis de casses 1	*OUT CONSISTENCY* (VC) = 4.0	IN1 VFLOW / KIC 2342 OUTPUT = 20	- Contrôleur KIC 2342 : VC = Var. Contrôlée VM = Var. Manipulée
812-162 (ADDER) (Pompe)	*IN1 : Eau blanche trouble* (VM) IN2 : Casses (reserv-eq)	OUT : Vers le cuvier de casses	*OUT CONSISTENCY* (VC) = 5.0	IN1 VFLOW / KIC 2320 OUTPUT = 50	- Contrôleur KIC 2320 : VC = Var. Contrôlée VM = Var. Manipulée
812-215 (ADDER) (Pompe)	*IN 1: Eau blanche trouble* (VM) IN2 : Casses (haute dens)	OUT : Vers le réservoir d'équilibre	*OUT CONSISTENCY* (VC) = 5.5	IN1 VFLOW / KIC 2255 OUTPUT = 40	- Contrôleur KIC 2255 : VC = Var. Contrôlée VM = Var. Manipulée
812-216 (ADDER) (Pompe)	IN 1: Eau blanche trouble IN2 : Casses (haute dens)	OUT : Sink_3	OUT VFLOW = 0.00		
812-221 (DYNTANK) (Cuvier de filtrat de l'épaississeur)	IN1 : Filtrat de l'épaississeur	OUT1: Débordement OUT2 : Au cuvier d'eau blanc trouble	Cross-Sect. Area = 80m² Start. Tot. Vol. = 1472E+03L *Niveau* (VC) = 75%	>> Linear: IN HDEBIT * (-0.01) + DUTY = 0.0 >> DIV7 OUT2 VFLOW / LIC 12259 OUTPUT = 100	- Conditions initiales: régime permanent - Mélange parfait - Perte de chaleur = 1% - Contrôleur LIC 12259 : VM = DIV7 OUT2
821-026 (ADDER) (Pompe)	*IN1: Eau blanche claire* (VM) IN2: Résineux	OUT1: Vers le réservoir de résineux	*OUT1 CONSISTENCY* (VC) = 4.5	IN1 VFLOW / KIC 7401 OUTPUT = 50	- Contrôleur KIC 7401 : VC = Var. Contrôlée VM = Var. Manipulée
ADD10	IN : Du ramasse pâte (OUT1) IN2 : Eau blanche de la machine	OUT : Vers le cuvier de ramasse pâte	OUT CONSISTENCY = 4.65		
ADD11	IN1 : Du cuvier de ramasse pâte *IN2 : Eau blanche de la machine* (VM)	OUT : À la colonne de mélange	*OUT CONSISTENCY* (VC) = 4.5	IN2 VFLOW / KIC 2391 OUTPUT = 50	- Contrôleur KIC 2391 : VC = Var. Contrôlée VM = Var. Manipulée
ADD12	IN1 : Eau blanche riche IN2 : Des épurateurs tertiaires IN3 : Des épurat. prim.	OUT : Vers les épurateurs secondaires	OUT CONSISTENCY = 0.535		

Unité	Entrée	Sortie	Spécifications / Consigne	Relations	Hypothèses / Commentaires
ADD13	IN1 : Eau blanche riche IN2 : Des épurat. quater. IN3 : Des épurat. second.	OUT : Vers les épurateurs tertiaires	OUT CONSISTENCY = 0.326		
ADD14	IN1 : Eau blanche riche IN2 : Des épurat. tertiair. IN3 : Du EPUR IN4 : Du EPUR	OUT : Vers les épurateurs quaternaires	OUT CONSISTENCY = 0.355		
ADD15	IN1: Eau blanche claire IN2: Du EPUR	OUT: Vers les épurateurs quaternaires	IN1 VFLOW = 10		
ADD16	IN1 : Du désaérateur IN2 : Eau blanche filtrée + produits chimiques	OUT : Au tamis prim.			
ADD18	IN1 : Eau blanche filtrée IN2 : Produits chimiques	OUT : Vers le ADD16 (entrée au tamis prim.)			
ADD2	IN1: Casses humides IN2 : Du ADD42	OUT : Vers les réservoirs de casses			- ADD42 = Casses secs
ADD21	IN1 : Du ADD26 IN2 : Du cuvier de la machine	OUT : À la pompe primaire		>>Ratio ADD21 IN2 VFLOW / SILO OUT2 VFLOW = 3.2	- ADD26 = Eau blanche claire
ADD23	IN1 : Eau blanche de la machine IN2 : Vapeur	OUT : Au silo	IN1 VFLOW = 999.871 IN2 VFLOW = 0.0		- IN1 : Vapeur, 150 °C, 550 kPa
ADD28	IN1 : Des pompes à haute pression, 4340 kPa IN2 : Eau tiède, 600 kPa	OUT : Vers le HEADER12	IN1 VFLOW : 154.993 IN2 VFLOW : 120		
ADD29	IN1 : Des pompes à haute pression, 4340 kPa IN2 : Eau tiède, 600 kPa	OUT : Vers le HEADER12	IN1 VFLOW : 143 IN2 VFLOW : 120		
ADD30	IN1 : Des pompes à haute pression, 6700 kPa IN2 : Des pompes à haute pression, 4340 kPa IN3 : Eau tiède, 600 kPa	OUT : Vers le HEADER12	IN1 VFLOW : 35 IN2 VFLOW : 155 IN3 VFLOW : 155		
ADD32	IN1 : De la fosse de coucheur IN2 : De la fosse - presse	OUT : Vers les réservoirs des casses			- Casses humides
ADD36	IN1 : De la fosse de la presse encolleuse IN2 : De la fosse de calandre	OUT : Vers le ADD37			

Unité	Entrée	Sortie	Spécifications / Consigne	Relations	Hypothèses / Commentaires
ADD37	IN1 : Du ADD36 IN2 : De la fosse de enrouleuse	OUT : Vers le ADD39			
ADD39	IN1 : Du ADD37 IN2 : De la fosse de bobineuse	OUT : Vers les réservoirs des casses			- Casses secs
ADD4	IN 1: Eau filtrée de l'épaississeur IN2 : Eau tiède IN 3: Pâte de l'épaississeur	OUT1 : Vers le réservoir de casses à haute densité	IN2 VFLOW = 1.0E-6		
ADD40	IN1: Résineux *IN2: Eau blanche trouble* (VM)	OUT: Vers la caisse de mélange	*OUT CONSISTENCY* (VC) = 4.2	IN1 VFLOW / KIC 2303 OUTPUT = 50	- Contrôleur KIC 2303 : VC = Var. Contrôlée VM = Var. Manipulée
ADD41	IN1: Casses hum (de la machine) IN2: Casses hum (FEED) IN3 : Casses de la machine 7 (FEED)	OUT : Vers les réservoirs de casses	IN2 VFLOW = 0.0 IN3 VFLOW = 0.0		ADD41 OUT = Casses secs totals
ADD42	IN1: Casses secs (de la machine) IN2: Casses secs (FEED)	OUT : Vers les réservoirs de casses	IN2 VFLOW = 0.0		- ADD42 OUT = Casses humides totals
ADD43	IN1 : Du réservoir equil. feuillus *IN2: Eau bl. trouble* (VM	OUT: Vers la caisse de mélange	*OUT CONSISTENCY* (VC) = 4.5	IN2 VFLOW / KIC 2309 OUTPUT = 50	- Contrôleur KIC 2309 : VC = Var. Contrôlée VM = Var. Manipulée
ADD6	IN1 : Eau tiède IN2 : Eau d'usine	OUT1 : Au réservoir d'eau filtrée	IN1 TEMP. = 35 IN1 VFLOW = 100 IN2 VFLOW = 100		
ADD7	IN 1 : Du cuvier de mélange IN2 : Eau filtré + Eau blanche de la machine	OUT : Vers le ramasse pâte		ADD7 IN1 VFLOW = ADD8 IN1 VFLOW * 0.05 + ADD8 IN2 VFLOW * 0.05	
AIDE_RET (Source)		OUT (FEED) : A la sortie du tamis prim.	FIN = 100 mass-% DISOL = 0 mass-% TEMPERATURE = 20	FEED FIN= PATE * 1.25E-03	
ALIM_RAM_PATE	IN1 : Du cuvier d'eau blanche de la machine IN2 : Du HEADER4 IN3 : Du réservoir d'eau des presses	OUT1 : Débordement OUT2 : Au ramasse pâte	Cross-Sect. Area = 20m^2 Start. Level = 10m OUT1 VFLOW = 0 *Niveau* (VC) = 60%	>> IN1 HDEBIT * (-5E-03) + IN2 HDEBIT * (-5E-03) + IN3 HDEBIT * (-5E-03) + IN4 HDEBIT * (-5E-03) + DUTY = 0.0	- Conditions initiales: régime permanent - Mélange parfait - Perte de chaleur = 0.5% - Contrôleur LIC8885 :

Unité	Entrée	Sortie	Spécifications / Consigne	Relations	Hypothèses / Commentaires
	IN4 : De la fosse du coucheur			>>DIV23 OUT2 VFLOW / LIC8885 OUTPUT = 300	VC = Var. Contrôlée VM = Var. Manipulée (DIV23 OUT2)
AMIDON (Source)		OUT (FEED) : Vers le DIV27	FIN = 100 mass-% DISOL = 0 mass-% TEMPERATURE = 20		- Amidon cationique
BENTONITE (Source)		OUT (FEED) : Bentonite	ASH = 100 mass-% DISOL = 0 mass-% TEMPERATURE = 20	FEED ASH = PATE*9.86E-4	
CAISSE_ARRIVÉE	IN1 : Du tamis prim.	OUT1 : À la machine OUT2 : Recirculation (vers le désaérateur)		>>Ratio COMPOSANT OUT2 / COMPOSANT IN1: VFLOW = 0.05 LAR = 0.05 MED = 0.05 FIN = 0.05 ASH = 0.05 DS_PPM = 1 TEMPERATURE = 1	-Pas des pertes de chaleur
CAISSE_MELANGE	IN1 : Casses IN2 : Résineux IN3 : Feuillus	OUT 1 : Vers le cuvier de mélange			-Perte de chaleur = 0 %
CASSES_HUM (Source)		OUT (FEED): Casses humides	TEMPERATURE = 47 CONSISTENCY= 4.5 L% = 13.00 M% = 73.00 DS_PPM = 340 ASH% = 15 TONNAGE = 0.00		F% est calculé
CASSES_MP7 (Source)		OUT (FEED): Casses de la machine 7	TONNAGE = 0.00		Pas de casses de la machine # 7
CASSES_SEC (Source)		OUT (FEED): Casses secs	TEMPERATURE = 49 CONSISTENCY= 4.5 L% = 11.00 M% = 80.00 DS_PPM = 450 ASH% = 15		F% est calculé
CHEST	IN1 : Du désaérateur	OUT1 : Débordement *OUT2 : Vers la pompe primaire* (VM)	Cross-Sect. Area = 2m^2 Start. Level = 1.5m *Niveau* (VC) = 70%	>> OUT2 VFLOW / LIC2466 OUTPUT = 400	-Pas des pertes de chaleur - Contrôleur LIC2466 : VC = Var. Contrôlée VM = Var. Manipulée

Unité	Entrée	Sortie	Spécifications / Consigne	Relations	Hypothèses / Commentaires
COL_MEL 812-037	IN1 : Du tamis de fente 2e stade IN2 : Du ramasse pâte IN3 : Du cuvier de mélange	OUT1 : Vers les tamis			- Perte de chaleur = 0%
COL_MEL 812-037	IN1 : Du cuvier de la machine	OUT1 : Au silo			- Perte de chaleur = 0%
CT	IN1 : Des SECHEURS45	OUT1 : Vers la presse encolleuse	DUTY = 1.273E03		- Correction de température
CUV_EAU_BL_ RICHE	IN1 : Débordement du silo IN2 : Du DIV28 IN3 : Du DIV28	OUT1 : Au cuvier d'eau blanche de la machine OUT2 : Vers les épurat. quaternaires + réservoir des rejets du tamis prim OUT3 : Vers les épurateurs secondaires OUT4 : Vers les épurateurs tertiaires	Cross-Sect. Area = 20m^2 Start. Level = 10m	>> Linear: IN1 HDEBIT * (-5E-03) + IN2 HDEBIT * (-5E-03) + IN3 HDEBIT * (-5E-03) + DUTY = 0.0	- Régime permanent - Mélange parfait - Perte de chaleur = 0.5%
CUV_EAU_BL_ MACH	IN1 : Du cuvier d'eau blanche riche IN2 : Du HEADER9 IN3 : Du HEADER10	OUT1 : Au cuvier d'alimentation au ramasse pâte OUT2 : Vers le DIV29	Cross-Sect. Area = 20m^2 Start. Level = 10m	>> Linear: IN1 HDEBIT * (-5E-03) + IN2 HDEBIT * (-5E-03) + IN3 HDEBIT * (-5E-03) + DUTY = 0.0	- Régime permanent - Mélange parfait - Perte de chaleur = 0.5%
CUVIER_CASSES	IN1 : Du tamis de casses 2 *IN2 : Pâte du réservoir d'équilibre* (VM)	OUT1 : Débordement OUT2 : Vers le tamis de casses 1	Cross-Sect. Area = 20m^2 Start. Tot. Vol. = 100E+03L *Niveau* (VC) = 75%	>> Linear: IN1 HDEBIT * (-0.01) + IN2 HDEBIT * (-0.01) + DUTY = 0.0 >> IN2 VFLOW / LIC2341 OUTPUT = 50	-Conditions initiales: régime permanent -Mélange parfait -Perte de chaleur = 1% - Contrôleur LIC2341 : VC = Var. Contrôlée VM = Var. Manipulée
CUVIER_EAU_ BL_CL	IN 1 : Du réservoir d'eau blanche claire IN2 : De la Fosse 1	OUT1 : Au cuvier d'eau blanche trouble *OUT2 : Au réservoir d'eau bl. claire* (VM) OUT3 : Au filtre d'eau blanche claire OUT4: Débordement	Cross-Sect. Area = 8m^2 Start. Tot. Vol. = 32E+03L IN1 VFLOW = 0 *Niveau* (VC) = 75%	>> Linear: IN2 HDEBIT * (-0.01) + DUTY = 0.0 >> OUT1 VFLOW / LIC2353 OUTPUT = 250	-Conditions initiales: régime permanent -Mélange parfait -Perte de chaleur = 1% - Contrôleur LIC2353 : VC = Var. Contrôlée VM = Var. Manipulée
CUVIER_EAU_ BL_TR	IN1 : Eau filtrée de l'épaississeur *IN2 : Du cuvier d'eau*	OUT1: Débordement OUT2 : Dilution dans plusieurs endroits	Cross-Sect. Area = 8m^2 Start. Tot. Vol. = 32E+03L	>> Linear: IN1 HDEBIT * (-0.01) + IN2 HDEBIT * (-0.01) +	- Conditions initiales: régime permanent - Mélange parfait

Unité	Entrée	Sortie	Spécifications / Consigne	Relations	Hypothèses / Commentaires
	blanche claire (VM) IN3 : Du réservoir d'eau blanche claire IN4 : Du filtre d'eau blanche claire IN5 : De la Fosse 2	OUT3 : Dilution de la pâte du tamis fente 3e stade	IN3 VFLOW = 0 *Niveau* (VC) = 65%	IN4 HDEBIT * (-0.01) + IN5 HDEBIT * (-0.01) + DUTY = 0.0 >> IN2 VFLOW / LIC2356 OUTPUT = 130	- Perte de chaleur = 1% - Contrôleur LIC2356 : VC = Var. Contrôlée VM = Var. Manipulée
CUVIER_MACHINE	IN1 : Amidon cationique *IN2 : Acceptés des tamis 1e et 2e stade* (VM)	OUT1: Débordement OUT2 : Vers la colonne de mélange 812-038	Cross-Sect. Area = 25m^2 Start. Tot. Vol. = 124E+03L *Niveau* (VC) = 70%	>> Linear: IN1 HDEBIT * (-0.01) + IN2 HDEBIT * (-0.01) + DUTY = 0.0 >> IN2 VFLOW / LIC2438A OUTPUT = 225	- Conditions initiales: régime permanent - Mélange parfait - Perte de chaleur = 1% - Contrôleur LIC2438A : VC = Var. Contrôlée VM = Var. Manipulée
CUVIER_MELANGE	IN1 : De la caisse de mélange	OUT1: Débordement OUT2 : Vers le DIV15	Cross-Sect. Area = 49m^2 Start. Tot. Vol. = 232E+03L *Niveau* (VC) = 70%	>> Linear : IN1 HDEBIT * (-0.01) + DUTY = 0.0 >> FURNISH U3 / LIC2431 OUTPUT = 10	- Conditions initiales: régime permanent - Mélange parfait - Perte de chaleur = 1 % - Contrôleur LIC2431 : VC = Var. Contrôlée VM = FURNISH U3
CUVIER_RAMASSE_ PATE	IN1 : Du ADD10 (pâte diluée du ramasse pâte)	OUT1: Débordement OUT2 : Vers la colonne de mélange (après dilution avec d'eau blanche de la machine)	Cross-Sect. Area = 12.584m^2 Start. Tot. Vol. = 60E+03L IN1 CONSIST (VC) = 4.65 *Niveau* (VC) = 70%	>> Linear: IN1 HDEBIT * (-0.01) + DUTY = 0.0 >> IN2 VFLOW / LIC2390 OUTPUT = 150	-Conditions initiales: régime permanent -Mélange parfait -Perte de chaleur = 1 % - Contrôleur LIC2390 : VC = Var. Contrôlée VM = ADD11 OUT
DEBIT_ PATE_SECHE				PATE = 812-049 OUT (pâte au silo) TONNAGE * 1	- Block workspace
DESAERATEUR	IN1: Du tamis second. IN2: De la caisse d'arrivée IN3: Des épurateurs primaires	OUT1: Débordement (CHEST) OUT2: Au tamis prim.	Cross-Sect. Area = 10m^2 Start. Tot. Vol. = 24E+03L	>> Linear: IN1 HDEBIT * (-5E-03) + IN2 HDEBIT * (-5E-03) + IN3 HDEBIT * (-5E-03) + IN4 HDEBIT * (-5E-03) + DUTY = 0.0	-Conditions initiales: régime permanent -Mélange parfait -Perte de chaleur = 0.5%
DIV11	IN : Pâte de la colonne de mélange 812-037	OUT1 : Vers le tamis 2e stade OUT2 : Vers le tamis 1e stade		>> Ratio OUT1 FLOW / IN FLOW = 50%	

Unité	Entrée	Sortie	Spécifications / Consigne	Relations	Hypothèses / Commentaires
DIV15	IN : Du cuvier de mélange	OUT1 : Au ramasse pâte OUT2 : Vers la colonne de mélange 812-037		DIV15 OUT1 VFLOW = ADD8 IN1 VFLOW * 0.05 + ADD8 IN2 VFLOW * 0.05	
DIV19	IN1 : Eau blanche filtrée	OUT1: À la machine OUT2: À la machine OUT3: dilution de produits chimiques	OUT1 VFLOW = 0 OUT2 VFLOW = 2770		
DIV2	IN: Du ADD2	OUT 1 : Vers le réservoir de cases colorées OUT2 : Vers le réservoir de cases propres	OUT1 = 45%		
DIV23	IN: Du cuvier eau bl. mach.	OUT1: Au cuvier ramasse pâte OUT2: Au ramasse pâte		OUT2 VFLOW / LIC8885 OUTPUT =300	
DIV27	IN : Amidon cationique	OUT1 : Au cuvier mach. OUT2 : Au tamis prim. OUT3 : Au presse encolleuse		OUT1 FIN = PATE * 2.78E-3 OUT2 FIN = PATE * 1.25E-3 OUT3 FIN = PATE * 1.0E-3	
DIV28	IN: Du PM2	OUT1: Vers le cuvier d'eau blanche riche OUT2: Vers le cuvier d'eau blanche riche		>>Ratio OUT1 VFLOW / IN VFLOW = 0.5	
DIV29	IN: Du cuvier d'eau blanche de la machine	OUT1 : À la dilution de la pâte OUT2 : Au silo	OUT2 VFLOW = 999.871		
DIV31	IN : Du PM2	OUT1 : Vers les presses OUT2 : À la fosse du coucheur	IN ASH% = 15	>>Ratio OUT2 VFLOW / IN VFLOW = 0.04	- Contenu de cendres dans la section de presses = 15% - Rognures = 4%
DIV32	IN : Du DIV31	OUT1 : Vers les presses OUT2 : À la fosse du coucheur	OUT2 VFLOW = 1.0E-6		- Pendant une casse : OUT1 VFLOW = 1.0E-6
DIV34	IN : Des presses	OUT1 : Vers les sécheurs45 OUT2 : À la fosse de presse		>>Ratio OUT2 TONNAGE / IN1 TONNAGE = 1.0E-6	- Pas de casses dans la section de presses
DIV41	IN1 : De la presse encolleuse	OUT1 : Vers les sécheurs67 OUT2 : À la fosse de la presse encolleuse		>>Ratio OUT2 TONNAGE / IN1 TONNAGE = 1.0E-6	- Pas de casses dans la presse encolleuse

Unité	Entrée	Sortie	Spécifications / Consigne	Relations	Hypothèses / Commentaires
DIV42	IN1 : Des SECHEURS67	OUT1 : Vers le DIV43 OUT2 : À la fosse de calandre	OUT1 TONNAGE = 870	>>Ratio OUT2 TONNAGE / IN TONNAGE = 1.0E-6	- Pas de casses dans la calandre
DIV43 (Refendeuse)	IN1 : Du DIV42	OUT1 : Vers le DIV44 OUT2 : À la fosse de enrouleuse		>>Ratio OUT2 TONNAGE / IN TONNAGE = 1.0E-6	-Pas de casses dans la enrouleuse
DIV44	IN1 : Du DIV43	OUT1 : Produit OUT2 : À la fosse de bobineuse		>>Ratio OUT2 TONNAGE / IN TONNAGE = 1.0E-6	-Pas de casses dans la bobineuse
DIV7	IN : Du cuvier de filtrat de l'épaississeur	OUT1 : Vers la dilution de la pâte concentrée de l'épaississeur OUT2 : Vers le cuvier d'eau blanche trouble	OUT1 VFLOW = 0.00		
DIV8	IN : Du réservoir de casses à haute densité	OUT1 : Vers la pompe 812-215 OUT 2 : Vers 812-216		DIV8 OUT2 = 812-216 OUT VFLOW / DIV8 IN CONSISTENCY * 0.0059	
EAU_BL_FIL	IN1: Eau d'usine + eau tiède IN2 : Du filtre d'eau blanche claire	OUT1: Débordement OUT2: Vers le DIV19 (À la machine et dilution de produits chimiques) OUT3: Au ramasse pâte et à la machine	Cross-Sect. Area = $10m^2$ Start. Tot. Vol. = 48E+03L OUT1 VFLOW = 0.0 *Niveau* (VC) = 60%	>>Linear: IN1 HDEBIT * (-5E-03) + IN2 HDEBIT * (-5E-03) + DUTY = 0.0 >> FILTRE_EAU_BL_CL IN1 VFLOW / LIC2 OUTPUT = 130	-Conditions initiales: régime permanent -Mélange parfait -Perte de chaleur = 0.5% - Contrôleur LIC2 : VC = Var. Contrôlée VM = Filtre eau Bl. claire IN1 VFLOW
EAU_CHAUDE (Source)		OUT (FEED) : Vers les sections de formation et pressage	TEMPERATURE = 80 DS_PPM = 100		-Eau chaude 300 kPa
EAU_TIÈDE (Source)		OUT (FEED) : Vers le DIV16	TEMPERATURE = 65 CONSISTENCY= 0 L% = 0 M% = 0 DS_PPM = 100 ASH% = 0		F% est calculé
EAU_TIEDE600 (Source)		OUT (FEED) : Vers la section de pressage	TEMPERATURE = 60 DS_PPM = 100		-Eau tiède, 600 kPa
EAU_USINE (Source)		OUT (FEED) : Vers le DIV21	TEMPERATURE = 15 CONSISTENCY= 0 L% = 0 M% = 0		F% est calculé

Unité	Entrée	Sortie	Spécifications / Consigne	Relations	Hypothèses / Commentaires
			DS_PPM = 100 ASH% = 0		
EPAISSISSEUR	IN 1: Pâte diluée IN2 : Eau tiède	OUT1 : Pâte concentrée OUT2 : Filtrat au Cuvier de filtrat du épaississeur		>> EPAISSEISSEUR IN1 = 812-142 OUT + 812-147 OUT >>Ratio COMPOSANT OUT1/ COMPOSANT IN1: WATER = 0.23021 LAR = 0.99883 MED = 0.99784 FIN = 0.99308 ASH = 0.99102 DISOL = 0.34028 TEMPERATURE = 0.95 >> Linear: IN1 HDEBIT * (-0.03) + IN2 HDEBIT * (-0.03) + DUTY = 0.0	-Perte de chaleur = 3%
EPUR	IN1 : Du réservoir de rejets des épurateurs quaternaires	OUT1 : Vers les épurateurs quaternaires OUT2 : Vers les épurateurs quaternaires	IN1 VFLOW = 200	>>Ratio COMPOSANT OUT1/ COMPOSANT IN1: WATER = 0.9 LAR = 0.85 MED = 0.85 FIN = 0.85 ASH = 0.85 DS_PPM = 1 TEMPERATURE = 1	-Pas des pertes de chaleur
EPUR_PRIM	IN1 : De la pompe primaire	OUT1 : Vers le désaérateur OUT2 : Vers les épurateurs secondaires		>>Ratio COMPOSANT OUT1/ COMPOSANT IN1: WATER = 0.91 LAR = 0.87 MED = 0.88 FIN = 0.94 ASH = 0.91 DS_PPM = 1 TEMPERATURE = 1	-Pas des pertes de chaleur
EPUR_QUAT	IN1 : Des épurateurs tertiaires	OUT1 : Vers les épurateurs tertiaires	IN1 CONSISTENCY = 0.355	>>Ratio COMPOSANT OUT1/	-Pas des pertes de chaleur

Unité	Entrée	Sortie	Spécifications / Consigne	Relations	Hypothèses / Commentaires
		OUT2 : Vers le réservoir de rejets des épurateurs quaternaires		COMPOSANT IN1: WATER = 0.9 LAR = 0.88 MED = 0.88 FIN = 0.86 ASH = 0.89 DS_PPM = 1 TEMPERATURE = 1	
EPUR_SEC	IN1: Des épurateurs primaires	OUT1: Vers la pompe primaire OUT2: Vers les épurateurs tertiaires	IN1 CONSISTENCY = 0.535	>>Ratio COMPOSANT OUT1/ COMPOSANT IN1: WATER = 0.9 LAR = 0.88 MED = 0.88 FIN = 0.86 ASH = 0.9 DS_PPM = 1 TEMPERATURE = 1	-Pas des pertes de chaleur
EPUR_TER	IN1 : Des épurateurs secondaires	OUT1 : Vers les épurateurs secondaires OUT2 : Vers les épurateurs quaternaires	IN1 CONSISTENCY = 0.326	>>Ratio COMPOSANT OUT1/ COMPOSANT IN1: WATER = 0.9 LAR = 0.87 MED = 0.89 FIN = 0.8 ASH = 0.84 DS_PPM = 1 TEMPERATURE = 1	-Pas des pertes de chaleur
FILTRE_EAU_BL_CL	IN2 : Du cuvier d'eau blanche claire	OUT1 : Au cuvier d'eau blanche trouble OUT2 : Au réservoir d'eau filtrée		>>Ratio COMPOSANT OUT2/ COMPOSANT IN1: WATER = 0.95007 LAR = 0.05521 MED = 0.33091 FIN = 0.83464 ASH = 0.67775 DISOL = 0.95007 TEMPERATURE = 1	-Pas des pertes de chaleur
FOSSE_ENROULOSE	IN1 : Casses de la refendeuse IN2 : Eau blanche claire	OUT1 : Vers le ADD37 + recirculation OUT2 : Débordement	Cross-Sect. Area = 20m^2 Start. Level = 10m	>>Ratio IN2 FLOW / IN1 FLOW = 30.352	-Régime permanent -Mélange parfait -Pas des pertes de chaleur

Unité	Entrée	Sortie	Spécifications / Consigne	Relations	Hypothèses / Commentaires
	IN3: Pâte recirculée		IN3 VFLOW = 999.762		-Pas de dilution de la pâte recirculée
FOSSE_BOBINEUSE	IN1 : Eau blanche claire IN2 : Casses de la bobineuse IN3: Pâte recirculée	OUT1 : Vers le ADD39 + recirculation OUT2 : Débordement	Cross-Sect. Area = 20m^2 Start. Level = 10m IN3 VFLOW = 999.797	>>Ratio IN2 FLOW / IN1 FLOW = 30.352	-Régime permanent -Mélange parfait -Pas des pertes de chaleur -Pas de dilution de la pâte recirculée
FOSSE_CALANDRE	IN1 : Casses dans la calandre IN2 : Eau blanche claire IN3: Pâte recirculée	OUT1 : Vers le ADD36 + recirculation OUT2 : Débordement	Cross-Sect. Area = 20m^2 Start. Level = 10m IN3 VFLOW = 999.801	>>Ratio IN2 FLOW / IN1 FLOW = 30.352	-Régime permanent -Mélange parfait -Pas des pertes de chaleur -Pas de dilution de la pâte recirculée
FOSSE_COUCHEUR	IN1 : Du HEADER11 IN2 : Du DIV31 (Rognures) IN3 : Du DIV32 (Casses) IN4 : Pâte recirculée IN5 : Eau blanche claire IN6: De la fosse de presse	OUT1 : Vers le ADD32 + recirculation OUT2 : Vers le cuvier d'alimentation au ramasse pâte (MV) OUT3 : Débordement	Cross-Sect. Area = 20m^2 Start. Level = 10m IN3 VFLOW = 1.0E-6 IN4 VFLOW = 500 IN6 VFLOW = 1.0E-6 Niveau (VC) = 30%	>>Linear IN1 HDEBIT * (-0.02) + IN2 HDEBIT * (-0.02) + IN4 HDEBIT * (-0.02) + IN5 HDEBIT * (-0.02) + DUTY = 0 >>Ratio IN5 FLOW / IN3 FLOW = 5.22	-Conditions initiales: régime permanent -Mélange parfait -Perte de chaleur = 2% -Pas de dilution de la pâte recirculée -LIC8800 : VC = Var. Contrôlée VM = Var. Manipulée
FOSSE_PRESSE	IN1: Casses des presses IN2: Eau blanche claire IN3: Pâte recirculée	OUT1: Vers la fosse de coucheur + ADD32 + recirculation OUT2 : Débordement	Cross-Sect. Area = 20m^2 Start. Level = 10m IN3 VFLOW = 500	>>Ratio IN2 FLOW / IN1 FLOW = 13.065	-Régime permanent -Mélange parfait -Pas des pertes de chaleur -Pas de dilution de la pâte recirculée
FOSSE_PRESSE_ ENCOLLEUSE	IN1 : Casses de la presse encolleuse IN2 : Eau blanche claire IN3: Pâte recirculée	OUT1 : Vers le ADD36 + recirculation OUT2 : Débordement	Cross-Sect. Area = 20m^2 Start. Level = 10m IN3 VFLOW = 999.827	>>Ratio IN2 FLOW / IN1 FLOW = 25.796	-Régime permanent -Mélange parfait -Pas des pertes de chaleur -Pas de dilution de la pâte recirculée
FOSSE1	IN : Du ramasse pâte (OUT3)	OUT1 : Vers le cuvier d'eau blanche claire			
FOSSE2	IN : Du ramasse pâte (OUT2)	OUT1 : Vers le cuvier d'eau blanche trouble			
FURNISH (BLOCK WORKSPACE)			CASSES = 20 HWRATIO = 85	>> FM = CAISSE_MELANGE OUT1 TONNAGE F1 = FM*CASSES F3 = U3 / IN3 VOLUME*1.44	-Feuillus = 85% de la fibre vierge -Casses = variable (par ex., 20% du total)

Unité	Entrée	Sortie	Spécifications / Consigne	Relations	Hypothèses / Commentaires
				FIB_VIERGE = F3 / HWRATIO * 100 F2 = FIB_VIERGE - F3 FEUILLUS = F3 / FM * 100 RESINEUX = F2 / FM * 100 CAISSE_MELANGE IN3 TONNAGE = F3	
HAUTE_PRESSION (Source)		OUT (FEED) : Vers les sections de formation et pressage	TEMPERATURE = 60 DS_PPM = 100		-Pompes à haute pression, 6700 kPa
HEADER10	IN1 : Eau blanche filtrée, 600 kPa IN2 : Eau chaude, 300 kPa IN3 : Des pompes à haute press., 6700 kPa	OUT1 : Au cuvier d'eau blanche de la machine	IN1 VFLOW : 100 IN2 VFLOW : 83.995 IN3 VFLOW : 50		-Nettoyage de la toile
HEADER11	IN1 : Eau blanche filtrée, 600 kPa IN2 : Eau blanche filtrée, 1800 kPa IN3 : Des pompes à haute press., 4340 kPa	OUT1 : À la fosse du coucheur	IN1 VFLOW : 50 IN2 VFLOW : 2470 IN3 VFLOW : 342		-Nettoyage de la toile
HEADER12	IN1 : Du ADD28 IN2 : Du ADD29 IN3 : Du ADD30 IN4 : Eau chaude, 300 kPa IN5 : Des presses	OUT1 : Au réservoir d'eau des presses	IN4 VFLOW : 100		-Nettoyage du feutre + filtrat
HEADER4	IN1, IN2, IN3 : Eau blanche filtrée, 600 kPa IN4: Eau blanche filtrée, 1800 kPa IN5 : Eau chaude, 300 kPa IN6 : Des pompes à haute press., 4340 kPa	OUT1 : Au cuvier d'alimentation au ramasse pâte	IN1 VFLOW : 100 IN2 VFLOW : 99.984 IN3 VFLOW : 100 IN4 VFLOW : 300.001 IN5 VFLOW : 150 IN6 VFLOW : 342		-Nettoyage de la toile
HEADER9	IN1 : Eau blanche filtrée, 600 kPa IN2 : Eau chaude, 300 kPa	OUT1 : Au cuvier d'eau blanche de la machine	IN1 VFLOW : 100 IN2 VFLOW : 165.99 IN3 VFLOW : 50		-Nettoyage de la toile

Unité	Entrée	Sortie	Spécifications / Consigne	Relations	Hypothèses / Commentaires
	IN3 : Des pompes à haute press., 6700 kPa				
HIGH_DENS (+MIXER#3)	IN 1 : Pâte de l'épaississeur IN2 : Eau blanche trouble	OUT1 : Débordement OUT2 : Vers le DIV8	Cross-Sect. Area = 110m^2 Start. Tot. Vol. = 3760E+03L	>> IN1 HDEBIT * (-0.02) + DUTY = 0.0 >> Eau bl_tr vers MIXER#3 VFLOW = 812-215 OUT VFLOW * 0.3 + 812-216 OUT VFLOW * 0.3	- Réservoir de casses à haute densité - Conditions initiales: régime permanent - Mélange parfait - Perte de chaleur = 2% - Control de niveau : manuel / automatique
INT69	IN1: Résineux	OUT1: Au Triturateur		>> OUT1 LAR = IN1 LAR * 0.5 >> OUT1 MED = IN1 MED * 1 + IN1 LAR * 0.45 >> OUT1 FIN = IN1 FIN * 1 + IN1 LAR * 0.05	50% de la fibre LAR est transformé en MED (45%) et FIN (5%) pendant la trituration
MIXER#1 (Dilution)	IN1: Pâte blanche IN2: Eau tiède IN3: Eau blanche trouble	OUT: MIXER#1 OUT	IN2 VFLOW = 100 OUT CONSISTENCY = 5.0		
PÂTE_BL (Source)		OUT (FEED): Pâte blanche	TEMPERATURE = 63 CONSISTENCY= 9.65 L% = 5.00 F% = 8.00 DS_PPM = 615 ASH% = 0.24		M% est calculé
PCC (Source)		OUT (FEED): PCC	ASH = 100 mass-% DISOL = 0 mass-% TEMPERATURE = 20		- Contenu de cendres de avant la section de presses = 15%
PECOL (Source)		OUT (FEED): Pecol	ASH = 0 mass-% DISOL = 1000 mass-% TEMPERATURE = 20	FEED DISOL= PATE * 1.25E-04	
PM1	IN1 : De la caisse d'arrivée	OUT1 : Canal d'amenée MK1 (Vers le Silo) OUT2 : Vers le PM2 OUT3 : Canal d'amenée MK2 (Vers le cuvier d'eau blanche riche)		>>Ratio COMPOSANT OUT1 (OUT3) / COMPOSANT IN1: WATER = 0.34219 (0.34213) LAR = 0 (6.5E-04) MED = 0.01222 (5.08E-03) FIN = 0.12211 (0.17504)	-Unité de drainage -Pas des pertes de chaleur

Unité	Entrée	Sortie	Spécifications / Consigne	Relations	Hypothèses / Commentaires
				ASH = 0.12099 (0.15169) DISOL = 0.33534 (0.33528) TEMPERAT. = 1 (1)	
PM2	IN1 : Du PM1	OUT1 : Vers la presse OUT2 : Vers le DIV28		>>Ratio COMPOSANT OUT2 / COMPOSANT IN1: WATER = 0.29043 LAR = 0 MED = 0.00786 FIN = 0.10191 ASH = 0.13092 DISOL = 0.2909 TEMPERATURE = 1	
POMPE_PRIM (ADDER)	IN1 : Du ADD21 IN2 : Du silo	OUT : Vers les épurateurs primaires			
PRESSE	IN1 : Du DIV32	OUT1 : Vers le DIV34 OUT2 : Eau filtrée vers le réservoir d'eau de presses	OUT1 CONSISTENCY = 42.0002	>>Ratio COMPOSANT OUT1 / COMPOSANT IN1: LAR = 1 MED = 1 FIN = 1 ASH = 1 TEMPERATURE = 1 >>Ratio OUT2 DS_PPM / IN1 DS_PPM =0.9	-Pas des pertes de chaleur
PRESSE ENCOLLEUSE	IN1 : De l'unité CT IN2 : Amidon cationique	OUT : Vers le DIV41			
RAMASSE_PATE	IN1 : Pâte IN2 : Eau blanche filtrée IN3 : Eau blanche trouble	OUT1 : Vers le cuvier de ramasse pâte après dilution avec d'eau blanche de la machine OUT2 : Vers la fosse 2 OUT 3 : Vers la fosse 1	IN2 VFLOW = 1000 IN3 VFLOW = 1000	>>Ratio COMPOSANT OUT1 (OUT2) / COMPOSANT IN1: WATER = 0.05133 (0.35165) LAR = 0.98097 (4.16E-03) MED = 0.9749 (8.49E-03) FIN = 0.96247 (1.74E-02) ASH = 0.91189 (4.767E-02) DISOL = 0.07348 (0.34285) TEMP. = 0.90854 (0.97) >> Linear : IN1 HDEBIT * (-0.03) +	-Régime permanent -Mélange parfait -Perte de chaleur = 3%

Unité	Entrée	Sortie	Spécifications / Consigne	Relations	Hypothèses / Commentaires
				IN2 HDEBIT * (-0.03) + IN3 HDEBIT * (-0.03) + DUTY = 0.0	
RESERV_CASS_ PROP	IN 1: Casses mélanges	OUT1 : Débordement OUT2: Vers la pompe 812-142	Cross-Sect. Area = 70m^2 Start. Tot. Vol. = 1472E+03L	>> IN1 HDEBIT * (-0.01) + DUTY = 0.0	-Conditions initiales: régime permanent -Mélange parfait -Perte de chaleur = 1%
RESERV_CASS_COL	IN 1: Casses mélanges	OUT1 : Débordement OUT2 : Vers la pompe 812-147	Cross-Sect. Area = 70m^2 Start. Tot. Vol. = 1472E+03L	>> IN1 HDEBIT * (-0.01) + DUTY = 0.0	-Conditions initiales: régime permanent -Mélange parfait -Perte de chaleur = 1%
RESERV_EAU_ BL_CL	*IN1 : Eau tiède + Eau d'usine* (VM) IN2: Vapeur IN3 : Du cuvier d'eau blanche claire	OUT1 : Vers les cuviers d'eau blanche claire et d'eau blanche trouble OUT2 : Débordement OUT3 : Excès OUT4 : Dilution dans plusieurs endroits	IN1 VFLOW = 100 IN2 TEMP. = 150 IN2 PRESSION = 550 OUT1 VFLOW = 0 OUT2 VFLOW = 0 OUT4 TEMP. = 48.5 Cross-Sect. Area = 113.097m^2 Start. Tot. Vol. = 2500E+03L Niveau (VC) = 60%	>>Eau tiède VFLOW = Eau d'usine VFLOW >> Linear: IN1 HDEBIT * (-0.04) + IN2 HDEBIT * (-0.04) + IN3 HDEBIT * (-0.04) + DUTY = 0.0 >> IN1 VFLOW / LIC2345 OUTPUT = 250	-Conditions initiales: régime permanent -Mélange parfait -Perte de chaleur = 4% -LIC2345 : VC = Var. Contrôlée VM = Var. Manipulée
RESERV_EAU_ PRESSES	IN1 : Du HEADER12	OUT1 : Débordement OUT2 : Vers le cuvier d'alimentation au ramasse pâte (VM)	Cross-Sect. Area = 1.767m^2 Start. Level = 2m Niveau (VC) = 60%	>> IN1 HDEBIT * (-5E-03) + DUTY = 0.0 >> OUT1 VFLOW / LIC8958 OUTPUT = 50	-Conditions initiales: régime permanent -Mélange parfait -Perte de chaleur = 0.5% -LIC8958 : VC = Var. Contrôlée VM = Var. Manipulée
RESERV_EQUIL	*IN 1 : Du réservoir de casses à haute densité* (VM)	OUT1 : Débordement OUT2 : Vers le cuvier de casses	Cross-Sect. Area = 70m^2 Start. Tot. Vol.= 1474E+03L Niveau (VC) = 95%	>> IN1 HDEBIT * (-0.02) + DUTY = 0.0 >> OUT1 VFLOW / LIC2319 OUTPUT = 120	-Conditions initiales: régime permanent -Mélange parfait -Perte de chaleur = 2 % -LIC2319 : VC = Var. Contrôlée VM = Var. Manipulée
RESERV_EQUIL_ FEUILLUS	IN1: MIXER#1 OUT	OUT1: Vers la caisse de mélange	Cross-Sect. Area = 50.265m^2 Start. Level = 14m	>> IN1 HDEBIT * (-0.02) + DUTY = 0.0	-Régime permanent -Mélange parfait -Perte de chaleur = 2%

Unité	Entrée	Sortie	Spécifications / Consigne	Relations	Hypothèses / Commentaires
RESERV_PÂTE_BL	IN1: Pâte blanche	OUT1: Au MIXER#1	Cross-Sect. Area = $110m^2$ Start. Tot.Vol.= 3760E3L	>> IN1 HDEBIT * (-0.02) + DUTY = 0.0	-Régime permanent -Mélange parfait -Perte de chaleur = 2%
RESERV_REJ_ EPUR_QUAT	*IN1 : Eau blanche trouble* (VM) IN2 : Des épurateurs quaternaires	OUT1 : Vers le EPUR OUT2 : Débordement	Cross-Sect. Area = $1m^2$ Start. Level = 2.44m OUT1 VFLOW = 200L Niveau (VC) = 60%	>> Linear: IN1 HDEBIT * (-0.01) + IN2 HDEBIT * (-0.01) + DUTY = 0.0 >> IN1 VFLOW / LIC2493 OUTPUT = 10	- Mélange parfait - Perte de chaleur = 1% -LIC2493 : VC = Var. Contrôlée VM = Var. Manipulée
RESERV_REJETS_ CASSES	IN1 : Eau blanche trouble IN2 : Casses du tamis de casses	OUT1 : Débordement *OUT2 : Vers le tamis de casses 2* (VM)	Cross-Sect. Area = $1.67m^2$ Start. Level = 0.75 m Niveau (VC) = 50%	>> IN1 VFLOW / IN2 VFLOW = 0.2 >> Linear: IN1 HDEBIT * (-0.01) + IN2 HDEBIT * (-0.01) + DUTY = 0.0 >> OUT2 VFLOW / LIC2293 OUTPUT = 10	- Perte de chaleur = 1% -LIC2293 : VC = Var. Contrôlée VM = Var. Manipulée
RESERV_REJETS_ TAMIS_1STADE	IN 1 : Eau blanche trouble IN2 : Du tamis 1e stade IN3 : Du tamis 2e stade	OUT1 : Vers le réservoir de rejets de tamis 2e stade OUT2 : Vers le tamis de fente 2e stade	Cross-Sect. Area = $5.91m^2$ Start. Tot. Vol. = 18E+03L Overflow (OUT1) = 3.81m	>> Linear: IN1 HDEBIT * (-0.01) + IN2 HDEBIT * (-0.01) + IN3 HDEBIT * (-0.01) + DUTY = 0.0 >> IN1 VFLOW = IN2 VFLOW * 0.23 + IN3 VFLOW * 0.23	-Régime permanent -Mélange parfait -Perte de chaleur = 1%
RESERV_REJETS_ TAMIS_2STADE	IN 1 : Eau blanche trouble IN2 : Du tamis fente 2e stade IN3 : Rejets tamis sec. IN4 : Du réservoir de rejets de tamis 1e stade	OUT1 : Vers le tamis fente 3e stade	Cross-Sect. Area = $9.235m^2$ Start. Tot. Vol. = 25E+03L	>> Linear: IN1 HDEBIT * (-0.01) + IN2 HDEBIT * (-0.01) + IN3 HDEBIT * (-0.01) + DUTY = 0.0 >> IN1 VFLOW / IN2 VFLOW = 3	-Régime permanent -Mélange parfait -Perte de chaleur = 1%
RESERV_REJETS_ TAMIS_PRIM	IN1 : Du tamis prim. *IN2 : Eau blanche riche* (VM)	OUT1 : Au tamis sec. OUT2 : Débordement	Cross-Sect. Area = $1.5m^2$ Start. Level = 1.5m Niveau (VC) = 70%	>> Linear: IN1 HDEBIT * (-5E-03) + IN2 HDEBIT * (-5E-03) + DUTY = 0.0 >> OUT1 VFLOW / IN1 VFLOW = 2.1 >> IN2 VFLOW / LIC2471 OUTPUT = 100	- Mélange parfait - Perte de chaleur = 0.5% -LIC2471 : VC = Var. Contrôlée VM = Var. Manipulée

Unité	Entrée	Sortie	Spécifications / Consigne	Relations	Hypothèses / Commentaires
RESERV_RESINEUX	IN1: Résineux	OUT1: Vers la dilution	Cross-Sect. Area = $50.265m^2$ Start. Tot. Vol. = 647E+03L	>> IN1 HDEBIT * (-0.02) + DUTY = 0.0	- Régime permanent - Mélange parfait - Perte de chaleur = 2%
RESINEUX (Source)		OUT (FEED): Résineux (Vers l'unité INTERCHANGE INT69)	TEMPERATURE = 15 CONSISTENCY = 90 M% = 16.05 F% = 2.08 DS_PPM = 4E+04 ASH% = 0.43		L% est calculé
SECHEURS45	IN1 : Du DIV34	OUT1 : Vapeur OUT2 : Vers l'unité CT	OUT2 CONSISTENCY = 80.0002 DUTY = 0.1157	>>Ratio COMPOSANT OUT2 / COMPOSANT IN1: LAR = 1 MED = 1 FIN = 1 ASH = 1 DISOL = 1 TEMPERATURE = 1	
SECHEURS45	IN1 : Du DIV41	OUT1 : Vapeur OUT2 : Vers le DIV42	OUT2 CONSISTENCY = 93.6	>>Ratio COMPOSANT OUT2 / COMPOSANT IN1: LAR = 1 MED = 1 FIN = 1 ASH = 1 DISOL = 1 TEMPERATURE = 1	-Pas des pertes de chaleur
SILO	IN1: Vapeur IN2: Du ADD23 IN3: Du canal d'amenée MK1 IN4: Du canal d'amenée MK2	OUT1 : Débordement au cuvier d'eau blanc riche OUT2 : À la pompe primaire	Cross-Sect. Area = $25m^2$ Start. Level = 6m IN1 TEMPERATURE = 150 IN1 PRESSION = 550	>> IN1 HDEBIT * (-5E-03) + IN2 HDEBIT * (-5E-03) + IN3 HDEBIT * (-5E-03) + IN4 HDEBIT * (-5E-03) + DUTY = 0.0 >>Ratio ADD21 IN2 VFLOW / SILO OUT2 VFLOW = 3.2	- Régime permanent - Mélange parfait - Perte de chaleur = 0.5%
TAMIS_1STADE	IN : Pâte de la colonne de mélange 812-037	OUT1 : Vers le réservoir de rejets de tamis 1[e] stade OUT2 : Vers le cuvier de machine	TAMIS_1STADE OUT1 VFLOW= 1200		

Unité	Entrée	Sortie	Spécifications / Consigne	Relations	Hypothèses / Commentaires
TAMIS_2STADE	IN : Pâte de la colonne de mélange 812-037	OUT1 : Vers le réservoir de rejets de tamis 1e stade OUT2 : Vers le cuvier de machine	TAMIS_2STADE OUT1 VFLOW= 1200		
TAMIS_CASSES	IN1 : Du cuvier de casses	OUT1 : À la caisse de mélange OUT2 : Vers le réservoir de rejets de casses	OUT2 VFLOW = 150	>>Ratio COMPOSANT OUT1 / COMPOSANT IN1: LAR = 0.8 MED = 0.88 FIN = 0.9 ASH% = 1 DS_PPM = 1 TEMPERATURE = 1	-Perte de chaleur = 0 %
TAMIS_CASSES2	IN1 : Vers le réservoir de rejets de casses	OUT1 : Vers le cuvier de casses			-Perte de chaleur = 0 %
TAMIS_FENTE_2STADE	IN : Du réservoir de rejets de tamis 1e stade	OUT1 : Vers le réservoir de rejets de tamis 2e stade OUT2 : Vers la colonne de mélange 812-037	OUT1 VFLOW = 800		
TAMIS_FENTE_3STADE	IN 1 : Du réservoir de rejets de tamis 2e stade	OUT1 : Vers la succion de la pompe 812-113 (Ramasse pâte)			-Perte de chaleur = 0%
TAMIS_PRIM	IN1 : Du ADD16	OUT1 : Vers la caisse d'arrivée OUT2 : Au réservoir de rejets du tamis primaire	OUT2 VFLOW = 5800	>> Ratio COMPOSANT OUT1 / COMPOSANT IN1: LAR = 0.85 MED = 0.9 ASH% = 1 DS_PPM = 1 TEMPERATURE = 1 >> OUT2 FIN = OUT2 FLOW * ADD16 OUT FIN / ADD16 OUT FLOW	-Pas des pertes de chaleur -Concentration de fines dans les rejets = concentration de fines à l'entrée du tamis
TAMIS_SEC	IN1 : Du réservoir de rejets du tamis primaire	OUT1 : Vers le désaérateur OUT2 : Vers le réservoir des rejets du tamis 2e stade		>> Ratio COMPOSANT OUT1/ COMPOSANT IN1: WATER = 0.94 LAR = 0.85 MED = 0.87 ASH% = 1	-Pas des pertes de chaleur -Concentration de fines dans le courant accepté = concentration de fines à l'entrée du tamis

Unité	Entrée	Sortie	Spécifications / Consigne	Relations	Hypothèses / Commentaires
				DS_PPM = 1 TEMPERATURE = 1 >> OUT1 FIN = OUT1 FLOW * IN1 FIN / IN1 FLOW	
TRITURATEUR	IN1: Eau blanche claire IN2: Vapeur IN3: Résineux	OUT1: Vers la pompe 821-026	IN2 TEMP = 156.153 IN2 PRESSION = 560 OUT1 TEMPERAT=50 OUT1 CONSIST= 4.8	>> IN1 HDEBIT * (-0.02) + IN2 HDEBIT * (-0.02) + IN3 HDEBIT * (-0.02) + DUTY = 0.0	- Perte de chaleur = 2 %
XX1 (Source)		OUT (FEED) : Vers le ADD24	TEMPERATURE = 50 CONSISTENCY= 0 L% = 0 M% = 0 DS_PPM = 100 ASH% = 0		F% est calculé
XX2 (Source)		OUT (FEED) : Vers le ADD25	TEMPERATURE = 50 CONSISTENCY= 0 L% = 0 M% = 0 DS_PPM = 100 ASH% = 0		F% est calculé

Table A4.3: Level controlled tanks

Tank	Capacity (m^3)	Height (m)	Residence Time* (min)
EPAISSISSEUR	100	5	27.9
RESERV_EQUIL	1474	14.74	511.8
CUVIER_CASSES	125	5	34.9
RESERV_REJETS_CASSES	2.5005	1.5	11.4
CUVIER_MELANGE	343	7	26.8
CUVIER_MACHINE	175	7	11.7
EAU_BL_FIL	48	4.8	6.1
RESERV_EAU_BL_CL	2827.425	25	293.5
CUVIER_EAU_BL_CL	32	4	1.4
CUVIER_EAU_BL_TR	32	4	1.4
CUVIER_RAMASSE_PATE	62.83	5	20.8
RESERV_REJ_EPUR_QUAT	2.5005	1.5	12.5
RESERV_REJETS_TAMIS_PRIM	2.5005	1.5	0.2
FOSSE_COUCHEUR	200	5	66.7
RESERV_EAU_PRESSES	3.534	2	1.5
CHEST_ DESAERATEUR	4	2	0.2
ALIM_RAM_PATE	200	10	9.5
CASSES_HAUT_DENS	3760	18.8	2372.2

* Residence time calculated for nominal steady-state conditions

(Broke ratio = 10%; no breaks)

Table A4.4. Parameters of level controllers

Controller	Set Point (%)	Gain (Controller Output%/Lev-%)	Reset Ratio (min^{-1})
LIC12259	75	0.800	0.02
LIC2319	95	8.189	0.01667
LIC2341	75	1.667	0.01667
LIC2293	50	0.500	0.05
LIC2431	70	1.715	0.025
LIC2438A	70	1.556	0.05
LIC2	60	1.477	0.1
LIC2345	60	7.540	0.01667
LIC2353	75	1.280	0.25
LIC2356	65	2.462	0.25
LIC2390	70	0.558	0.03333
LIC2493	60	0.500	0.05
LIC2471	70	0.250	0.25
LIC8800	30	1.600	0.02
LIC8958	60	0.707	0.25
LIC2466	70	0.100	0.25
LIC8885	60	1.333	0.05
LIC1	50	50.133	0.01667

Table A4.5: Consistency control loops

Controller	Controlled Variable	Gain (Controller Output%/Cons-%)	Reset Ratio (min^{-1})
KIC2270	RESERV_PATE_BL outlet	9.231	20
KIC2309	RESERV_EQUIL_FEUILLUS outlet	13.636	20
KIC7401	TRITURATEUR outlet	2.422	20
KIC2303	RESERV_RESINEUX outlet	0.750	20
KIC2335	RESERV_CASS_PROP outlet	3.927	20
KIC2339	RESERV_CASS_COL outlet	3.927	20
KIC2255	CASSES_HAUTEDENS outlet	2.143	20
KIC2320	RESERV_EQUIL outlet	0.9724	20
KIC2342	CUVIER_CASSES outlet	4.4248	20
KIC2433	CUVIER_MELANGE outlet	30.303	20
KIC2439	CUVIER_MACHINE outlet	31.579	20
KIC2391	CUVIER_RAMASSE_PATE	3.871	20

APPENDIX A5

LIST OF CONFERENCES

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APPENDIX B: OPERABILITY ANALYSIS

APPENDIX B1

BACKGROUND

Vinson and Georgakis (2000) introduced a geometric approach for the assessment of the operability of a process. Their approach aims at quantifying the inherent controllability of the process. According to Vinson (2000), a process is said to be operable if the available set of inputs is capable of satisfying the desired steady-state and dynamic performance requirements defined at the design stage, in the presence of the set of anticipated disturbances, without violating any process constraints. The availability of a mathematical model relating inputs and disturbance to outputs is a prerequisite of this approach.

Operating spaces

To develop their controllability concepts, Vinson and Georgakis (2000) introduced a number of *operating spaces*. They are defined as the ranges over which inputs, outputs and disturbances can vary. The first set is the Available Input Space (*AIS*), which is defined as the set of values that the input variable can take. Analogously, the Desired Output Space (*DOS*) is defined as the set of desired values of the process outputs. For setpoint tracking problems, the Achievable Output Space (AOS_u) can be calculated by mapping *AIS* onto the output space, when the disturbances are at their nominal values. The mathematical relationship between inputs and outputs is used to perform this calculation. For disturbance rejection problems, the authors defined two additional operating spaces, the Expected Disturbance Space (*EDS*), defined as the set of expected disturbances that can affect the system, and the Desired Input Space (DIS_d), calculated as the required inputs to compensate the disturbances that enter the system.

Output controllability index

Vinson and Georgakis proposed a steady-state, multivariable and nonlinear measure for assessing the input-output, open-loop controllability of a process. This measure, called

Output Controllability Index (OCI), does not take into account the effect of process dynamics on the achievable performance. Instead, it focuses on the input-output relations and aims at quantifying the effect of limited ranges of the inputs on the achievable performance.

The calculation of OCI involves the combination of operating spaces by projecting one operating space onto another and the calculation of the intersection, thereafter. Depending on the objectives of the application, a number of output controllability indices can be defined. The best and worst values of these indices are 1 and 0, respectively. For the purposes of this work, the following two indices are relevant.

a. For *setpoint tracking problems*, the servo output controllability index (*s–OCI*) is defined by:

$$s - OCI = \frac{\mu[AOS_u \cap DOS]}{\mu[DOS]} \tag{B1.1}$$

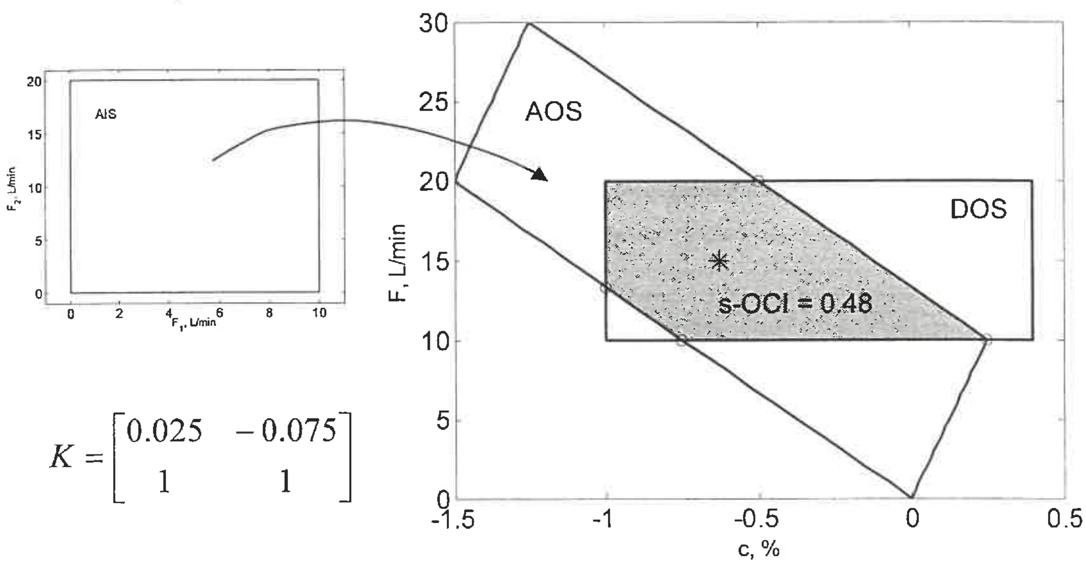
where μ represents a function calculating the size of the corresponding space. This index quantifies how much of the desired output space can be achieved with the available input space. If this value is less than 1, it indicates that the available input space is not enough to achieve the entire desired output space. **Figure B1.1** shows an example for the linear model of the blending process of two streams. ***K*** is the steady-state gain matrix used to calculate the AOS from the AIS.

b. For *disturbance rejection problems*, the regulatory output controllability index (*r–OCI*) is defined by:

$$r - OCI = \frac{\mu[AIS \cap DIS_d]}{\mu[DIS_d]} \tag{B1.2}$$

This index quantifies the ability of the plant to reject a disturbance entering the system. Similar to the previous case, a value less than 1 indicates that the required inputs to compensate the effect of a disturbance are not covered by the available inputs.

For 2x2 systems the intersection represents an area, in three dimensions, it represents a volume.



$$K = \begin{bmatrix} 0.025 & -0.075 \\ 1 & 1 \end{bmatrix}$$

Figure B1.1: Servo Output Controllability Index (s-OCI) of a linear system.

APPENDIX B2

LINEARIZED MODEL OF SUB-SYSTEM

Table B2.1: High density broke storage tank

$$\frac{dh_1}{dt} = \frac{1}{A_1}(F_1 - F_2)$$
$$\frac{dc_2}{dt} = \frac{F_1}{V_1}(c_1 - c_2)$$
$$\frac{dc_{f2}}{dt} = \frac{F_1}{V_1}(c_{f1} - c_{f2})$$
$$\frac{dc_{A2}}{dt} = \frac{F_1}{V_1}(c_{A1} - c_{A2})$$
$$\frac{dc_{DS2}}{dt} = \frac{F_1}{V_1}(c_{DS1} - c_{DS2})$$

Table B2.2: Dilution point

$$F_4 = F_2 + F_3$$
$$c_4 = \left(\frac{F_2}{F_4}\right)c_2 + \left(\frac{F_3}{F_4}\right)c_3$$
$$c_{f4} = \left(\frac{F_2}{F_4}\right)c_{f2} + \left(\frac{F_3}{F_4}\right)c_{f3}$$
$$c_{A4} = \left(\frac{F_2}{F_4}\right)c_{A2} + \left(\frac{F_3}{F_4}\right)c_{A3}$$
$$c_{DS4} = \left(\frac{F_2}{F_4}\right)c_{DS2} + \left(\frac{F_3}{F_4}\right)c_{DS3}$$

Table B2.3: Mixing chest

$$\frac{dh_2}{dt} = \frac{1}{A_2}(F_4 + F_5 + F_6 - F_7)$$
$$\frac{dc_7}{dt} = \frac{F_4}{V_2}(c_4 - c_7) + \frac{F_5}{V_2}(c_5 - c_7) + \frac{F_6}{V_2}(c_6 - c_7)$$
$$\frac{dc_{f7}}{dt} = \frac{F_4}{V_2}(c_{f4} - c_{f7}) + \frac{F_5}{V_2}(c_{f5} - c_{f7}) + \frac{F_6}{V_2}(c_{f6} - c_{f7})$$
$$\frac{dc_{A7}}{dt} = \frac{F_4}{V_2}(c_{A4} - c_{A7}) + \frac{F_5}{V_2}(c_{A5} - c_{A7}) + \frac{F_6}{V_2}(c_{A6} - c_{A7})$$
$$\frac{dc_{DS7}}{dt} = \frac{F_4}{V_2}(c_{DS4} - c_{DS7}) + \frac{F_5}{V_2}(c_{DS5} - c_{DS7}) + \frac{F_6}{V_2}(c_{DS6} - c_{DS7})$$

Table B2.4: Pulp ratios

Hardwood – to – softwood ratio :	$R_1 = \frac{F_6 c_6}{F_5 c_5} \times 100$
Broke ratio :	$R_2 = \frac{F_4 c_4}{F_7 c_7} \times 100$

Table B2.5: Dimensionless variables

$x_{1i} = \frac{h_i}{h_i^R}$	$x_{2j} = \frac{c_j}{c^R}$	$x_{3j} = \frac{c_{fj}}{c_f^R}$	$x_{4j} = \frac{c_{Aj}}{c_A^R}$	$x_{5j} = \frac{c_{DSj}}{c_{DS}^R}$
$q_j = \frac{F_j}{F^R}$	$v_i = \frac{V_1^R}{V_i^R}$	$a_i = \frac{A_i}{A_i^R}$	$\tau = \frac{tF^R}{V_1^R}$	$r_n = \frac{R_n}{R^R}$

Table B2.6: High density broke storage tank

$$\frac{dx_{11}}{d\tau} = \frac{v_1}{a_1}(q_1 - q_2)$$

$$\frac{dx_{22}}{d\tau} = \frac{q_1 v_1}{a_1 x_{11}}(x_{21} - x_{22})$$

$$\frac{dx_{32}}{d\tau} = \frac{q_1 v_1}{a_1 x_{11}}(x_{31} - x_{32})$$

$$\frac{dx_{42}}{d\tau} = \frac{q_1 v_1}{a_1 x_{11}}(x_{41} - x_{42})$$

$$\frac{dx_{52}}{d\tau} = \frac{q_1 v_1}{a_1 x_{11}}(x_{51} - x_{52})$$

Table B2.7: Dilution point

$$\frac{dx_{12}}{d\tau} = \frac{v_2}{a_2}(q_4 + q_5 + q_6 - q_7)$$

$$\frac{dx_{27}}{d\tau} = \frac{q_4 v_2}{a_2 x_{12}}(x_{24} - x_{27}) + \frac{q_5 v_2}{a_2 x_{12}}(x_{25} - x_{27}) + \frac{q_6 v_2}{a_2 x_{12}}(x_{26} - x_{27})$$

$$\frac{dx_{37}}{d\tau} = \frac{q_4 v_2}{a_2 x_{12}}(x_{34} - x_{37}) + \frac{q_5 v_2}{a_2 x_{12}}(x_{35} - x_{37}) + \frac{q_6 v_2}{a_2 x_{12}}(x_{36} - x_{37})$$

$$\frac{dx_{47}}{d\tau} = \frac{q_4 v_2}{a_2 x_{12}}(x_{44} - x_{47}) + \frac{q_5 v_2}{a_2 x_{12}}(x_{45} - x_{47}) + \frac{q_6 v_2}{a_2 x_{12}}(x_{46} - x_{47})$$

$$\frac{dx_{57}}{d\tau} = \frac{q_4 v_2}{a_2 x_{12}}(x_{54} - x_{57}) + \frac{q_5 v_2}{a_2 x_{12}}(x_{55} - x_{57}) + \frac{q_6 v_2}{a_2 x_{12}}(x_{56} - x_{57})$$

Table B2.8: Mixing chest and ratios

$$q_4 = q_2 + q_3$$

$$x_{24} = \left(\frac{q_2}{q_4}\right)x_{22} + \left(\frac{q_3}{q_4}\right)x_{23}$$

$$x_{34} = \left(\frac{q_2}{q_4}\right)x_{32} + \left(\frac{q_3}{q_4}\right)x_{33}$$

$$x_{44} = \left(\frac{q_2}{q_4}\right)x_{42} + \left(\frac{q_3}{q_4}\right)x_{43}$$

$$x_{54} = \left(\frac{q_2}{q_4}\right)x_{52} + \left(\frac{q_3}{q_4}\right)x_{53}$$

$$r_1 = \frac{q_6 x_{26}}{q_5 x_{25}} \cdot \frac{100}{R^R}$$

$$r_2 = \frac{q_4 x_{24}}{(q_4 x_{24} + q_5 x_{25} + q_6 x_{26})} \cdot \frac{100}{R^R}$$

APPENDIX B3

A new tool for assessing closed-loop dynamic operability of process designs for a desired control performance

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Abstract

This paper offers a new perspective of the dynamic operability of processes, based on the idea of moving operating ranges, called dynamic operating spaces. The concept of *Operable Fraction* (f_{op}) is introduced and defined, for open-loop conditions, by combination of these spaces. This fraction is a measure of the inherent operability of a process. A new control performance index is proposed and this index is included in the definition of a new measure of the dynamic operability. This is a measure of the operable fraction that a process can achieve within the desired performance. A simple linear model is used to demonstrate the properties of this *dynamic Operability Measure* (*dOM*) and its applicability to process design is illustrated with a distillation control problem.

Keywords: Operability; Controllability; Control performance; Index; Linear and nonlinear systems

1. **Introduction**

The ever-increasing demands of global competition and stricter environmental regulations have transformed chemical processes into complex, highly integrated systems that are difficult to operate. Operational requirements include operability, controllability, flexibility, switchability, availability, reliability, maintainability and resiliency (for an extensive overview, see e.g., Perkins and Walsh, 1996; Van Schijndel and Pistikopoulos, 1999). Unfortunately, there is no agreement as to the exact definition of these terms. Some are used as synonyms, or with just slight nuances in the meaning. Meeuse and Grievink (2000) reserve the term operability for the ability to cope with all these operational requirements. Thus, operational requirements like controllability (in simple terms, the ability of the plant to meet specifications in spite of disturbances) and switchability (the ability to switch economically between operating points) are subsets of operability.

In addition to the terms used to characterize operability, a large number of operability tools and measures have been proposed. Usually, they quantify specific characteristics of process operability. Operability evaluation methods may be classified into three categories, according to the model used in the evaluation procedure: steady-state model-based, linear dynamic model-based, or nonlinear dynamic model-based (Lee *et al.*, 2001).

Georgakis *et al.* (2001) made a broad classification of the different approaches to the operability analysis and categorized them as either linear or nonlinear model-based methods, depending upon the system structure. Most of these measurements were developed for linear process models assuming steady-state conditions, and some others explicitly take the process dynamics into account.

Vinson and Georgakis (2000) proposed a geometric approach to assess process controllability of steady-state systems. They introduced a new controllability index, the output controllability index (OCI), to characterize the inherent ability of a process to track a set point change or to reject disturbances when the process is open-loop controlled, i.e., in the absence of any regulatory control structure. This OCI, designated as the operability index (OI) in later publications (Georgakis *et al.*, 2001; Vinson and Georgakis, 2002), aims at quantifying the effect of a limited range of inputs on the achievement of performance objectives for the process.

Uztürk and Georgakis (2002) extended this approach to the dynamic case for linear systems using an optimal-control-based technique. Thus, this approach does not assume any control structure. The performance measure used is the shortest time required for a system to settle to the desired setpoint after a setpoint change and/or a disturbance. A dynamic operability index is defined, which quantifies the achievable performance of the process using an open-loop optimal controller. The same methodology was used by Subramanian *et al.* (2001) for a more general, nonsquare nonlinear system.

Ekawati and Bahri (2003) integrated Vinson's OCI within the Dynamic Operability Framework (DOF), developed previously by Bahri (1996). The operating spaces and the operability index, however, are not the same as defined by Vinson (2000). The authors used dynamic nonlinear programming (NLP) to calculate the optimal operating conditions and the feasible operating region, and a projection of disturbance space into output space to assess the controllability.

Noticeably, most of the proposed measures of controllability and operability are based on optimization techniques and are more suited for the screening of design alternatives. However, many operating problems in existing plants require adequate tools to analyze the capacity of the plant to move from one operating condition to another, and to deal effectively with disturbances. Since process and control systems form an indissoluble unit, it is not possible to assess this capacity by observing only one element. Any measure or index of the dynamic operability of a process should explicitly take into account the process related *and* control system characteristics.

Some proposed methods emphasize only one aspect of process operability, or they are not practical enough to be implemented by the practising engineer. Furthermore, it is difficult to link dynamic operability and performance with many of the proposed tools. These considerations motivated us to develop a different route for the assessment of dynamic operability. Our approach combines well-established methods and some new ideas.

In this work, we seek to develop a general framework to assess the dynamic operability of processes that can be applied to a wide range of processes, including first-principles and empirical models, linear and nonlinear systems, as well as time-domain and transfer-domain models. Our aim is to propose a simple, yet accurate, measure of dynamic operability that can be applied in process design and for retrofit purposes. For the sake of simplicity, only linear examples are considered. However, general guidelines are also provided for nonlinear systems. Although the methodology has been developed using a standard feedback structure (with a PI controller), this approach can be applied to other control strategies and controller algorithms.

The scope of this study only includes deterministic process changes. The important and broad area of stochastic objects, intensively investigated in recent years, is not addressed here.

This paper is organized as follows. In section 2, a general methodology to assess the dynamic operability of single-input single-output systems is developed. In section 3, this approach is expanded to a multi-input multi-output system, and in section 4, some conclusions are drawn.

2. **Dynamic Operability of a SISO System**

The definition of operability given by Vinson (2000) is used throughout this work. We also adopted some of his notation.

Process Operability

A process is defined as operable if the available set of inputs is capable of satisfying the desired steady-state and dynamic performance requirements defined at the design stage, in the presence of the set of anticipated disturbances, without violating any process constraints.

This definition provides a steady-state operability framework for generic nonlinear systems, regardless of the control system configuration. The first step in any operability analysis is to evaluate whether or not the process will be able to meet design specifications in the face of desired process output changes and expected disturbances. This work aims at expanding this approach for dynamic systems.

The first requirement is to have a mathematical model that relates inputs and disturbances to outputs. If real data are available, they also can be used to evaluate the dynamic operability of an existing plant, provided that plant model mismatches are small.

A nonlinear single-input single-output (SISO) system can be represented by

$$\begin{aligned} \dot{x} &= f(x,u,d) \\ y &= g(x,u,d) \end{aligned} \tag{B3.1}$$

where x is the state variable $(\dot{x} = dx/dt)$, u and y are the input and output variables, respectively, and d is a known disturbance.

The classical representation of a linear SISO system is

$$y(s) = g_p(s)u(s) + g_d(s)d(s) \tag{B3.2}$$

where $u(s)$, $y(s)$ and $d(s)$ are the Laplace transforms of $u(t)$, $y(t)$ and $d(t)$, respectively. Here $g_p(s)$ and $g_d(s)$ are the scalar transfer functions relating them, as shown inside the box of **Figure B3.1**.

The closed-loop relationship of **Figure B3.1** can be easily derived:

$$y(s) = \frac{g_p(s)g_c(s)}{1+g_p(s)g_c(s)}r(s) + \frac{g_d(s)}{1+g_p(s)g_c(s)}d(s) \tag{B3.3}$$

where $g_c(s)$ is the controller transfer function and $r(s)$ is the reference value of the output variable or setpoint. In principle, any controller algorithm can be used, but for most of this study, we used only a PI controller.

There are two main problems in process control: The *servo* problem or *setpoint tracking,* and the *regulatory* problem or *disturbance rejection*. In the first case, we are assuming that there is no disturbance entering the system ($d(s)$ = 0) and the main objective of the control system is to bring the controlled variable fast and smoothly to its new value after a set point change. In the second case, we assume that there is no setpoint change ($r(s)$ = 0) and the main control objective is to bring the controlled variable back to its initial value after a disturbance.

2.1. **Dynamic Operating Spaces**

Vinson *et al.* (2000) introduced a number of operating spaces for the steady-state operability analysis. These operating spaces are defined as ranges that the inputs, outputs and the expected disturbances can take, and the operability index is calculated by mapping one variable onto another, using the mathematical model for this purpose. The procedure involves finding the intersection of two polyhedral spaces. This intersection represents an area in two dimensions, a volume in three dimensions, and a convex hull in n dimensions. They used the software Geometric Bounding Toolbox, developed by Veres (1995), to perform the calculations.

Assuming perfect control, the static operating spaces have been adapted to the dynamic case:

For setpoint tracking problems ($d = 0$):

- The dynamic Desired Output Space, $DOS(t)$, is defined as the set of values that the output variable y takes as a function of the time.
- The dynamic Available Input Space, $AIS(t)$, is defined as the set of values of u and its variation over time.
- The dynamic Achievable Output Space, denoted by $AOS_u(t)$, is calculated by solving the model (**Eq. B3.1 or B3.2**) for the output y, given the input u. $AOS_u(t)$ can be thought as the dynamic mapping of u onto y, that is $y = g(x, u)$, for a nonlinear system and $y(s) = g_p(s)u(s)$ for a linear system.

For disturbance rejection problems ($y = 0$), two additional operating spaces are required:

- The dynamic Expected Disturbance Space, $EDS(t)$, is defined as the set of values that d can take over time.
- The dynamic Desired Input Space, $DIS_d(t)$, is formed by all values of u required to compensate for a known disturbance d that is occurring. The input variable u can be back calculated from $g(x,u,d) = 0$, for a nonlinear system, or using the relation $u(s) = -[g_p(s)]^{-1}[g_d(s)d(s)]$, for a linear system.

It must be noted that the inversion of $g_p(s)$ requires factoring the process model into invertible and noninvertible parts. Noninvertible elements include: time delays and RHP zeros.

Since any process variable can move inside its one-dimensional range of variation as time passes, the operating spaces in this framework are considered to be two-dimensional space-time entities. The output and input variables could be any physical variable, such as flow rates, temperatures, concentrations.

In this work, we are only considering deterministic changes in the process in the form of step changes. Thus, $DOS(t)$ and $AIS(t)$ will have the shape of a rectangle, whose base consists of the time span under consideration.

2.2. **Operable Fraction**

Definition 1: The *operable fraction*, f_{op}, is defined as the fraction of the desired or requested operating spaces that can be achieved with the available dynamic input space ($AIS(t)$) or for the expected dynamic disturbance space ($EDS(t)$) for open-loop conditions.

Since no control structure is assumed at this stage, this fraction depends exclusively on process characteristics. Indeed, it measures the inherent ability of the process to track set point changes and to reject disturbances. It also represents the highest achievable performance that only a perfect controller can achieve, that is, when there is perfect tracking after a set point change or when there is an instantaneous response of the manipulated variable after a perturbation has entered the system.

Setpoint tracking

Mathematically, the operable fraction for the servo case can be defined as

$$f_{op}\Big|_{d=0} = \frac{\int_0^{t_{ss}} \left[AOS_u(t) \cap DOS(t)\right] dt}{\int_0^{t_{ss}} \left[DOS(t)\right] dt} \qquad \text{(B3.4)}$$

where the upper limit of the integrals, t_{ss}, is the 'time to steady-state', defined as the time when the output variable y is within 0.1% of the vicinity of its final value. This final value was calculated by applying the final value theorem.

This fraction indicates how much of the desired process output is covered by the achievable output with the available input. This can be considered the dynamic version of the servo output controllability index (s-OCI) developed by Vinson (2000).

Since we are comparing areas, scaling of variables is not a requirement of this approach and variables could be used directly with their engineering units. However, the use of normalized, dimensionless variables has the advantage of making the comparison of results easier.

Consider the illustrative example depicted in **Figure B3.2**. The intersection between $DOS(t)$ and $AOS_u(t)$ was calculated using linear interpolation and the integrals were approximated using Simpson's method. The shaded area represents the highest performance that a perfect controller could achieve if the available input space is defined by the set $AIS(t) = \{u(t)| \ 0 \leq u(t) \leq 1\}$. Since dead time cannot be removed from the process, the operable fraction will be always less than 1 for a process with dead time. The highest value of f_{op} for the servo case can be calculated from $(1 - t_d/t_{ss})$, where t_d is the time delay. In general, f_{op} will vary between 0 and 1, with 1 as the best value.

Disturbance rejection

The operable fraction for the regulatory case is expressed as

$$f_{op}\Big|_{y=0} = \frac{\int_0^{t_{ss}} [AIS(t) \cap DIS_d(t)]dt}{\int_0^{t_{ss}} [DIS_d(t)]dt} \tag{B3.5}$$

Here t_{ss} is the time required to bring $DIS_d(t)$ within 0.1% of the vicinity of its final value.

This fraction measures how much of the desired input, required to reject an expected disturbance, is achievable with the available input. Similar to the servo case, the best and worst values of f_{op} in the regulatory case are 1 and 0, respectively. A value of f_{op} less than 1 indicates that the available input needs to be incremented in order to compensate the expected disturbance. The corresponding index in the approach for steady-state operability analysis described by Vinson (2000) is the regulatory output controllability index (r-OCI).

In **Figure B3.3** the intersection points between $AIS(t)$ and $DIS_d(t)$ as well as the integrals, were calculated similarly to the servo case. Again, the shaded area represents the performance of an optimal controller for the available input and a known disturbance. In this example, for $|u| \geq 2.5$, $DIS_d(t)$ will lie entirely inside $AIS(t)$ and the operable fraction will attain the value 1.

2.3. **Control Performance**

There is a close relationship between process controllability and control performance under closed-loop conditions. Indeed, both open-loop factors (inherent to the process) and closed-loop characteristics (related to the control system) determine how well (or poorly) a process can be operated. Assuming that the closed-loop control system is stable, the next most important characteristic is the performance. A large number of methods have been proposed to measure the control performance. The minimum variance control (MVC) has been the most widely used tool to monitor industrial processes, since its introduction by Åstrom (1967) as performance benchmark. This method is naturally suited for the performance assessment of stochastic disturbances. Several authors (Eriksson and Isaksson, 1994; Tyler and Morari, 1995) have pointed out that MVC is not adequate to assess control performance if only deterministic changes in the process are considered. More recently, however, Huang and Shah (1999) showed that the setpoint tracking problem can be re-formulated as a regulatory problem. Consequently, MVC-based methods can handle deterministic disturbance rejection as well as setpoint tracking problems, if we consider deterministic disturbances at random time. A number of methods have been proposed for assessing the control performance of deterministic disturbances and set point changes. Some of these monitoring criteria have been used for process controllability studies. In particular, we can mention the Integral

Absolute Error (IAE), the Integral Squared Error (ISE) and the settling time. One shortcoming of these measurements is that only the controlled variable is taken into consideration. However, the manipulated variable also affects the control performance and needs to be considered as well.

Manipulated variable (MV) performance

MV performance is of concern because fast and large variations of the MV are associated with a shortening of the lifespan of actuators, usually valves. Moreover, as Wilton (1999) states, in complex processes the MV for one loop is often a disturbance to another loop. Therefore, it is important to take the MV into consideration. The rate of change and the largest variation are usually used as indication of the MV performance. In many cases, the industrial experience tells that an overshoot of 170% can be allowed (Marlin, 2000), but in general, little or no overshoot is desirable. The selection of a suitable value of the overshoot for each specific case is recommended.

To define a performance index for MV, we use a relative error, similar to the overshoot, calculated at each time step, k:

$$\varepsilon_u(k) = \left|\frac{u(k) - u(k-1)}{\Delta u^0}\right| \tag{B3.6}$$

where $\Delta u^0 = u_f^0 - u_i^0$ is the difference between the final and initial steady-state value of MV.

The MV performance is defined by

$$\eta_u = \left|1 - \frac{\bar{\varepsilon}_u}{\varepsilon_u^*}\right| \tag{B3.7}$$

where $\bar{\varepsilon}_u$ is the average value of the relative error over the transient period, t^*, and $\varepsilon_u^* = 2.7$ is a reference value corresponding to a maximal overshoot of 170%. The transient period for this variable has been defined as
$t^* = \{t \mid |\Delta u| = 10^{-3}\}$.

Figure B3.4 shows an example of a calculation for the same process treated in the previous section. η_u results 0.95 and 0.94, for the regulatory case and for setpoint tracking, respectively.

Controlled variable (CV) performance

Many controllability approaches focusing on the states of the system, and on the dynamics of the process and the control system, are based on the minimization of some performance measure. Since larger deviations of the CV from the desired set point are associated with greater performance degradation, in most cases the objective is to minimize this deviation. Our first objective in this work was to find a bounded performance index that could be used within this operability framework. We are using a modified form of the IAE. First, let us define a relative error of the CV expressed by

$$\varepsilon_y(t) = 100\left(\frac{r(t) - y(t)}{B}\right) \tag{B3.8}$$

where B is the step change in the set point (Δr) for the servo case or in the disturbance ($K_d \Delta d$) for the regulatory case, with K_d and d as the gain of the disturbance transfer function and the disturbance magnitude, respectively.

The tolerance band for $\varepsilon_y(t)$ has been fixed to 5%. A first factor, α_A, of the CV performance is calculated as the fraction of the area under the curve $\varepsilon_y(t)$ that lies within the tolerance band. Mathematically,

$$\alpha_A = \frac{\int_0^{t_f} \left|\varepsilon_y^*(t)\right| dt}{\int_0^{t_f} \left|\varepsilon_y(t)\right| dt} \tag{B3.9}$$

where $\varepsilon_y^*(t)$ is a function including all values of $\varepsilon_y(t)$ that not surpass the selected limit of 5% (solid line in **Figure A2.5**), that is

$\varepsilon_y^*(t)=\{\varepsilon_y(t) \mid |\varepsilon_y(t)| \leq 5\ \%\}$

Both functions, $\varepsilon_y(t)$ and $\varepsilon_y^*(t)$ are integrated over the interval $[0, t_f]$, where the final time t_f, the duration of the transient period, has been selected so that the total area under the curve $\varepsilon_y(t)$ equals the area of the rectangle whose base and height are t_f and the limit of 5%, respectively, that is

$$t_f = \left\{ t \mid \int_0^{t_f} |\varepsilon_y(t)| dt = 5t_f \right\}$$

Alternatively, one could select the final time for an adequately small value of $\varepsilon_y(t)$, e.g. 10^{-3}%. However, this criterion can cause the simulation to stop too early, such as in cases when there is still some oscillation after the error ε_y has been brought within the tolerance band of the final value.

The factor α_A accounts for the size of the error and the time that the CV spends outside the limits, but this factor does not account for the other important parameter that affects the CV performance, the settling time. It is possible to have the same α_A for very different settling times. Based on this consideration we are introducing another factor, α_t, that accounts explicitly for the settling time, t_s.

$$\alpha_t = 1 - \frac{t_s}{t_f} \tag{B3.10}$$

The contribution of α_A and α_t on the CV performance can be expressed as the geometric mean of both factors:

$$\eta_y = \sqrt{\alpha_A \alpha_t} \tag{B3.11}$$

Figure B3.5 shows the results of these factors and η_y for the case of disturbance rejection. Here again, the same methods used in the previous subsection were used to calculate the intersection points and the area. For the servo case we get: $\eta_y = 0.38$.

One way to combine the controlled and manipulated variable performances to calculate the overall closed-loop performance, η, is by using the following relationship:

$$\eta = \sqrt{\eta_y \eta_u} \tag{B3.12}$$

Both MV and CV performances are bounded by the interval [0, 1]. Thus, the inequality $0 \le \eta \le 1$ also holds. The highest performance (i.e., a value of 1) can only be achieved by an optimal controller. For any physically realisable feedback controller, in general $\eta < 1$. In the example, the controller performance obtained is 0.60 and 0.61, for the servo and regulatory case, respectively.

2.4. **Dynamic Operability Measure**

Definition 2: The *dynamic operability measure*, *dOM*, is defined as the achievable operable fraction within the desired control performance.

Both open-loop and closed-loop aspects of a process will define and shape the achievable output space in the servo case or the required input space in the regulatory case. The dynamic operability measure is an index that represents that space and it is calculated in this framework by taking into account the contributions of the operable fraction, f_{op}, and the control system performance, η:

$$dOM = \sqrt{f_{op}\,\eta}\,, \qquad 0 \le dOM \le 1 \qquad \text{(B3.13)}$$

This index is a measure of the ability of a controlled process to achieve the desired outputs and to reject expected disturbances within the specified performance, with 1 and 0 as the best and worst values, respectively. It also provides information about the sensitivity of the process and control system to changes in the setpoint and to disturbances. In this framework the operable fraction accounts for the process dynamics; it can be seen as the inherent operability index. On the other hand, the second factor, the controller performance accounts for the control system dynamics. This factor imposes a limit to the dynamic operability that could potentially be achieved with a perfect controller.

Using the results from the preceding example, we obtain a slight difference in the *dOM* for setpoint tracking and disturbance rejection, with values of 0.727 and 0.728, respectively. This small difference between the servo and regulatory *dOM* is expected for a linear system.

2.5. **Example 1: First-Order + Dead Time Process**

Many processes can be described as first order plus time delay

$$g_p(s) = \frac{K_p e^{-t_d s}}{\tau_p s + 1} \qquad \text{(B3.14)}$$

where K_p is the process gain, τ_p the process time constant and t_d the time delay. We are also using here this type of process to illustrate the properties of the dynamic operability measure.

To tune the PI controller in the following examples, the internal model control (IMC) (Morari and Zafiriou, 1989) based tuning method was used. In this method, a unique parameter, Lambda (λ), which is the time constant of the closed loop, needs to be selected.

MATLAB® software was used to perform all calculations, and although SIMULINK® was used to simulate process models, the simulation was controlled from within the MATLAB® program.

For the sake of clarity, we have divided this study into two separate cases, according to the main problems that occur in process control.

Setpoint tracking

The dynamic Available Input Space is specified as

$$AIS(t) = \{u(t) | -1 \le u(t) \le 1, \forall t\} \tag{B3.15}$$

A setpoint step change of magnitude Δr at $t = 0$ is considered in each of the cases studied below. Thus, the dynamic Desired Output Space, is defined as the set

$$DOS(t) = \{y(t) | (y(t) = 0, t < 0) \cup (y(t) = \Delta r, t \ge 0)\} \tag{B3.16}$$

Process dynamics

Figure B3.6 shows an initial improvement in the *dOM* as K_p increases up to around $K_p = 3$. The dominant open-loop dynamics are responsible for this behaviour. In general, however, the dynamic operability measure decreases with increasing values of K_p and τ_p. The closed-loop performance explains this trend.

Figure B3.7 shows the expected negative effect of time delay on the achievable dynamic operability. Dead time affects the control performance more at smaller setpoint changes but it produces larger variations of f_{op} in the opposite direction. As a result, the negative effect of time delay on the *dOM* becomes slightly more pronounced at larger setpoint changes.

Input constraints

Input variables are always constrained in a real plant. Some of these constraints, called *soft constraints*, are imposed on the process based on quality considerations. In contrast, other constraints, called *hard constraints*, are critical to the process because they are related to the security of personnel and equipment. Two types of constraints are considered here:

1. The input variable u may be limited by upper and lower bounds, that is, $u_{min} \leq u \leq u_{max}$
2. The rate of change of u may be limited as well, that is, $|\Delta u| = |u(k) - u(k\text{-}1)| \leq \delta\Delta t$, $0 < \delta < 1$, with Δt as the time step.

The achievable operable fraction decreases continuously for smaller ranges of *AIS*(*t*), for any setpoint change, but the trend for the control performance is the opposite. If the available set of inputs is large enough and there are no rate-of-change constraints, the control performance (and consequently *dOM*) improves at larger setpoint changes (**Figure B3.8**). Larger ranges of *AIS*(*t*) deteriorate the performance since larger changes in the manipulated variable are allowed. If the available input is too small (dashed line in this example), this can severely affect the dynamic operability of the process for setpoint changes larger than 0.5 and less than -0.5.

Figure B3.9 shows that smaller rate-of-change constraints are more restrictive in the range of setpoint changes (-1, -0.5) and (0.5, 1). At smaller changes of the setpoint, the controller performance is more greatly affected by the faster and larger changes of the MV. This causes a similar effect on the *dOM*.

Controller

At smaller values of λ, the closed-loop response to changes in r is faster, causing larger changes in the MV. The deterioration of the control performance by aggressive controller tuning is reflected in a significant drop of the *dOM* for λ = 0.5 at small changes of the setpoint. When the controller tuning is slow enough ($\lambda = 2$), no significant changes in the dynamic operability measure are observed (**Figure B3.10**).

As we stated earlier, this approach is not limited to a certain control system configuration or type of controller. The following example discusses the effect of two controller algorithms, PI and IMC, on the *dOM*. A brief description of the IMC algorithm (Morari and Zafiriou, 1989) is given in the Appendix.

Figure B3.11 shows that rate-of-change constraints of the input variable ($|\Delta u| \leq 0.1\Delta t$) are more restrictive when a PI controller is used (lines with markers). When no rate-of-change constraints are imposed (lines without markers), the IMC controller responds faster than the PI controller, for the same value of λ. The larger variations in the MV for the IMC controller cause a larger drop of *dOM* at smaller changes of r.

Disturbance Rejection

The dynamic Available Input and Expected Disturbance Spaces are specified as follows

$$\begin{aligned} AIS(t) &= \{u(t) | -1 \leq u(t) \leq 1, \forall t\} \\ EDS(t) &= \{d(t) | \left(d(t) = 0, t < 0\right) \cup \left(d(t) = \Delta d, t \geq 0\right)\} \end{aligned} \tag{B3.17}$$

Process dynamics

It is known that higher values of K_p and smaller values of τ_p contribute to a better rejection of disturbances. **Figure B3.12** clearly shows this trend for the dynamic operability of a process, for the regulatory case.

Figure B3.13 shows a clear trend of the effect of time delay on the *dOM*. Since dead time in the presence of a disturbance affects the achievable operable fraction more severely at larger magnitudes of the perturbation, the deterioration of *dOM* for the regulatory case is also more pronounced for higher values of Δd.

Input constraints

The same types of constraints considered for the servo case are investigated in the following examples.

In general, larger disturbances are more difficult to reject in the presence of input constraints. When the constraints of the magnitude of *AIS*(t) or the rate of change of *AIS*(t) are too narrow (i.e., dashed line in **Figure B3.14** and dotted line in **Figure B3.15**), the system will react too slowly in the face of a disturbance and a significant deterioration of the control performance and the achievable dynamic operability is to be expected.

Controller

If the objective of the control system is to reject disturbances, a faster response (smaller λ) is desirable to improve the control performance. This heuristic is observed in relation to the *dOM* (**Figure B3.16**).

It can be seen that PI and IMC controllers behave similarly in the regulatory case for almost the entire range of *EDS*(t) (lines with no markers in **Figure B3.17**). The IMC controller shows, however, a higher robustness in the presence of rate-of-change constraints of the input variable ($|\Delta u| \leq 0.1\Delta t$). Consequently, the *dOM* for this controller is also higher (thin line with markers in **Figure B3.17**).

3. Dynamic Operability of a MIMO System

In this section we shall expand the dynamic operability approach to multi-input multi-output (MIMO) systems. The analysis of such systems may be an extremely difficult undertaking, even for low dimensional systems. Therefore, it is common to consider a MIMO system as a sum of n SISO systems. This assumption simplifies enormously the analysis of n dimensional systems. The simplifying assumption is rigorously valid for linear systems. However, it also can be applied to nonlinear systems, provided the nonlinearity is not significant, which is the case in many real systems.

The state-space representation of a nonlinear system is

$$\begin{aligned} \dot{\mathbf{x}} &= \mathbf{F}(\mathbf{x},\mathbf{u},\mathbf{d}) \\ \mathbf{y} &= \mathbf{G}(\mathbf{x},\mathbf{u},\mathbf{d}) \end{aligned} \qquad \text{(B3.18)}$$

where $\mathbf{x}$, $\mathbf{y}$, $\mathbf{u}$ and $\mathbf{d}$ are vectors of states, outputs, inputs and disturbances.

Linear lumped models are represented in the time-domain by

$$\begin{aligned} \dot{\mathbf{x}} &= \mathbf{Ax} + \mathbf{Bu} + \mathbf{\Gamma d} \\ \mathbf{y} &= \mathbf{Cx} + \mathbf{D_u u} + \mathbf{D_d d} \end{aligned} \tag{B3.19}$$

where $\mathbf{A}$, $\mathbf{B}$, $\mathbf{\Gamma}$, $\mathbf{C}$, $\mathbf{D_u}$ and $\mathbf{D_d}$ are constant matrices if the system is time invariant (LTI). Alternatively, the model can be represented in the transform-domain by

$$\mathbf{y}(s) = \mathbf{G}(s)\mathbf{u}(s) + \mathbf{G_d}(s)\mathbf{d}(s) \tag{B3.20}$$

If there are m inputs, n outputs and l disturbances, $\mathbf{G}(s)$ is an $n \times m$ matrix, while $\mathbf{G_d}(s)$ is an $n \times l$ matrix.

Dynamic Operating Spaces

We shall limit our analysis to square systems, that is, to systems with equal number of inputs and outputs. The extension of this approach to nonsquare systems should not be difficult. Using the assumption that an n-dimensional MIMO system is composed of n SISO systems, dynamic Input and Desired Output Spaces can be defined for each input, u_j, and output, y_i as the ranges of all values of u_i and y_i as a function of the time, that is

$$AIS_j(t) = \left\{ u_j(t) \middle| \, u_{j,\min} \le u_j(t) \le u_{j,\max}, \forall t \right\} \tag{B3.21}$$

and

$$DOS_i(t) = \left\{ y_i(t) \middle| \, y_{i,\min} \le y_i(t) \le y_{i,\max}, \forall t \right\} \tag{B3.22}$$

For *setpoint tracking* problems ($\boldsymbol{d} = \mathbf{0}$), Achievable Output Spaces, $AOS_{ij}(t)$, can be calculated for each pair $\{y_i - u_j\}$ using the relation $\mathbf{y} = \mathbf{G}(\mathbf{x},\mathbf{u})$, for nonlinear systems, or $\mathbf{y}(\mathrm{s}) = \mathbf{G}(\mathrm{s})\mathbf{u}(\mathrm{s})$, for linear systems.

In *disturbance rejection* problems ($y = \mathbf{0}$), the ranges of expected disturbances are used to define the Expected Disturbance Space:

$$EDS_i(t) = \left\{ d_i(t) \middle| \, d_{i,\min} \le d_i(t) \le d_{i,\max}, \forall t \right\} \tag{B3.23}$$

Desired Input Spaces, $DIS_i(t)$, are calculated for each pair $\{u_i - d_i\}$ with **Eq. (B3.18)** for nonlinear systems, or **Eq. (B3.20)** for linear systems, and solving for u_i:

$$\begin{aligned}&\mathbf{G}(\mathbf{x},\mathbf{u},\mathbf{d}) = \mathbf{0}\\ &\mathbf{u}(s) = [\mathbf{G}(s)]^{-1}[\mathbf{G}_{\mathrm{d}}(s)\mathbf{d}(s)]\end{aligned} \qquad \text{(B3.24a, B3.24b)}$$

The calculation of $[\mathbf{G}(s)]^{-1}$ in **Eq. (B3.24b)** is possible, provided the system has no RHP transmission zeros. Calculating the inverse of a transfer function matrix can be very tedious, but it is a straightforward task when the appropriate software is used, e.g., MATLAB®'s Process Control Toolbox.

Suggested method

The suggested procedure to calculate the dynamic operability measure for a linear, square, MIMO system consists of the following steps.

1.Calculate the Relative Gain, λ_{ij}, for each pair $\{y_i - u_j\}$.

2.Since steady-state interactions are present in a MIMO system, even before closing the control loops (open-loop interactions), it is necessary to take this into account, by calculating the effective gain matrix whose elements are:

$$K_{ij,eff} = \frac{K_{ij}}{\lambda_{ij}} \qquad \text{(B3.25)}$$

3.Calculate the operable fraction, $f_{op}(i)$, for each single loop.

4.For each single loop, calculate the controller parameters (K_c, τ_I), using any tuning method (e.g., λ-tuning).

5.The calculating controller parameters may be too aggressive, when loops are closed. Hence, it is necessary to "detune" the controllers using any detuning method. McAvoy (1981) suggested, for a 2x2 system, the following relationships:

$$K_c^* = \begin{cases}\left(\lambda_{ij} - \sqrt{\lambda_{ij}^2 - \lambda_{ij}}\right)K_c, & \lambda_{ij} > 1.0\\ \left(\lambda_{ij} + \sqrt{|\lambda_{ij}^2 - \lambda_{ij}|}\right)K_c, & \lambda_{ij} < 1.0\end{cases} \qquad \text{(B3.26)}$$

where λ_{ij} is the relative gain relating the jth input and the ith output.

6.Calculate the control performance of each single loop i, η_i, using K_c^*, when all other single loops are *closed*.

7.Calculate the dynamic Operability Measure, *dOM*(i), for each pair $\{y_i - u_j\}$.

For nonlinear systems, steps 1 and 2 are skipped, and the loop interactions can be taken into account if the model is solved using an equation-based approach.

3.1. **Two Input-Two Output Processes**

In this sub-section we show a procedure to calculate the operable fraction for a 2 x 2 system (inside the box in **Figure B3.18**). The corresponding feedback control system for the pairings $\{y_1 - u_1\}$ and $\{y_2 - u_2\}$ is also depicted in **Figure B3.18**.

The transfer function of the open-loop system is

$$\begin{bmatrix} y_1(s) \\ y_2(s) \end{bmatrix} = \begin{bmatrix} g_{11}(s) & g_{12}(s) \\ g_{21}(s) & g_{22}(s) \end{bmatrix} \begin{bmatrix} u_1(s) \\ u_2(s) \end{bmatrix} + \begin{bmatrix} g_{d1}(s) \\ g_{d2}(s) \end{bmatrix} d(s) \qquad \text{(B3.27)}$$

Setpoint tracking

For the servo case we assume that there are no disturbances entering the system ($d = 0$) and it can be seen from **Figure B3.18** or **Eq. B3.27** that each output variable is influenced by both input variables. For example, the total dynamic Achievable Output Space for the output y_1, $AOS_1(t)$, is composed of two sub-spaces, $AOS_{11}(t)$ and $AOS_{12}(t)$, which are the achievable output spaces for each input, u_1 and u_2, respectively. Thus, the operable fraction for the output y_1 is calculated as

$$f_{op}(1)\big|_{d=0} = \frac{\int_0^{t_{ss}} \left[\left(AOS_{11}(t) \cup AOS_{12}(t) \right) \cap DOS_1(t) \right] dt}{\int_0^{t_{ss}} \left[DOS_1(t) \right] dt} \qquad \text{(B3.28)}$$

Similarly, the total dynamic Achievable Output Space for the output y_2, $AOS_2(t)$, is calculated. The same results can be achieved, inverting the steps in the calculation, that is, by calculating first partial operable fractions for each input, and then summing them up.

This can be generalized to an n-dimensional MIMO system. In this case, the total dynamic Achievable Output Space for each output y_i, $AOS_i(t)$, is composed of n sub-spaces, $AOS_{ij}(t)$, each of them calculated mapping u_j onto y_i. For each output y_i we get

$$f_{op}(i)\Big|_{d=0} = \frac{\int_0^{t_{ss}} \left[\left(\bigcup_{j=1}^{n} AOS_{ij}(t) \right) \cap DOS_i(t) \right] dt}{\int_0^{t_{ss}} \left[DOS_i(t) \right] dt} \tag{B3.29}$$

Disturbance rejection

In the regulatory case we want to keep all output variables at their nominal value $(y_i = 0, \forall i)$. Combining **Eqs. B3.24b** and **B3.27**, we get for $\mathbf{u}$:

$$\mathbf{u} = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = -\frac{1}{\Delta} \begin{bmatrix} g_{22} & -g_{12} \\ -g_{21} & g_{11} \end{bmatrix} \begin{bmatrix} g_{d1} \\ g_{d2} \end{bmatrix} d = \frac{d}{\Delta} \begin{bmatrix} g_{12}g_{d2} - g_{22}g_{d1} \\ g_{21}g_{d1} - g_{11}g_{d2} \end{bmatrix} \tag{B3.30}$$

where $\Delta = \det(\mathbf{G}) = g_{11}g_{22} - g_{12}g_{21}$ is the determinant of the process transfer function matrix.

Applying **Eq. B3.5**, the regulatory operable fraction for each input u_i can be then calculated as

$$f_{op}(j)\Big|_{y=0} = \frac{\int_0^{t_{ss}} \left[AIS_j(t) \cap DIS_j(t) \right] dt}{\int_0^{t_{ss}} \left[DIS_j(t) \right] dt} \tag{B3.31}$$

This relationship is also applicable for an n-dimensional MIMO system.

3.2. **Example 2: Distillation Control**

This example, taken from Marlin (2000), demonstrates that in a multiloop control system, the assumption that pairing input-output variables with a relative gain closest to 1.0 gives the best performance is not always valid.

Two configurations are considered. The first (**Figure B3.19a**) uses the reflux flowrate to control the top product composition and the distillate flowrate to control the overhead drum level. In the second (**Figure B3.19b**), these pairings have been interchanged.

The transfer functions of the two configurations are:

Configuration A

$$\begin{bmatrix} x_D \\ x_B \end{bmatrix} = \begin{bmatrix} \dfrac{0.0747e^{-3s}}{12s+1} & \dfrac{-0.0667e^{-2s}}{15s+1} \\ \dfrac{0.1173e^{-3.3s}}{11.75s+1} & \dfrac{-0.1253e^{-2s}}{10.2s+1} \end{bmatrix} \begin{bmatrix} F_R \\ F_V \end{bmatrix} + \begin{bmatrix} \dfrac{0.70e^{-5s}}{14.4s+1} \\ \dfrac{1.3e^{-3s}}{12s+1} \end{bmatrix} x_F \qquad \text{(B3.32a)}$$

Configuration B

$$\begin{bmatrix} x_D \\ x_B \end{bmatrix} = \begin{bmatrix} \dfrac{-0.0747e^{-2s}}{10s+1} & \dfrac{0.008e^{-2s}}{15s+1} \\ \dfrac{-0.1173e^{-2s}}{9s+1} & \dfrac{-0.008e^{-2s}}{3s+1} \end{bmatrix} \begin{bmatrix} F_D \\ F_V \end{bmatrix} + \begin{bmatrix} \dfrac{0.70e^{-5s}}{14.4s+1} \\ \dfrac{1.3e^{-3s}}{12s+1} \end{bmatrix} x_F \qquad \text{(B3.32b)}$$

Figures B3.20a and **B3.20b** show the transient responses for a feed composition disturbance and a setpoint change in the distillate product composition. In order to compare our results with those reported in Marlins textbook, the PI controllers were tuned the same way.

The performances of both design alternatives based on the Integral Absolute Error are given in **Table B3.1**. Our results for dynamic operability of these processes are given in **Table B3.2**.

Table B3.3 shows the total IAE values for both of the considered design configurations, as well as the average values of the dynamic Operability Measures and their factors. It can be seen that configuration A gives the best performance (smaller

IAE) in the regulatory case (Δx_F). However, **Table B3.1** implies that configuration B, whose relative gain is closer to 1.0, should have a higher performance. As Marlin concludes, the best-performing multi-loop control system is not always the system with least transmission interaction, that is, the pairing with the relative gain closest to 1.0. The approach developed in this work also leads to the same conclusion, if we compare the performances or the *dOM* of both designs ($dOM_A > dOM_B$). But our approach gives additional information related to the operability of these processes. The low values of f_{op} (0.45) in the bottom concentration control loop of both designs, for the case of feed composition disturbance, indicate that the specified inputs need to be incremented in order to improve the dynamic operability for good disturbance rejection. By taking the factors involved in the calculation of the performance into account in the analysis, it is possible to find out which factor plays the most important role in these results. For the top composition control loop in the regulatory case, the factor α_A is the key factor, with a value of 0.61 and 0.18 for configurations A and B, respectively. This, in turn, means that the time spent outside the specified bounds was much longer for configuration B than for configuration A. This was most likely caused by too sluggish a tuning of the top concentration controller.

4. **Discussions and Conclusions**

A new approach to assess the dynamic operability of processes was developed. The operating spaces, introduced originally by Vinson (2000) to analyse the steady-state operability, were extended to dynamic systems, then these dynamic operating spaces were used to define operable fractions. Also, a new performance index, which is calculated by considering the contribution of both the manipulated and the controlled variable, was proposed. A new measure of the dynamic operability (*dOM*) is presented by combining the operable fraction for open-loop conditions and the closed-loop performance.

The properties of *dOM* are illustrated with a simple SISO system. A number of factors affecting the dynamic operability are studied, including process dynamics and constraints, as well as control system characteristics. Then, this approach is extended to MIMO systems and an example of its application was presented for the screening of control configuration alternatives in a distillation process. Since this method involves calculating the inverse of a matrix for MIMO systems, this inverse matrix should not contain unstable poles.

Summarizing the results for the SISO system, we can conclude that closed-loop systems in general show higher sensitivity to larger setpoint changes and disturbances, but the dynamic operability of processes (given by the *dOM*) is more severely affected by small changes in the setpoint and larger disturbances.

This approach can be widely applied to different types of process models, including linear and nonlinear processes. Although the emphasis was placed on design problems, it should be also possible to use this approach to analyze the dynamic operability of exiting plants for retrofit purposes, e.g., to analyze the effect of a new equipment on the dynamic operability. Another potential application on a real plant is the analysis of the relationship between dynamic operability and process variability for different control strategies. Real process data can be used directly after pre-treatment as needed (filtering, reconciliation) or they can be used to develop first semi-empirical models. The last alternative is especially useful if the input-output relationship is not known, or to make an estimation of the disturbance model.

It has been shown that the proposed dynamic Operability Measure effectively captures different aspects of the dynamic operability of processes, but additional work is necessary to study other aspects not investigated here. This study should address important questions, such as determining how this measure is affected by model incertitude, and which specific issues need to be taken into account when dealing with real systems, e.g., requirements of process data. Since in many real processes the number of manipulated variables is higher than the controlled variables, it is important to extend this framework to non-square systems. The increasingly growing research field of process optimization is another area to be considered in relation to the dynamic operability. Certainly, an operability index will be really useful only if it helps to find the economically optimal design configuration and/or to achieve the optimal solution for an existing plant. The economic considerations in relation to the dynamic operability of a process are an important subject that remains open.

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Table B3.1: Tuning and performance data for distillation dynamics

		Configuration A	Configuration B
$\lambda_{XD\text{-}FB}$		6.09	
$\lambda_{XD\text{-}FD}$			0.39
K_{cD}		10.4	-9.35
τ_{ID}		9.0	10.0
K_{cB}		-6.8	-68.7
τ_{IB}		6.1	6.7
$\Delta x_F = -0.04$	IAE_{XD}	0.17	0.45
	IAE_{XB}	0.35	0.31
$\Delta r_{xD} = 0.005$	IAE_{XD}	0.35	0.0585
	IAE_{XB}	0.34	0.0456

Table B3.2: Operable fraction, control performance and dynamic operability measure

		Configuration A		Configuration B	
		XD	XB	XD	XB
$\Delta x_F = -0.04$	f_{op}	1.00	0.45	1.00	0.45
	η	0.85	0.70	0.62	0.69
	dOM	0.92	0.56	0.79	0.56
$\Delta r_{xD} = 0.005$	f_{op}	0.92	0.95	0.97	0.88
	η	0.48	0.48	0.64	0.69
	dOM	0.66	0.67	0.79	0.78

Table B3.3: Summary of results for distillation process

		IAE		Dynamic OM	
		A	B	A	B
$\Delta x_F = -0.04$	f_{op}			0.72	0.72
	η	0.52	0.76	0.78	0.66
	dOM			0.74	0.68
$\Delta r_{xD} = 0.005$	f_{op}			0.94	0.92
	η	0.69	0.10	0.48	0.66
	dOM			0.66	0.78

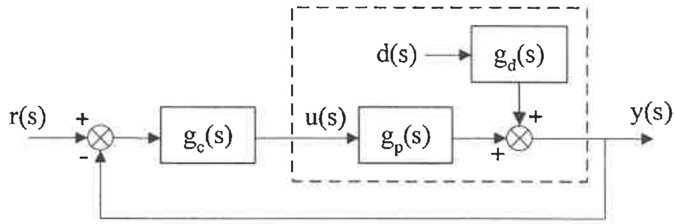

Figure B3.1: Generalized closed-loop control system including a load disturbance

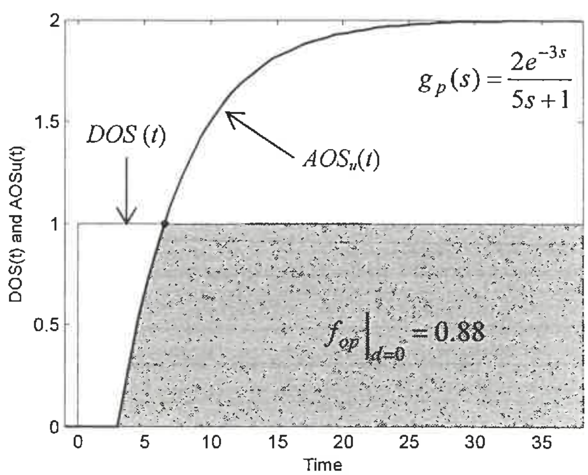

Figure B3.2: Servo operable fraction of a first-order plus time delay process

$(d = 0, |\Delta u| = 1)$

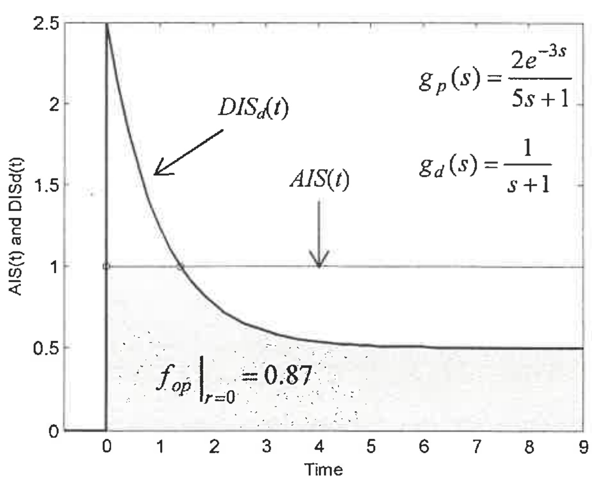

Figure B3.3: Regulatory operable fraction of a first-order plus time delay process

$(r = 0, |d| = 1)$

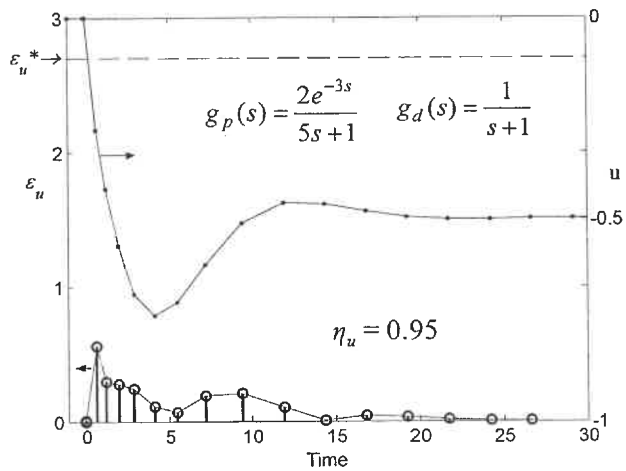

Figure B3.4: Manipulated variable performance for a disturbance rejection problem

($|d| = 1$, PI controller: $K_c = 0.542$, $\tau_I = 6.5$)

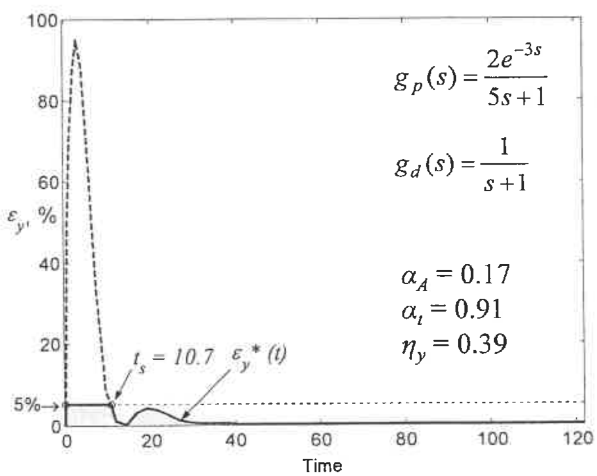

Figure B3.5: Controlled variable performance for the regulatory case

($|d| = 1$, PI controller: $K_c = 0.542$, $\tau_I = 6.5$)

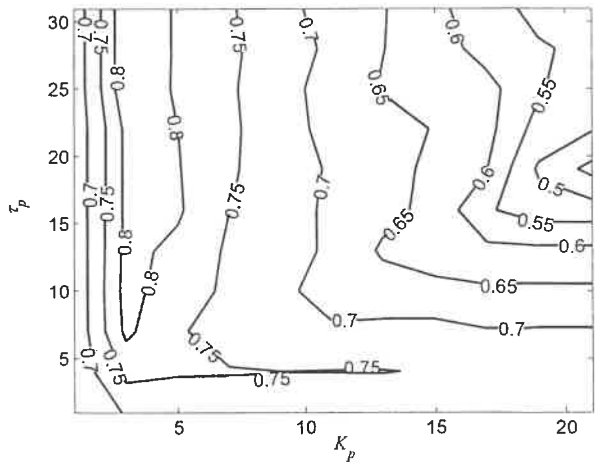

Figure B3.6: Effect of process gain and time constant on the dynamic operability measure (*dOM*) – Servo case. ($t_d = 0$; $\lambda = 1$)

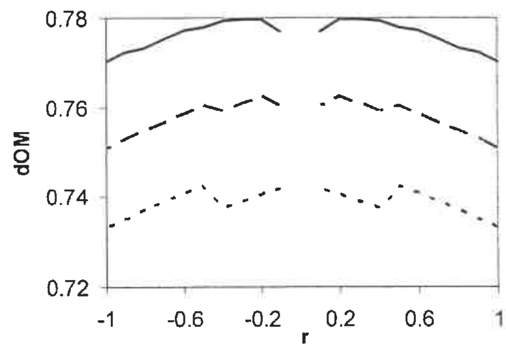

Figure B3.7: Effect of time delay on the dynamic operability measure - Servo case

$K_p = 2$, $\tau_p = 5$, $\lambda = 3$ (solid line: $t_d = 0$, dashed line: $t_d = 1$, dotted line: $t_d = 2$)

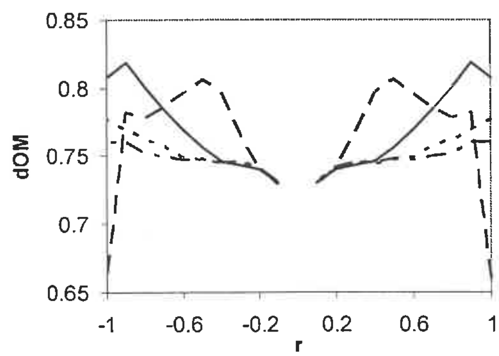

Figure B3.8: Effect of input constraints on the dynamic operability measure - Servo case

$K_p = 2$, $\tau_p = 5$, $t_d = 0$; $\lambda = 1$

(dashed line: $|u| \leq 0.5$, solid line: $|u| \leq 1$, dotted line: $|u| \leq 1.5$, dash-dotted line: $|u| \leq 2$)

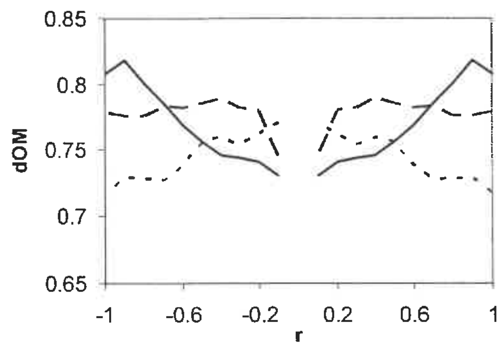

Figure B3.9: Effect of rate-of-change constraints in the input variable on the dynamic operability measure – Servo case

$K_p = 2$, $\tau_p = 5$, $t_d = 0$; $\lambda = 1$

(dotted line: $|\Delta u| \leq 0.1\Delta t$, dashed line: $|\Delta u| \leq 0.5\Delta t$, solid line: No constraints)

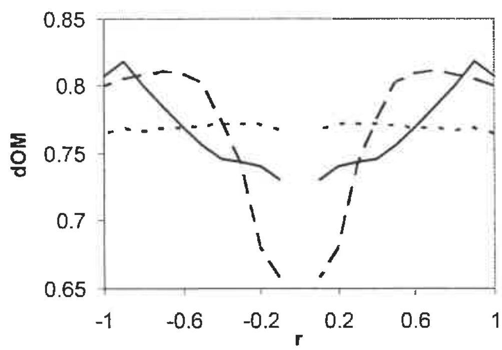

Figure B3.10: Effect of PI controller tuning on the *dOM* - Servo case

$K_p = 2$, $\tau_p = 5$ (dashed line: $\lambda = 0.5$, solid line: $\lambda = 1$, dotted line: $\lambda = 2$)

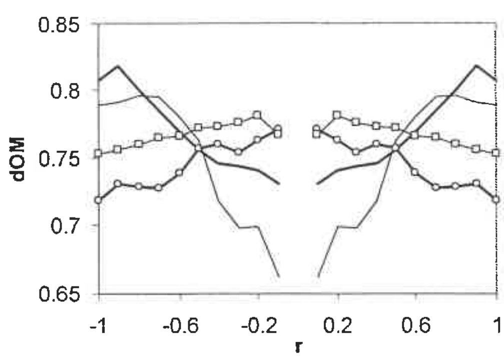

Figure B3.11: Comparison of *dOM* for two different feedback controllers – Servo case

$K_p = 2$, $\tau_p = 5$, $t_d = 0$; $\lambda = 1$ (thick line, no markers: PI; thick line, with markers: PI with constrained input; thin line, no markers: IMC; thin line, with markers: IMC with constrained input)

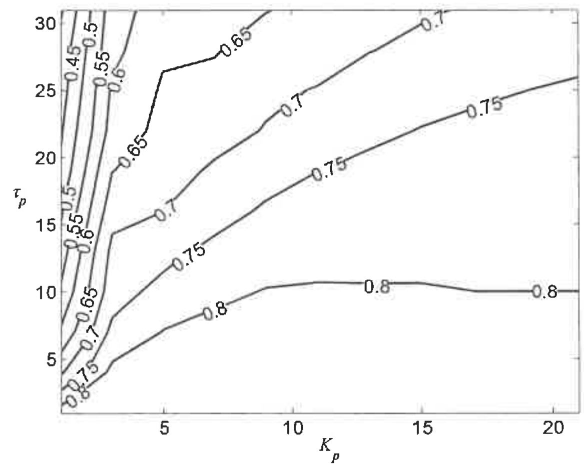

Figure B3.12: Effect of process gain and time constant on the dynamic operability measure (*dOM*) – Regulatory case. ($t_d = 0$; $\lambda = 1$)

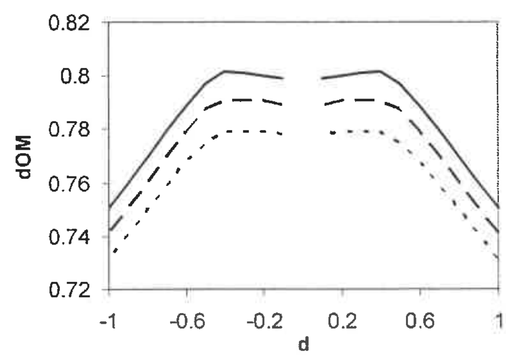

Figure B3.13: Effect of time delay on the dynamic operability measure - Regulatory case

$K_p = 2$, $\tau_p = 5$, $t_d = 0$; $\lambda = 1$ (solid line: $t_d = 0$, dashed line: $t_d = 1$, dotted line: $t_d = 2$)

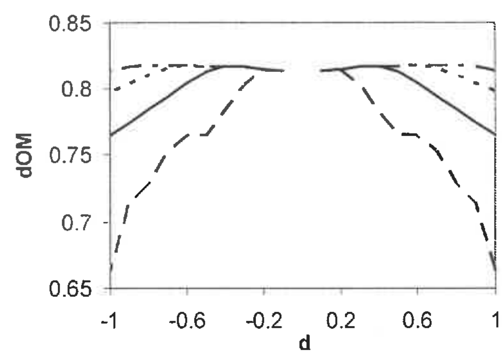

Figure B3.14: Effect of input constraints on the *dOM* - Regulatory case

$K_p = 2$, $\tau_p = 5$, $t_d = 0$; $\lambda = 1$

(dashed line: $|u| \leq 0.5$, solid line: $|u| \leq 1$, dotted line: $|u| \leq 1.5$, dash-dotted line: $|u| \leq 2$)

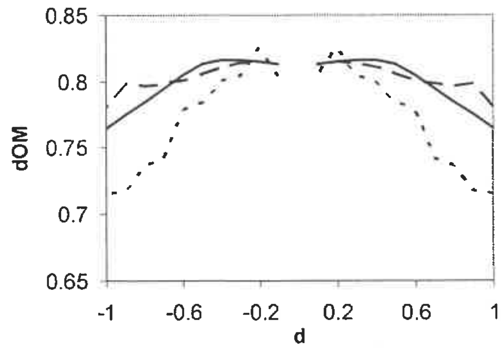

Figure B3.15: Effect of rate-of-change constraints in the input variable on the dynamic operability measure - Regulatory case

$K_p = 2$, $\tau_p = 5$, $t_d = 0$; $\lambda = 1$

(dotted line: $|\Delta u| \leq 0.1\Delta t$, dashed line: $|\Delta u| \leq 0.5\Delta t$, solid line: No constraints)

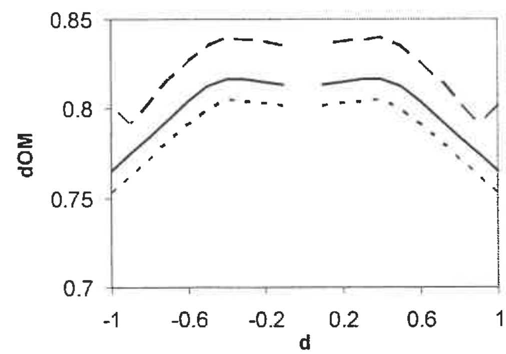

Figure B3.16: Effect of controller tuning on the *dOM* - Regulatory case

$K_p = 2$, $\tau_p = 5$ (dashed line: $\lambda = 0.5$, solid line: $\lambda = 1$, dotted line: $\lambda = 2$)

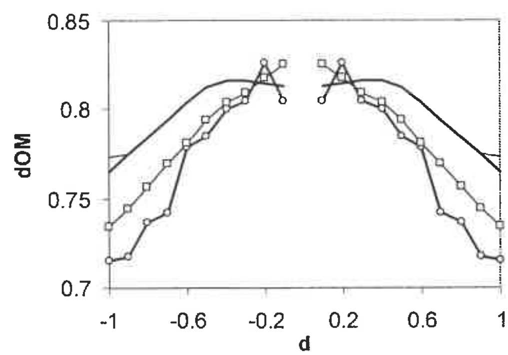

Figure B3.17: Comparison of the *dOM* for two different controllers - Regulatory case

$K_p = 2$, $\tau_p = 5$, $t_d = 0$; $\lambda = 1$ (thick line, no marks: PI; thick line, with marks: PI with constrained input; thin line, no marks: IMC; thin line, with marks: IMC with constrained input)

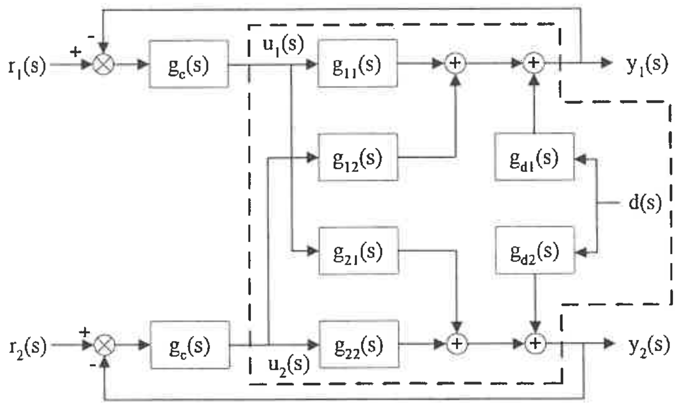

Figure B3.18: Feedback block diagram of a 2 x 2 system

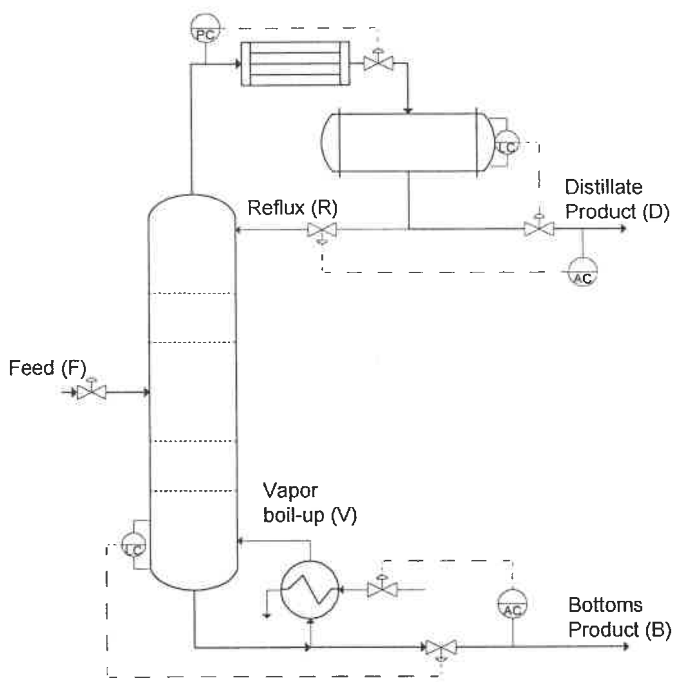

Figure B3.19: Distillation control: Distillate product concentration paired with reflux flowrate

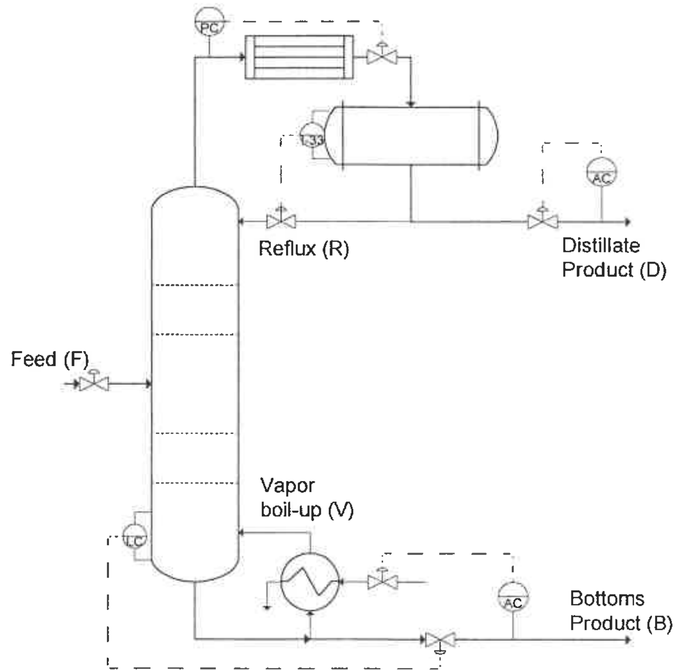

Figure B3.20: Distillation Control: Distillate product concentration paired with distillate product flowrate

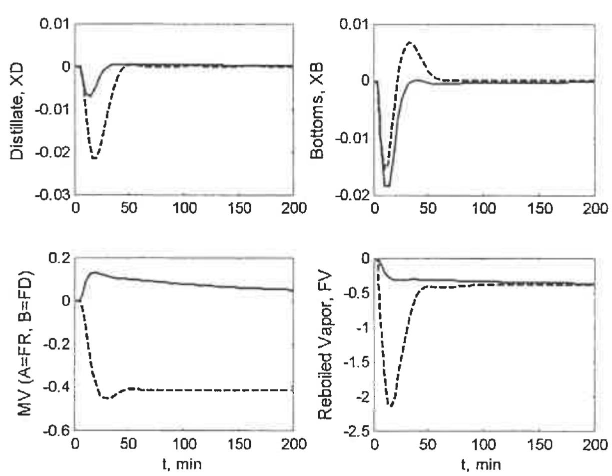

Figure B3.21: Closed loop responses after a feed composition disturbance (Δx_F = -0.04). Left column = distillate product, right column = bottoms product; upper graphs = controlled variables, lower graphs = manipulated variables (FR = Reflux flowrate, FD = Distillate product flowrate); solid lines = Configuration A, dashed lines = Configuration B

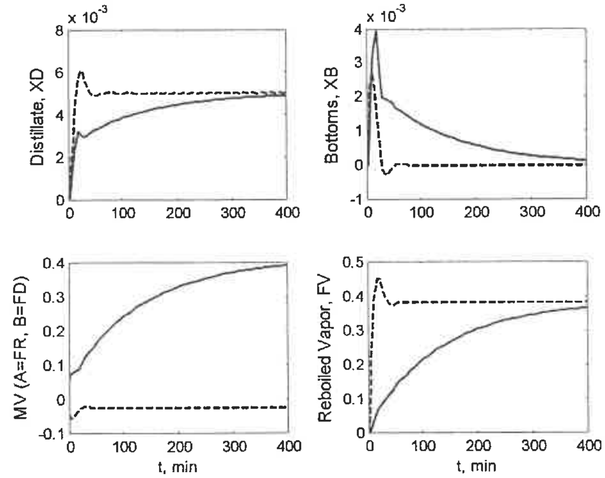

Figure B3.22: Closed loop responses for a set point disturbance

(Δr_{xD} = 0.005): Left column = distillate product, right column = bottoms product; upper graphs = controlled variables, lower graphs = manipulated variables (FR = Reflux flowrate, FD = Distillate product flowrate); solid lines = Configuration A, dashed lines = Configuration B

Appendix I: Internal Model Structure (IMC)

Figure I-1 shows a feedback IMC structure.

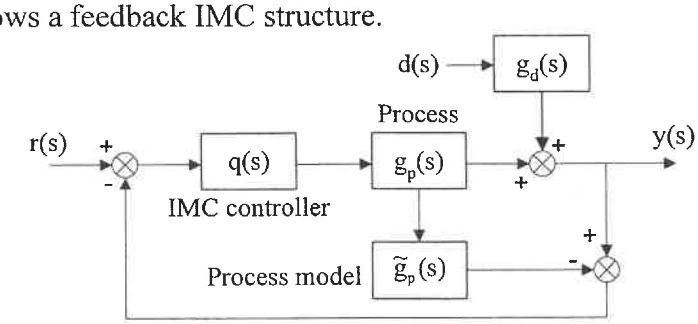

Figure I-1: The internal model control structure

The corresponding closed-loop transfer function is

$$y(s) = \frac{g_p(s)q(s)}{1 + q(s)\left[g_p(s) - \tilde{g}_p(s)\right]} r(s) + \frac{\left[1 - \tilde{g}_p(s)q(s)\right]}{1 + q(s)\left[g_p(s) - \tilde{g}_p(s)\right]} d(s) \tag{I-1}$$

The IMC controller is calculated as

$$q(s) = [\tilde{g}_p^-(s)]^{-1} f(s) \tag{I-2}$$

where $\tilde{g}_p^-(s)$ is the invertible portion of the process model and $f(s)$ a filter that makes $q(s)$ proper. A filter of the form $f(s) = 1/(\lambda s+1)$ was used in the examples of this study.

For the servo case ($d = 0$), and assuming that the model is perfect ($\tilde{g}_p(s) = g_p(s)$) and the process is open-loop stable, the closed-loop relationship becomes

$$y(s) = g_p(s)q(s)r(s) \tag{I-3}$$

Assuming again a perfect model, the closed-loop relationship of a feedback IMC structure (**Eq. I-1**) for the regulatory case ($r = 0$) becomes

$$y(s) = [1 - \tilde{g}_p(s)q(s)]d(s) \tag{I-4}$$

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