Optimization Approaches for Process Engineering Problems Under Uncertainty

by

Marianthi G. Ierapetritou

1995

A thesis submitted for the degree of Doctor of Philosophy of the University of London and for Diploma of Membership of the Imperial College

Department of Chemical Engineering and Chemical Technology
Imperial College of Science, Technology and Medicine
London SW7 2BY, U.K.

BIBL. LONDIN. UNIV.

Abstract

Production systems typically involve significant uncertainty in their operation due to either external or internal sources. The existence of uncertainty transforms conventional deterministic process models to stochastic/parametric problems, the solution of which requires the application of specialized optimization techniques.

The main objective of this thesis is to develop suitable algorithms and numerical techniques for the efficient solution of process engineering problems involving uncertain parameters. Based on modelling issues regarding uncertainty classification (deterministic and stochastic uncertain parameters) and design objectives with respect to uncertainty (fixed degree of flexibility and optimal degree of flexibility), a unified multiperiod/stochastic two-stage optimization formulation is proposed and a decomposition based algorithmic procedure is developed for its efficient solution. The proposed algorithm forms the basis for addressing process design problems, planning and scheduling problems and problems related to behavioural analysis under uncertainty.

For batch plant design problems involving uncertainty in the description of process parameters such as transfer coefficients, kinetic constants, etc., as well as variability of external parameters such as product demand, economic cost data etc., the exploitation of the special structure coupled with the relaxation of feasibility requirement regarding product demands enables the transformation of the stochastic two-stage programming problems to a single optimization model where the structure of the deterministic problem is fully preserved. For the case of continuous size of equipments, an efficient global optimization procedure is proposed, whereas for the case of discrete equipment sizes the algorithm reduces to the solution of a mixed integer linear programming problem. For short term production planning and long-range planning problems including capacity expansion options, the application of the proposed approach results in the optimal production plan (i.e. process utilization levels, purchases and sales of materials) and/or an optimal capacity expansion policy that maximize an expected profit and ensure an optimal level of future feasibility.

Finally, an attempt to address the question of the future "value" of uncertainty is presented based on the concept of value of perfect information. It is shown that the proposed algorithmic developments can be effectively extended to include both the solution of the *here-and-now* and the *wait-and-see* models in order to analyze and integrate the

Acknowledgements

I would like to thank my supervisor Dr. Stratos Pistikopoulos for his excellent guidance throughout my PhD. His strong support and continuous motivation helped me to refine my ideas and was instrumental in accomplishing this work.

I wish to acknowledge the constant challenges of Dr. Costas Pantelides and Professor Chris Floudas that kept me wondering about too many things and provided their own ideas to a challenging subject.

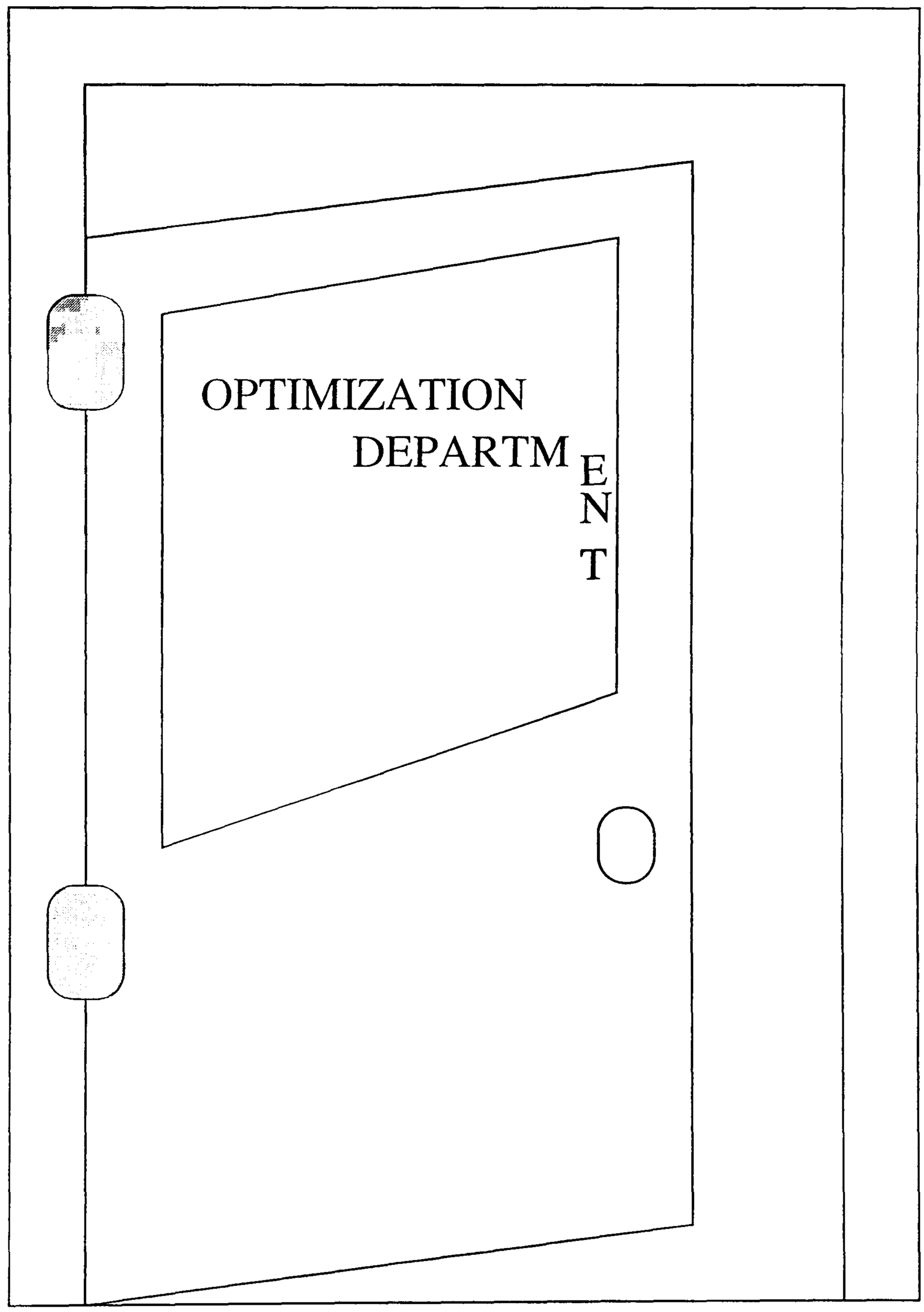
Financial support from the Centre for Process Systems Engineering and the Commission of European Communities under grant ERB CHBI CT93 0484 is gratefully acknowledged.

Among the many friends I made at Imperial College I would like to mention Thomas, Katerina, Lazaros, Vassilis, Benjamin, Mathaios, Joaquin, Stavros and Costas for creating a pleasant working environment and having many interesting discussions.

Special thanks to my friend Yannis Androulakis who although 3000 miles away helped me cope with the difficulties of academic research. He has been a source of strength for me and inspiration for my research.

Last but not least I wish to express my gratitude to my parents Yorgos and Anna, my brother Yannis and my aunt Eleni for their invaluable support and encouragement all these years.

To my parents
Γιώργο και Αννα


OPTIMIZATION
DEPARTMENT

Contents

List of Figures 7

List of Tables 9

1 Introduction and Project Aims 11
- 1.1 Introduction . . . 11
- 1.2 Motivating example . . . 12
  - 1.2.1 Deterministic case . . . 12
  - 1.2.2 Uncertainty consideration . . . 15
- 1.3 Project Aims . . . 21

2 An algorithm for Design Optimization involving Uncertain Parameters 24
- 2.1 Introduction . . . 24
- 2.2 Mathematical Formulation . . . 27
  - 2.2.1 Uncertainty Classification . . . 27
  - 2.2.2 Combined Multiperiod/Stochastic Programming Formulation . . . 28
- 2.3 Proposed Approach . . . 31
  - 2.3.1 Stochastic Uncertain Parameters . . . 31
  - 2.3.2 Extended Algorithmic Procedure . . . 44
- 2.4 Applications . . . 48
- 2.5 Summary . . . 64

3 Batch Plant Design and Operations under Uncertainty 66
- 3.1 Introduction . . . 66
  - 3.1.1 Deterministic Design Problem . . . 67
  - 3.1.2 Batch Plant Design Problem under Uncertainty . . . 67
- 3.2 A Conceptual Mathematical Formulation . . . 69
- 3.3 Continuous equipment sizes . . . 78
- 3.4 Discrete equipment sizes . . . 81
- 3.5 Examples . . . 83
- 3.6 Concluding Remarks . . . 97

4 Production and Capacity Planning Under Uncertainty **100**
4.1 Introduction 100
4.2 Two-stage Stochastic Formulation 104
4.3 Proposed Approach 108
4.4 Examples 112
4.5 Summary 124

5 Value of Perfect Information and Decision Flexibility **125**
5.1 Introduction 125
5.2 Value of Information 129
5.3 An Integrated Strategy for Operational planning under uncertainty 133
5.4 Combined flexibility-VPI metrics 135
5.4.1 Flexibility Index 135
5.4.2 Flexibility-VPI metric 137
5.4.3 Trade-off Curve of VPI vs Flexibility 146
5.4.4 Stochastic flexibility-VPI metric 151
5.5 Examples 153
5.6 Summary 176

6 Conclusions and Future Directions **178**
6.1 Conclusions 178
6.2 Recommendations for Future work 181

Appendix A **192**
A.1 Equivalence of problems (PD5) and (P5′) for fixed design variables 192
A.2 Correction Factors 193
A.2.1 Derivation of the Correction factors 193
A.2.2 Generalized Correction Factors 196
A.3 Sign of multipliers in problem (P5′) 197
A.4 Uncertain prices 198

Appendix B **200**
B.1 Capacity Expansion Consideration 200
B.2 Evaluation of critical value of γ 201
B.3 Feasibility property for Multiproduct Batch plant operating in Single Product Campaign 203
B.3.1 V_j continuous 203
B.3.2 V_j discrete 204
B.4 Steps of Global Optimization Algorithm 205

Appendix C **208**
C.1 Solution of Multi-Parametric LP problems 208
C.2 Evaluation of VPI function 211

List of Figures

1.1 Batch Plant of Motivating Example 12
1.2 Feasible region (in production space) for two alternative batch plants for motivating example 14
1.3 Expected Profit vs Capital Cost - Motivating example 17
1.4 Results from different formulations 19
1.5 Effect of penalty coefficient 19

2.1 Block diagonal structure of problem (2.5) 30
2.2 Design under Uncertainty Algorithm - problem (2.6) 42
2.3 Expanded block diagonal structure of profit optimization subproblem 45
2.4 Unified Algorithm of Combined Multiperiod/stochastic Programming Problem 47
2.5 Feasible region of the initial design - Example 1 50
2.6 Feasible region of the optimal design - Example 1 50
2.7 Convergence of the algorithm - Example 1 51
2.8 Feasible region of the initial design - Example 2 54
2.9 Feasible region of the optimal design - Example 2 55
2.10 Convergence of the algorithm - Example 2 55
2.11 Process superstructure - Example 3 56
2.12 Convergence of the algorithm - Example 3 58
2.13 Process Superstructure - Example 4 59
2.14 Benzene chlorination process 63
2.15 Expected profit vs. Reactor capacity - Example 5 64

3.1 Different demand constraints 72
3.2 Effect of penalty coefficient γ 73
3.3 Global Optimization Algorithm 82
3.4 Batch Plant - Example 1 84
3.5 Feasible region (in production space) for two alternative batch plants - Example 1 86
3.6 Expected Profit vs Capital Cost - Example 1 87
3.7 Results from different formulations - Example 1 89
3.8 Batch Plant - Example 3 90

3.9 Plant layout for Example 5 92
3.10 Gantt charts for different demand values - Example 6 95
3.11 Plant superstructure of Example 7 96
3.12 State task network of Example 7 96
3.13 Gantt charts for different demand values (Example 7) 98
3.14 One schedule for different demand values (Example 7) 99

4.1 Production Network 104
4.2 Quadrature Points inside Feasible Region 110
4.3 New planning under uncertainty Algorithm 113
4.4 Chemical Complex - Example 1 114
4.5 Progress of bounds - Example 1 117
4.6 Chemical Complex - Example 2 117
4.7 Progress of bounds - Example 2 120
4.8 Refinery input and output schematic - Example 3 121
4.9 Progress of bounds - Example 3 123

5.1 Flexibility index proposed by Saboo et al. 126
5.2 Flexibility index proposed by Swaney and Grossmann 126
5.3 Stochastic Flexibility Index 127
5.4 Wait-and-see and here-and-now models 131
5.5 Value of information 131
5.6 Expected value of information 132
5.7 A strategy for Operational Planning under Uncertainty 134
5.8 Material flow 141
5.9 Feasible region of plan (5,4) 143
5.10 Feasibility function of plan (5,4) 143
5.11 VPI function of plan (5,4) 145
5.12 Combined Flexibility-VPI metric vs. VIP target 151
5.13 Trade-off Curves - Example 1 156
5.14 Combined metrics - Example 1 159
5.15 Chemical Complex - Example 2 160
5.16 Trade-off Curves - Example 2 164
5.17 Expected profit for different demand levels - Example 3 165
5.18 Stochastic Flexibility versus demand - Example 3 166
5.19 Expected profit vs Stochastic Flexibility - Example 3 166
5.20 Value of Information versus demand - Example 3 167
5.21 Expected Value of Information vs. first-stage decision - Example 3 167
5.22 Expected Profit vs. Capacity expansion - Example 4 169
5.23 EVPI vs. Capacity expansion - Example 4 169
5.24 Value of Perfect Information for different structures - Example 5 171
5.25 EVPI vs. SF - Example 5 173
5.26 Expected profit vs. Reactor capacity - Example 6 174
5.27 Wait-and-see and Here-and now profit vs. purity - Example 6 174
5.28 Value of Perfect Information for Optimal Plant - Example 6 175
5.29 VPI results for a different plant - Example 6 176
5.30 VPI results for a different plant in example 6 - the consideration of a second distillation column 177

List of Tables

1.1 Data for motivating example 13
1.2 Uncertain demand consideration 15
1.3 Data for uncertain demands 16
1.4 Results of motivating example 19
1.5 Uncertain process parameters 20
1.6 Results of motivating example 21

2.1 Bounds for θ_2 at $\theta_1^{q_1}$ of initial design 49
2.2 Optimal revenue at the quadrature points (5x5 grid) 49
2.3 Bounds for θ_2 at $\theta_1^{q_1}$ of optimal design 50
2.4 Results for different number of quadrature points - Example 1 52
2.5 Data for uncertain parameters - Example 1 52
2.6 Data for uncertain parameters - Example 2 53
2.7 Convergence of the algorithm from different starting points - Example 2 . . 56
2.8 Data for Example 3 57
2.9 Mathematical model of Example 3 57
2.10 Data for uncertain parameters - Example 3 58
2.11 Data for Example 4 62
2.12 Data for uncertain parameters - Example 4 62

3.1 Stochastic Models for Multiproduct Batch Plant Design 75
3.2 Stochastic Models for Multipurpose Batch Plant Design 76
3.3 Stochastic Models for Multipurpose Batch Plant Design 77
3.4 Data for example 1 84
3.5 Uncertain demand consideration - Example 1 87
3.6 Results of example 1 88
3.7 Uncertain process parameters - Example 1 88
3.8 Results of Global Optimization Algorithm - Example 2 90
3.9 Data for Example 3 91
3.10 Data for Example 5 93
3.11 Horizon Constraints for Example 5 93
3.12 Recipe Data for Example 6 94
3.13 Equipment Data for Example 6 95

3.14 Equipment Data for Example 7 97

4.1 Bounds for θ_2 at θ_1^{q1} for the initial plan 115
4.2 Optimal profit at the quadrature points (5x5 grid) 115
4.3 Bounds for θ_2 at θ_1^{q1} for the optimal plan 116
4.4 Data for uncertain parameters for Example 2 119
4.5 Convergence of the algorithm for different starting points - example 2 . . . 120
4.6 Data for the refinery crudes and products 121
4.7 Bounds for θ_2 at θ_1^{q1} for the initial plan 122
4.8 Optimal profit at the quadrature points 122
4.9 Bounds for θ_2 at θ_1^{q1} for the initial plan 123

5.1 Flexibility-VPI analysis results for plan (5,4) 146
5.2 F1 expressions as a function of uncertain parameters - Example 1 156
5.3 First-period plan - Example 1 156
5.4 F2 expressions as a function of uncertain parameters - Example 1 157
5.5 VPI expressions as a function of uncertain parameters - Example 1 158
5.6 Results for Flexibility-VPI analysis - Example 1 158
5.7 Combined metrics - Example 1 159
5.8 Economic data of chemical processes - Example 2 160
5.9 Economic data of materials for the first time period for Example 2 161
5.10 Economic data of materials for the second time period - Example 2 162
5.11 F1 expressions as a function of uncertain parameters - Example 2 162
5.12 Two alternative first period plans - Example 2 163
5.13 F2 expressions as a function of θ for plan I - Example 2 163
5.14 F2 expressions as a function of θ for plan II - Example 2 164
5.15 Results of Flexibility-VPI analysis - Example 2 164
5.16 Convergence of the Algorithm - Example 5 170
5.17 Summary of results - Example 5 171

B.1 Solutions of the Relaxed Dual Problems - Example 2 206
B.2 Results of GOP application - Example 2 207

Chapter 1

Introduction and Project Aims

1.1. Introduction

In chemical process design the goal is to obtain a plant design that is optimal with respect to cost and performance. However, plant performance can be characterized by several criteria. Since design specifications such as product demands, reaction constraints, inlet temperature, ambient conditions will normally vary during the operation of the process, a "good" design must not only be economically optimal but also capable to operate in a steady-state mode for a range of uncertain conditions that may be encountered during plant operation. Consequently, flexibility objectives should be also considered together with economic criteria at the design stage if the goal of producing an effective design is to be achieved.

Moreover, due to the competitive environment, any industrial sector should realize the importance of managing efficiently the available resources and accomplishing production requirements and product specifications by developing flexible planning strategies as well as identifying and accessing the potential benefits of exploring new resources (in conjunction with the existing ones) and manufacturing new products.

In the last two decades the problem of developing quantitative techniques for planning the selection of new processes, the expansion of existing ones and the production of chemicals under changing conditions has received an increasing attention in the open literature. Two main directions can be distinguished:

- the design of flexible process plants

- the planning and scheduling of existing processes under an uncertain environment.

It is well understood that the consideration of uncertainty aspects transforms the problem from a deterministic one, where standard methods of mathematical programming can be applied, to a stochastic problem where special techniques are required. It is the main objective of this work to develop suitable mathematical tools enabling feasibility objectives to be systematically embodied in process optimization for design and operations; a second objective is then to analyze the sensitivity of optimal decision making to uncertainty.

An example of a multiproduct batch plant design will be first presented to motivate the need for such tools and introduce some key ideas, which provide the basis for the developments outlined in this thesis.

1.2. Motivating example

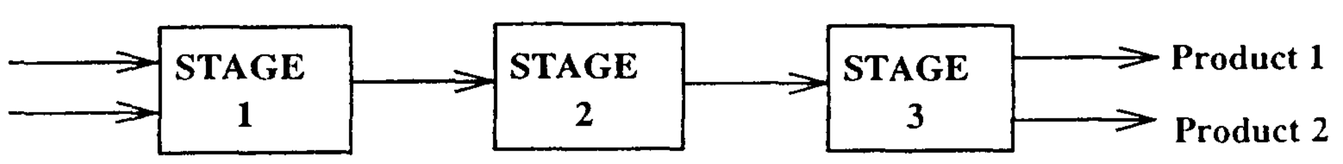


Figure 1.1: Batch Plant of Motivating Example

Consider a simplified multiproduct batch plant, shown in Figure 1.1 where two products are produced in three stages with a single equipment per stage (a single product campaign is assumed, with no intermediate storage). Data regarding size factors, processing times and equipment cost are given in Table 1.1.

1.2.1. Deterministic case

Assume that there is a demand for products 1 and 2 of 200 and 100 units, respectively. Consider a specific design d_1 with (V_1, V_2, V_3)=(1618,2428,3237). Then:

$$B_1 = \min\{\frac{V_1}{S_{11}}, \frac{V_2}{S_{12}}, \frac{V_3}{S_{13}}\} = 809$$

$$B_2 = \min\{\frac{V_1}{S_{21}}, \frac{V_2}{S_{22}}, \frac{V_3}{S_{23}}\} = 405$$

with which the horizon constraint

$$\frac{Q_1}{B_1}T_{L1} + \frac{Q_2}{B_2}T_{L2} \leq H$$

(a) Size factors				(b) Processing times			
	Stage				Stage		
Product	1	2	3	Product	1	2	3
1	2	3	4	1	8	20	8
2	4	6	3	2	16	4	4
(c) Investment cost coefficients				(d) Prices of products			
Stage j	α_j		β_j	Product	P_i		
1	5		0.6	1	5.5		
2	5		0.6	2	7.0		
3	5		0.6				
Time horizon H=8							

Table 1.1: Data for motivating example

is violated for Q_1=200, Q_2=100 (see also Figure 1.2); thus, the suggested design cannot fully accommodate the demands for products 1 and 2. However, with the cost data of Table 1.1, the solution of the following problem:

$$\max_{Q_1,Q_2} P_1Q_1 + P_2Q_2$$

$$\text{subject to:} \quad \frac{Q_1}{809}20 + \frac{Q_2}{405}16 \leq 8$$
$$Q_1 \leq D_1$$
$$Q_2 \leq D_2$$

results in the production of $Q_1^* = 200, Q_2^* = 77$ units of products with a revenue of 1641 units; i.e. by relaxing the requirement to produce at least as much as demanded, a better utilization of the available "recourses" was achieved. The "loss" incurred due to the plant incapability to meet product demands can be approximated by the following penalty term:

$$(P_1D_1 + P_2D_2) - (P_1Q_1^* + P_2Q_2^*) = 1800 - 1641 = 159 \text{ units}$$

If a different design $d_2 = (V_1, V_2, V_3)$=(1907,2861,3815) is considered with larger volumes (and thus larger investment cost), as shown in Figure 1.2, it can accommodate both demands with maximum revenue of 1800 units (zero losses); therefore, there are trade-offs between investment cost and revenues (including "losses" due to design insufficiency) which have to be explored in the design of multiproduct batch plants. This suggests that a more appropriate formulation for the design problem is as follows:

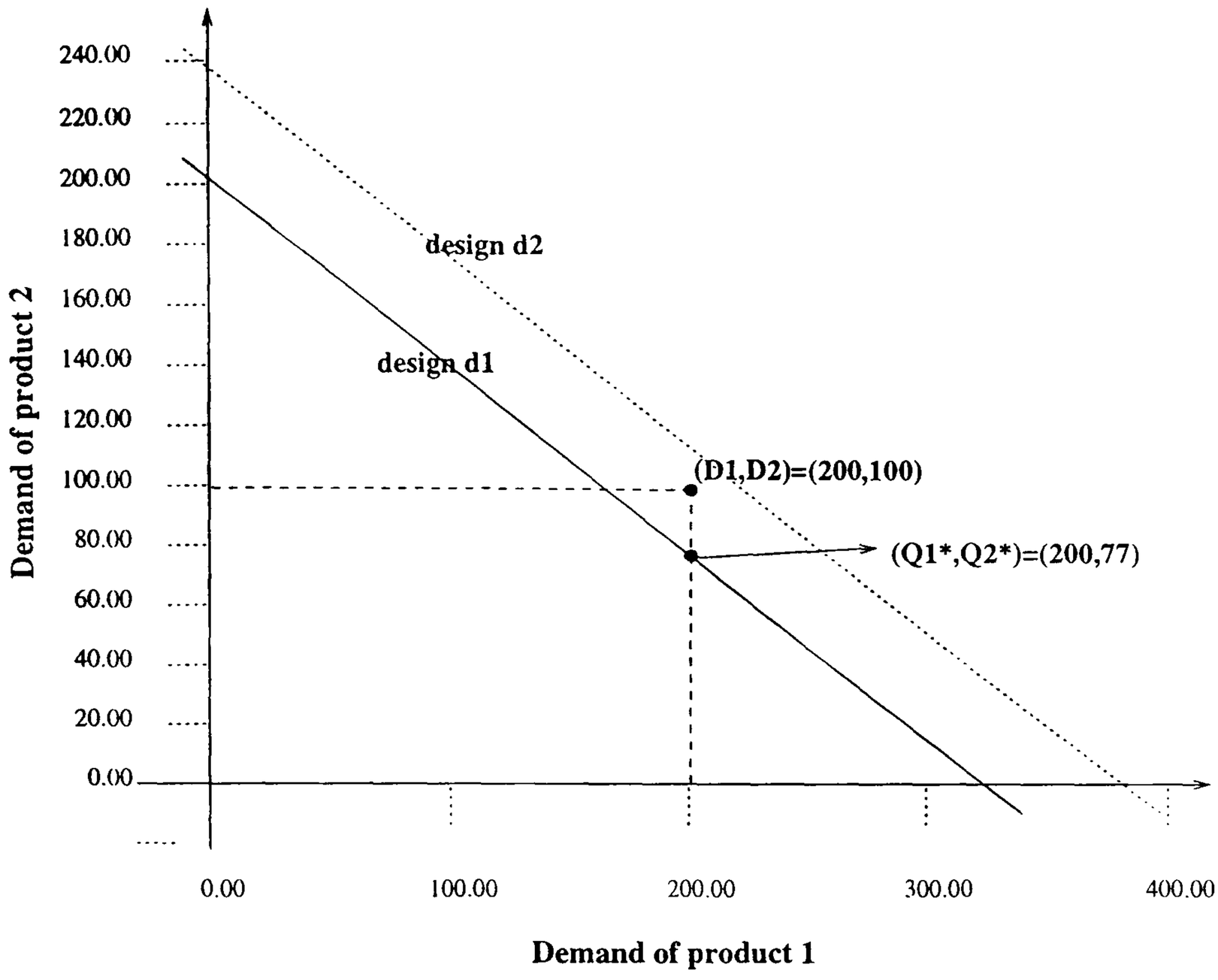


Figure 1.2: Feasible region (in production space) for two alternative batch plants for motivating example

Problem (1.1)

$$\max_{V_j,Q_1,Q_2} \{\underbrace{P_1Q_1 + P_2Q_2}_{Revenue} - \underbrace{\sum_{j=1}^{3}\alpha_j V_j^{\beta_j}}_{Investment\ Cost} - \underbrace{\gamma[(P_1D_1 + P_2D_2) - (P_1Q_1 + P_2Q_2)]}_{Penalty\ term}\}$$

subject to:

$$\left.\begin{array}{l} \dfrac{Q_1}{B_1}T_{L1} + \dfrac{Q_2}{B_2}T_{L2} \leq H \end{array}\right\} \begin{array}{l}\text{Horizon}\\ \text{Constraint}\end{array}$$

$$\left.\begin{array}{l} Q_1 \leq D_1 \\ Q_2 \leq D_2 \end{array}\right\} \text{Demand Constraints}$$

$$\left.\begin{array}{l} B_1 = \min\{\dfrac{V_1}{S_{11}}, \dfrac{V_2}{S_{21}}, \dfrac{V_3}{S_{31}}\} \\ B_2 = \min\{\dfrac{V_1}{S_{21}}, \dfrac{V_2}{S_{22}}, \dfrac{V_3}{S_{32}}\} \end{array}\right\} \begin{array}{l}\text{Batch size}\\ \text{Constraints}\end{array}$$

$$\left.\begin{array}{l} T_{L1} = \max\{t_{11}, t_{12}, t_{13}\} \\ T_{L2} = \max\{t_{21}, t_{22}, t_{23}\} \end{array}\right\} \text{Cycle time Constraints}$$

where γ is a penalty coefficient used to monitor the effect of penalty term. The above formulation features an explicit penalty term to account for the possibility of not fully meeting the demand constraints.

Table 1.2 summarizes the results of problem (1.1) for different values of demand (D_1, D_2). It is clear that the requirement of accommodating larger demand values leads to plants with increased revenues, albeit involving larger units and thus requiring more investment cost. If one considers the fact that typically product demands can only be forecasted (rather than known with certainty), a natural question that arises is what is a suitable formulation when uncertainty is involved.

Demand		Design			Revenue	Investment	Expected	Flexibility
D_1	D_2	V_1	V_2	V_3		Cost	Profit	
240	140	2400	3600	4500	2300	1992	1421.3	1.0
200	100	1800	2700	3600	1800	1702	1489.7	0.5
160	60	1280	1920	2560	1300	1387	1092.5	0.0

Table 1.2: Uncertain demand consideration

1.2.2. Uncertainty consideration

Consider the case of product demands given by some probability distributional form, for example a normal probability density function as shown in Table 1.3. Then, the formulation in problem (1.1) must be modified to account for:

(i) the uncertainty in product demand realizations

(ii) proper estimation of the plant profitability in this case.

One way to achieve this is shown in the following formulation in which the expected profit is evaluated within the corresponding feasible region of the batch plant design.

Uncertain demand	Distribution function	Mean value	Positive deviation	Negative deviation
θ_1	N(200, 10)	200	40	40
θ_2	N(100, 10)	100	40	40

Table 1.3: Data for uncertain demands

Problem (1.2)

$$\max_{V_j} -\sum_{j=1}^{3}\alpha_j V_j^{\beta_j} + E_{\theta\in R(V)}\max_{Q_1,Q_2}\{P_1Q_1+P_2Q_2\}$$
$$-\gamma E_{\theta\in R(V)}\{\max_{Q_1,Q_2}[(P_1D_1+P_2D_2)-(P_1Q_1+P_2Q_2)]\}$$

subject to:

$$\frac{Q_1}{B_1}T_{L1}+\frac{Q_2}{B_2}T_{L2}\le H$$
$$B_1=\min\{\frac{V_1}{S_{11}},\frac{V_2}{S_{21}},\frac{V_3}{S_{31}}\}$$
$$B_2=\min\{\frac{V_1}{S_{21}},\frac{V_2}{S_{22}},\frac{V_3}{S_{32}}\}$$
$$T_{L1}=\max\{t_{11},t_{12},t_{13}\}$$
$$T_{L2}=\max\{t_{21},t_{22},t_{23}\}$$
$$Q_1\le D_1$$
$$Q_2\le D_2$$
$$D_1=\theta_1$$
$$D_2=\theta_2$$
$$\theta_1^L\le\theta_1\le\theta_1^U,\ \theta_1=(\theta_1^N,\sigma_1);\ \theta_1^{U,L}=\theta_1^N\pm 4\sigma_1$$
$$\theta_2^L\le\theta_2\le\theta_2^U,\ \theta_2=(\theta_2^N,\sigma_2);\ \theta_2^{U,L}=\theta_2^N\pm 4\sigma_2$$
$$V_j^{LO}\le V_j\le V_j^{UP}$$
$$\theta_1,\theta_2\in R(V_j)\ \gamma\ge 0$$
$$R(V)=\{\theta_i\mid\forall\,\theta_i\in R(V_j)\ \exists\,Q_i\ :\text{model constraints are satisfied}\}$$

The solution of problem (1.2) with the data of Tables 1.1 and 1.3 and $\gamma = 0$ results in a plant (V_1, V_2, V_3)=(1800,2700,3600) with the maximum expected profit equal to 1489 units at the optimal level of flexibility (0.5) (see Figure 1.3).

The following points, however, should be emphasized here. First, regarding the consideration of uncertain product demand: the following alternatives can in fact be distinguished reflecting the decision maker's (DM) own preference and judgement and the available information of demand variation:

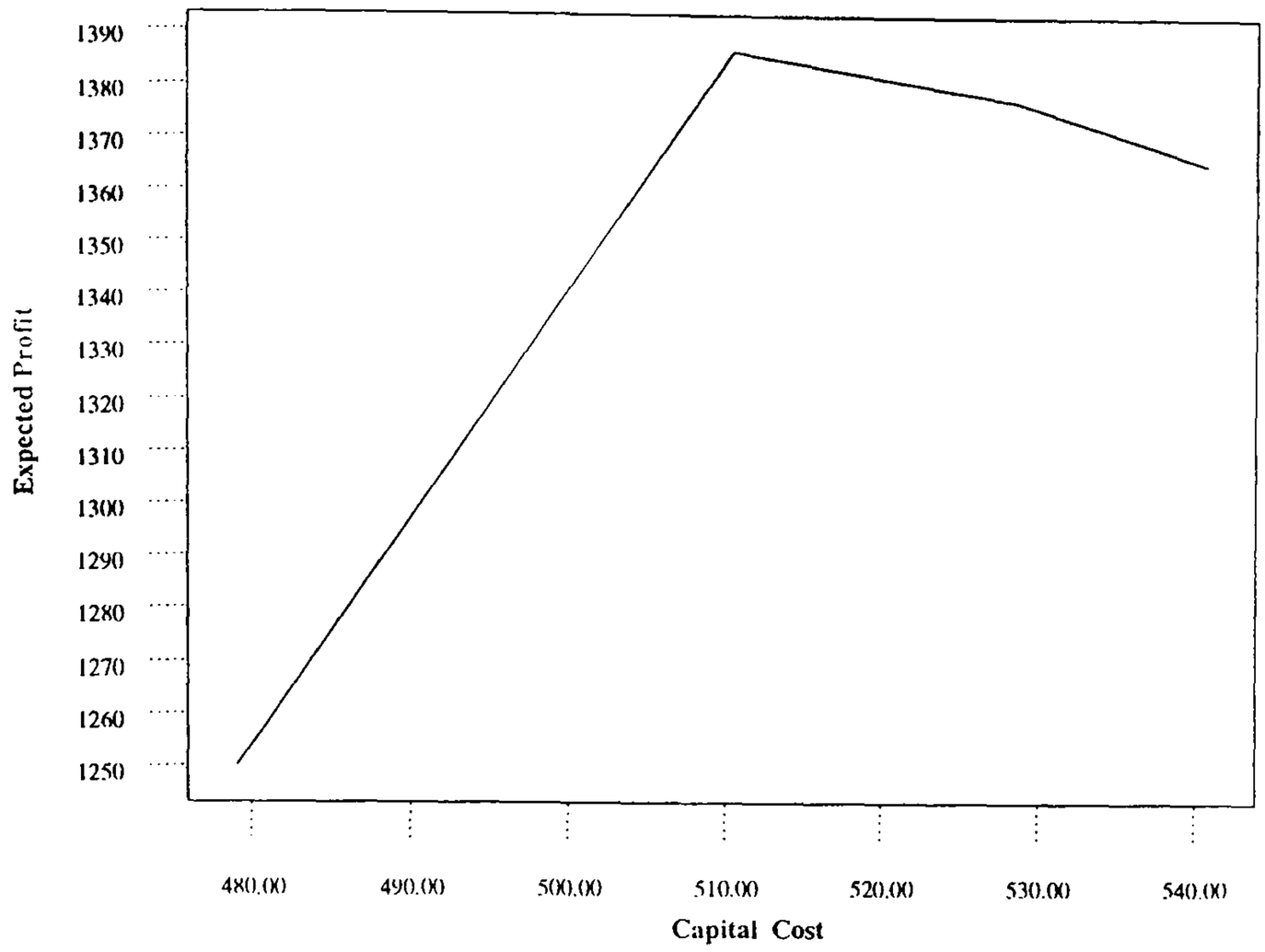


Figure 1.3: Expected Profit vs Capital Cost - Motivating example

- $Q_i = \theta_i, \theta_i \in R(V_j)$ representing the decision maker's choice to meet always the demand within plant's feasible region

- $Q_i = \theta_i, \theta_i \in T(\theta_i)$ (scenario approach) representing the DM requirement of demand satisfaction within a specified range $T(\theta_i)$ defined by appropriate lower and upper bounds

- $Q_i \leq \theta_i, \theta_i \in R(V_j)$ representing the DM attitude for the best possible production

Second, the introduction of uncertainty transforms the deterministic problem (1.1) to the stochastic one (1.2) which cannot be directly solved, since it involves the evaluation of the expected profit within the unknown,at the design stage,feasible region of the plant; moreover, it requires an integration (expectation evaluation) over an optimization problem (maximization of revenue with respect to production variables). The basic ideas to overcome the above difficulties as well as the steps of the proposed algorithmic procedure are presented in chapter 2.

Furthermore, for the case of multiproduct/multipurpose batch plant design formulation with uncertain demands, it will be shown in chapter 3 that the relaxation of the demand constraints allows for the evaluation of the objective function within the region depicted by the bounds of the uncertain demands (thus, avoiding an integration over an unknown at the design stage feasible region) leading to the following formulation:

Problem (1.3)

$$\max_{V_j, Q_i^q} \{-\delta \sum_{j=1}^{3} \alpha_j V_j^{\beta_j}) + \sum_{q=1}^{Q} w^q J^q \{P_1 Q_1^q + P_2 Q_2^q\}$$
$$-\gamma \sum_{q=1}^{Q} w^q J^q \{\sum_{i=1}^{2} p_i \theta_i^q - \sum_{i=1}^{2} p_i Q_i^q\}\}$$

subject to: $B_i = \min_j \{\frac{V_j}{S_{ij}}\}$; $i = 1, 2,\ j = 1, .., 3$

$$T_{Li} = \max_j \{t_{ij}\}\ ;\ i = 1, 2,\ j = 1, .., 3$$

$$\frac{Q_1^q}{B_1} T_{L1} + \frac{Q_2^q}{B_2} T_{L2} \leq H\ ;\ i = 1, 2,\ q = 1, .., Q$$

$$Q_i^q \leq \theta_i^q\ ;\ i = 1, 2,\ q = 1, .., Q$$

$$V_j^{LO} \leq V_j \leq V_j^{UP}$$
$$\theta_i^q \in T(\theta),\ \gamma \geq 0$$

In order to compute different problem formulations regarding the strategy for dealing with uncertain demands, problem (1.3) is solved for the other two cases, i.e. strict demand satisfaction and scenario-based approach, respectively. The results are graphically shown in Figure 1.4, where it can be seen that the optimal plants obtained P2: (V_1, V_2, V_3) = (2128,3194, 4260) and P3:(V_1, V_2, V_3) = (2295,3442,4500) respectively, are more conservative with larger equipments per stage, yet they can accommodate larger demand variations (larger feasible regions) compared to plant P1 (the solution of problem 1.3). However, the proposed formulation in (1.3), based on the relaxation of demand constraint and the incorporation of a penalty term in the objective function to penalize the partial order fulfillment, results in a proper balance of the above trade-offs. As shown in Table 1.4 and Figure 1.5, as the value of penalty coefficient γ increases (corresponding to more severe penalization) we move towards the direction of complete demand satisfaction which coincides with the result of scenario-based approach; i.e. the formulation in (1.3) is general enough to capture the various strategies regarding the uncertainty in demand. These issues are discussed in detail in Chapter 3.

Note however, that although the special structure of batch problem enables the transformation of problem (1.2) to a deterministic equivalent (1.3), the consideration of uncertain demands introduces extra non-convexities of the following form (since in this

γ values	Optimal Plant (V_1, V_2, V_3)
0	(1800, 2700,3600)
1	(1908, 2862,3815)
10	(1972, 2958,3954)
100	(2080, 3120,4160)
1000	(2090,3135,4180)
10000	(2198,3297,4395)
100000	(2295, 3442, 4500)

Table 1.4: Results of motivating example

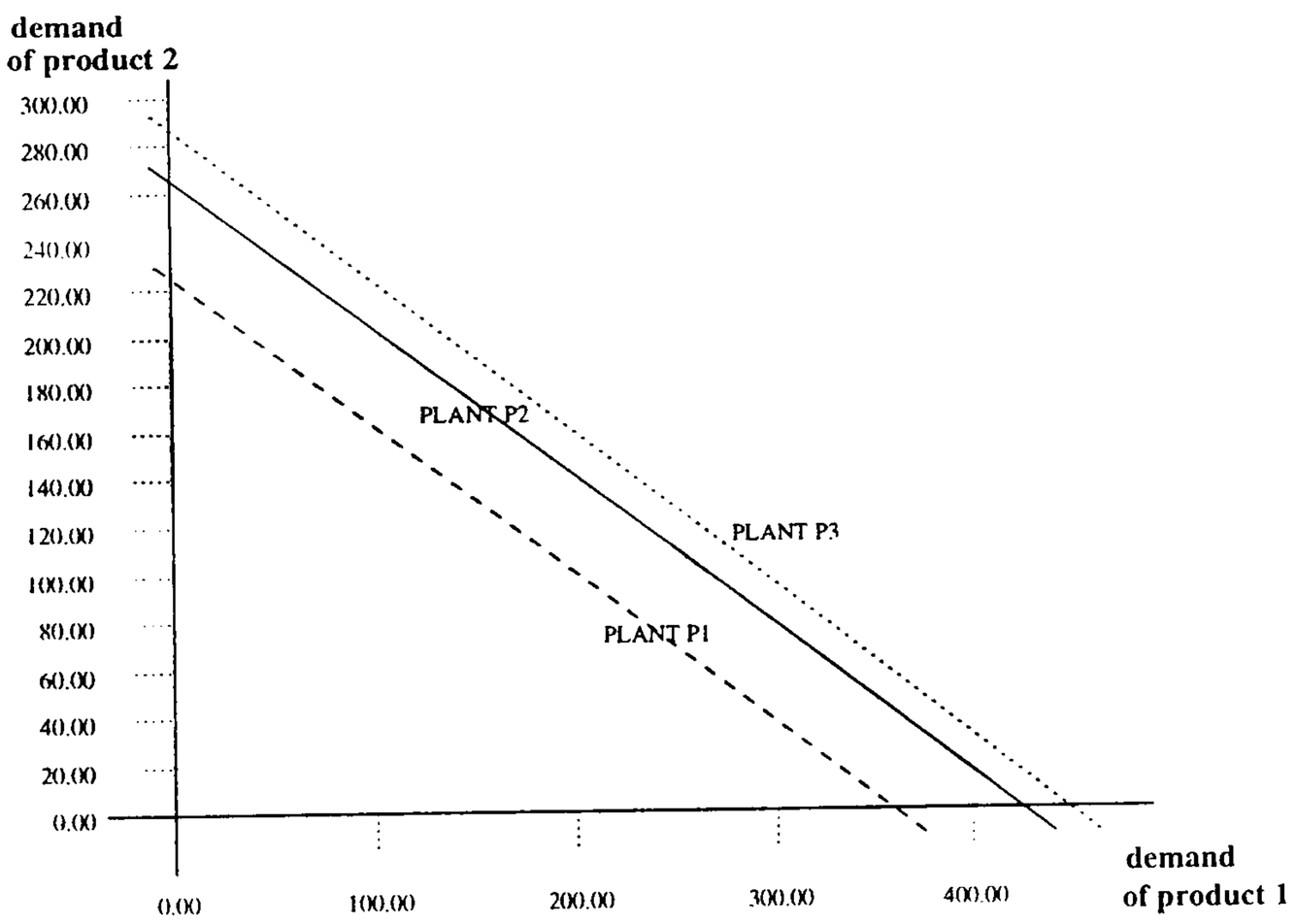


Figure 1.4: Results from different formulations

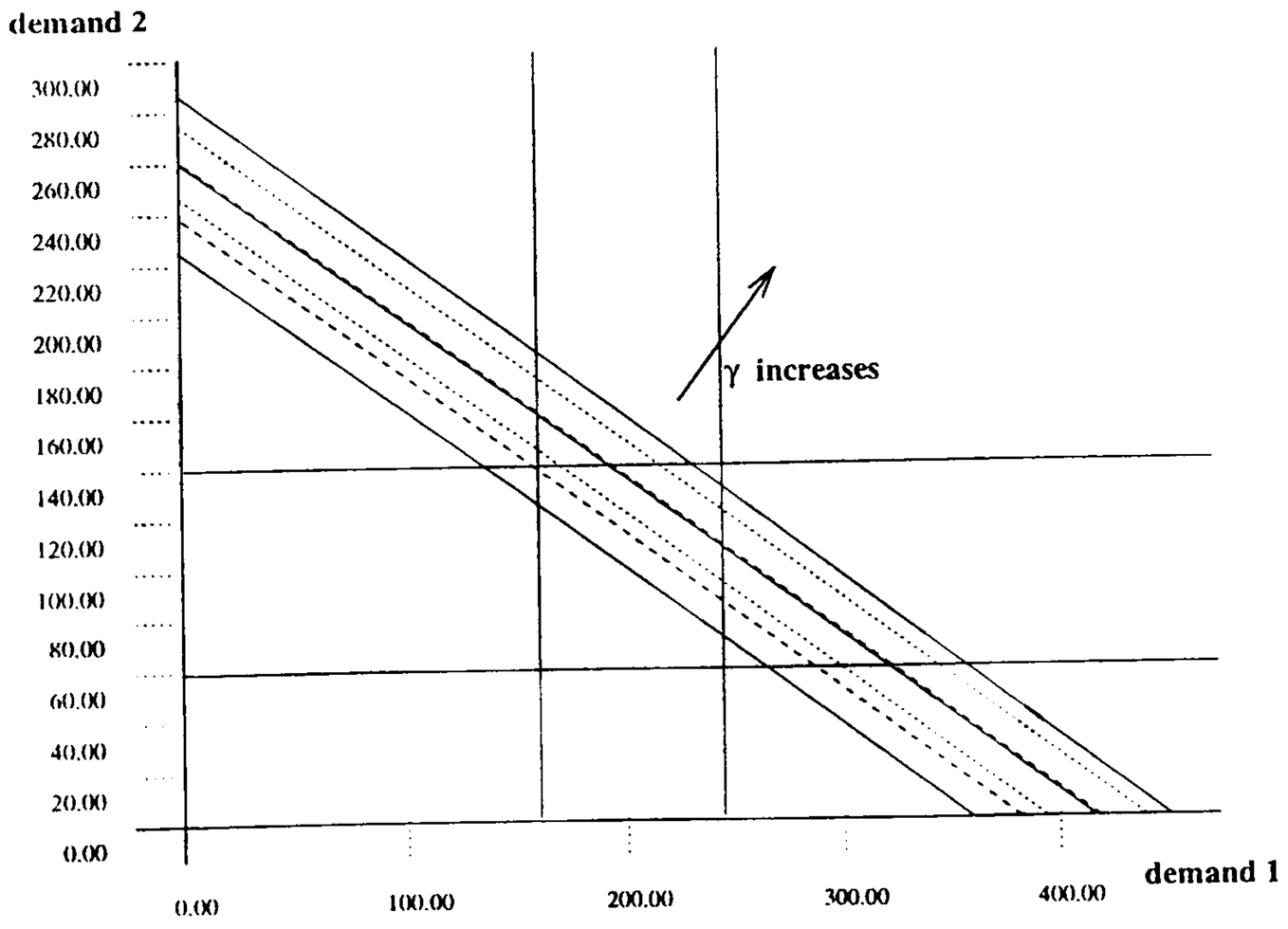


Figure 1.5: Effect of penalty coefficient

case the plant production (Q_1, Q_2) are optimization variables):

$$Q_1 \exp(-b_1) T_{L1} + Q_2 \exp(-b_2) T_{L2} \leq H,$$

$$B_1 = \exp(b_1), B_2 = \exp(b_2)$$

which cannot be convexified through the exponential transformations (as used in Kocis and Grossmann, 1988 for the deterministic model). Consequently, there is need for global optimization solution approaches as also discussed in chapter 3.

Periods	Product	t_{ij}			S_{ij}		
		Stage 1	Stage 2	Stage 3	Stage 1	Stage 2	Stage 3
1	1	7	19	7	2.5	3.5	4.5
	2	15	3	3	4.5	6.5	3.5
2	1	9	21	9	1.5	2.5	3.5
	2	17	5	5	3.5	5.5	2.5
3	1	8	20	8	2	3	4
	2	16	4	4	4	6	3

Table 1.5: Uncertain process parameters

Another important issue with respect to uncertainty consideration involves the modelling of the other uncertain parameters that appear in the problem formulation, such as processing times and size factors. As discussed in chapter 2, one can distinguish between "stochastic" uncertain parameters such as product demands and "deterministic" uncertainties such as size factors which can be considered via a multiperiod-based approach (see for example Table 1.5.

Finally, more involved scheduling models concerning plant operation in multiple product campaign with zero wait (ZW) or unlimited intermediate storage (UIS) can be also considered, where the possibility of having more than one units per stage also incorporated. The results are summarized in Table 1.6. Notice that the consideration of more detailed scheduling models leads to more optimistic plants due to better utilization of processing equipments. Also as far as the uncertainty aspects are concerned, in order to achieve the best utilization of the proposed plant, schedule patterns can be considered to change with respect to demand realization. These ideas are discussed in detail in chapter 3.

Stochastic or deterministic uncertainty models only represent an approximation of the true model-plant mismatch, the potential variability and disturbances of the true

Single Product Campaign			Multiple Product Campaign			
			Zero Wait (ZW)		Unlimited Intermediate Storage (No Clean-up times)	
Stage J	No of units	Equipment Size	No of units	Equipment Size	No of units	Equipment Size
J1	3	1200	3	800	2	1200
J2	3	1200	3	800	2	1200
J3	3	1200	3	800	2	1200
Capital Cost:		7900	6300		5300	
Expected Profit:		1.2E+3	1.4E+3		1.5E+3	

Table 1.6: Results of motivating example

process. The selection of a realistic type and extent of uncertainty representation requires a careful balance between robustness and conservativeness regarding the extent of possible variations: this may be achieved through an estimation of the "price" of uncertainty in the sense of knowing whether further information about future parameter realization is indeed worth acquiring - the sensitivity of decision making to uncertainty. Chapter 5 introduces the Value of Perfect Information (VPI), used in the field of behaviour analysis. as a measure for the "price" of uncertainty and tool to analyze the effect of uncertainty in decision making analysis.

1.3. Project Aims

As motivated by the example problem in section 1.2, due to lack of accurate process models and the variability of environmental data (external parameters), it becomes indispensable to establish systematic ways to incorporate flexibility objectives at the decision stage as well as to identify and analyze the effects of uncertainty within the decision making process. It is the focal point of this research to develop suitable algorithms and numerical techniques for the efficient solution of process engineering problems involving uncertain parameters. In particular, the main objectives of this thesis have been:

1. The consideration of uncertain parameters in a unified stochastic programming formulation.

2. The development of an efficient solution procedure for the resulting problem formulation.

3. The exploitation of the batch plant problem special structure and characteristics.

4. The derivation of flexible production plans and capacity expansion policies.

5. The introduction of quantitative measures for the "price" of the uncertainty and the analysis of the effects of uncertainty in decision making process.

For the first objective, in chapter 2 modelling issues regarding uncertainty classification (deterministic and stochastic uncertain parameters) and design objectives with respect to uncertainty (fixed degree of flexibility and optimal degree of flexibility) are discussed and a unified multiperiod/stochastic two-stage optimization formulation is proposed for the determination of the optimal design with the maximum expected profit at an optimal level of flexibility.

For the second objective, in chapter 2 a decomposition based algorithmic procedure is developed for the efficient solution of the resulting formulation based on the following ideas:

(i) the multiple integral for the expected profit evaluation over the feasible region of the plant is approximated through a Gaussian quadrature formula with **unknown** quadrature points

(ii) the unknown quadrature points are determined as part of the optimization procedure through the solution of a sequence of feasibility subproblems

(iii) a modified (Generalized) Benders Decomposition is employed where the first-stage design variables are selected as "complicating variables".

The key feature of the proposed approach is that it allows for the economic optimization and design feasibility to be performed simultaneously without requiring an "a priori" discretization of the uncertainty. The proposed algorithm forms the basis for addressing process design problems, planning and scheduling problems and problems related to behavioural analysis under uncertainty.

For the third objective, in chapter 3 we deal with the problem of batch plant design involving uncertainty in the description of process parameters such as transfer coefficients, kinetic constants, etc., as well as variations of external parameters such as product demands, economic cost data etc. The exploitation of the special problem structure coupled with the relaxation of feasibility requirement regarding product demands enables the transformation of the stochastic two-stage programming problems to a single optimization model where the structure of the deterministic problem is fully preserved.

For the case of continuous equipment sizes, an efficient global optimization procedure is proposed, whereas for the case of discrete equipment sizes the algorithm reduces to the solution of a mixed integer linear programming problem.

For the fourth objective, in chapter 4 the problem of short-term production planning and long-range planning problems including capacity expansion options is addressed. The application of the proposed approach in this case results in the optimal production plan (i.e. process utilization levels, purchases and sales of materials) and/or an optimal capacity expansion policy that maximize an expected profit and ensures an optimal level of future feasibility.

Finally, for the last objective, in chapter 5 the question of the future "value" of uncertainty is addressed based on the concept of value of perfect information. It is shown that the proposed algorithmic developments in chapters 2,3 and 4 can be effectively extended to include both the solution of the *here-and-now* and the *wait-and-see* models in order to quantify the VPI and use this information to analyze and integrate the decision maker's attitude towards risk.

Chapter 2

An Algorithm for Design Optimization involving Uncertain Parameters

A decomposition-based approach is presented in this chapter for the optimization of design/planning models involving stochastic parameters. The problem is formulated as a two-stage stochastic programming problem where the objective is to determine the design that maximizes an expected profit while simultaneously measuring design feasibility. A number of example problems illustrate the steps of the proposed algorithmic procedure.

2.1. Introduction

In the design of chemical plants, there are usually a number of technical and commercial parameters which are subject to significant uncertainty. These uncertainties can correspond to variations either in internal process parameters such as transfer coefficients, reaction constants, efficiencies and physical properties or external parameters such as quality of the feedstreams, product demand, environmental conditions and economic cost data. Therefore, it is clear that some degree of flexibility must be introduced at the design stage to ensure that the plant will be able to handle uncertain parameters during operation.

A general representation of the problem of design under uncertainty is of the following form:

Problem (2.1)

$$\max_{d,z,x} P(d,z,x,\theta)$$

$$s.t.\ h(d,z,x,\theta) = 0$$

$$g(d,z,x,\theta) \leq 0$$

$$x \in X,\ z \in Z,\ d \in D$$

where d,z,x are the vectors of design, control and state variables, respectively; θ is the vector of uncertain parameters which is assumed to follow a continuous distribution function J(θ); P(d,z,x,θ)is a profit function; h(d,z,x,θ), g(d,z,x,θ) are the vectors of model equality and inequality constraints, respectively. Qualitatively, the design optimization problem (2.1) corresponds to selecting the vector of design variables d so as to maximize a profit function while ensuring an optimal level of feasible operation (see section 2.2 for a formal mathematical representation).

Several approaches have been reported in the literature addressing the problem of design under uncertainty in (2.1); extensive overviews are given by Grossmann et al. (1983), and recently by Grossmann and Straub (1991). Three main directions can be broadly distinguished: (i) deterministic, (ii) probabilistic and (iii) flexibility analysis.

The basic idea of the deterministic-based approaches is to transform the original (semi-infinite in θ) optimization problem to a deterministic approximation, by specifying in advance a number of uncertain parameter realizations in a sequence of time periods or stages. The optimal design problem can then be approximated by the following "multi-period" program:

Problem (2.2)

$$\max_{d,z^i,x^i} \sum_{i=1}^{N} P(d,z^i,x^i,\theta^i)$$

$$\left.\begin{array}{r} s.t.\ h^i(d,z^i,x^i,\theta^i)=0 \\ g^i(d,z^i,x^i,\theta^i)\le 0 \end{array}\right\} \quad i=1,..,N$$

Problem (2.2) exhibits a block diagonal structure which can be exploited for computational efficiency (Grigoriadis, 1971; Grossmann and Sargent, 1978; Grossmann and Halemane, 1982). More recently, Paules and Floudas (1992) have developed a nested solution procedure combining Generalized Benders Decomposition (GBD) and Outer Approximation (OA) algorithms to address the problem of multiperiod design of heat integrated distillation sequences. Varvarezos et al. (1992) have also developed an Outer Approximation based decomposition method for the solution of multiperiod design optimization problems. Although the formulation in (2.2) represents an important class of design problems, its major limitation as an approximation to problem (2.1) (due to its discretization nature) is how to select a finite number of points in θ-space so as to ensure feasible and optimal operation inside "some" continuous range of interest. In an attempt

to circumvent the above limitation, Halemane and Grossmann (1983) proposed a successive iterative scheme between a feasibility subproblem and a multiperiod design step (i.e. problem P′). In spite of the computational evidence, which has shown that commonly only a few iterations need be performed to achieve feasibility (see for example Floudas and Grossmann, 1987, Papalexandri and Pistikopoulos, 1993), the iterative procedure still remains an approximation to the direct solution of problem (2.1).

The most common probabilistic approach is the two-stage stochastic programming (among others Birge, 1982, 1985, Reinhart and Rippin, 1986, Pai and Hughes, 1987, Wallace, 1987, Birge and Wets, 1989, Dantzig, 1989), which is based on selecting here-and-now (first-stage) an optimal vector of the design variables d while seeking for operational feasibility/flexibility in the second-stage; i.e. the control variables z can be manipulated with the prevailing values of θ. Here, the question of feasibility has been addressed, either via the additional consideration of penalty functions or through the postulation of a finite number of discrete θ points and the transformation to a deterministic "multiperiod" problem, similar to the one in (2.2) (see for example Walkup and Wets, 1967). Pereira and Pinto (1991) presented a method based on the application of dynamic programming where the second stage objective function is approximated by a piecewise linear function.

Flexibility analysis has also evolved as a tool for designing under uncertainty. Pistikopoulos and Grossmann (1988a) have formulated the linear problem of redesigning existing plants in order to achieve a specified degree of flexibility at minimum cost as a single LP/MILP problem where flexibility constraints have been explicitly included. By exploiting the properties of linear constraints, they have derived analytical expressions of the flexibility index of Swaney and Grossmann, (1985) in terms of the changes of the design variables for each active set (see also Grossmann and Floudas, 1987). In their later work (1988b), the same authors have proposed an iterative procedure to obtain the optimal degree of flexibility for linear systems by constructing the trade-off curves relating retrofit cost and expected revenue to flexibility. Their approach consists of two phases: first the trade-off curve of retrofit cost and flexibility is determined; from this curve a number of redesigns are obtained for which at the second phase the expected revenue is evaluated by employing a modified Cartesian integration method. Their work has also been extended to nonlinear constraints (Pistikopoulos and Grossmann, 1989a,b). As far as flexibility metrics are concerned, except of the (deterministic) flexibility index (Swaney and Grossmann, 1985), other metrics which have been appeared in the literature for the quantification of

the system ability to cope with future uncertainties include: the Resilience Index (Saboo et al. 1983), the design "reliability" index (Kubic and Stein, 1988) and the Stochastic Flexibility Index (Pistikopoulos and Mazzuchi, 1990, Straub and Grossmann, 1990).

The approaches discussed above share a number of common characteristics and limitations. Most of them address a special case of problem (2.1); i.e. the design optimization with fixed degree of feasibility/flexibility (Grossmann and Straub, 1991), where the designer either specifies a finite number or more generally a bounded range of operating conditions and specifications that the design must satisfy. However, the main goal of the design optimization in (2.1) is to determine the design with an optimal degree of feasibility; i.e. a design that maximizes an expected profit. As will be shown later in this chapter, the direct consideration of problem (2.1) is not straightforward since it requires a measure for plant feasibility/flexibility. Pistikopoulos and Grossmann (1988b, 1989b) deal with the solution of problem (2.1), but in their approximation economic optimization and design feasibility are performed separately.

This chapter presents a unified approach for process optimization problems involving stochastic parameters. Modelling issues regarding process uncertainty and its sources are first examined in detail in an attempt to classify the types of uncertainty that can be treated as "deterministic" and those which have to be treated in a "stochastic" manner. Issues related to permanent feasibility and optimal flexibility are also addressed. A comprehensive combined multiperiod/stochastic optimization formulation is then presented together with a decomposition based algorithm for its solution. Finally, a few examples are presented to illustrate the analytical steps of the proposed approach and its potential for addressing different types of process engineering problems under uncertainty.

2.2. Mathematical Formulation

2.2.1. Uncertainty Classification

Based on the nature of the source of uncertainty in a process, described by the mathematical model in (2.1), a suitable classification can be proposed as follows:

(i) Model-inherent uncertainty; it includes kinetic constants, physical properties, transfer coefficients. Information regarding this type of uncertainty is usually obtained from experimental and pilot-plant data; a typical description form can be supplied

via either a range of possible realizations or some approximation of a probability distribution function.

(ii) Process-inherent uncertainty; flowrate and temperature variations, stream quality fluctuations and so on fall into this category which is usually described by a probability distributional form obtained from (on-line) measurements. Any desired range of these uncertain parameter realizations could in principle be achieved through the implementation of a suitable control scheme.

(iii) External uncertainty, including feedstream availability, product demands, prices and environmental conditions. Forecasting techniques based on historical data, customers orders and market indicators are usually used to obtain approximate ranges of uncertainty realizations or a probability distributional form.

(iv) Discrete uncertainty, for equipment availability and other random discrete events. A (discrete) probability distribution function can commonly be obtained from available data and manufacturer's specifications. Discrete uncertainty is not considered in this thesis (see Thomaidis and Pistikopoulos, 1994).

Dealing with the above types of uncertainty in process design and operations gives rise to two distinct design objectives, reflecting the decision maker's own preference and judgement as well as the available information regarding the uncertainty itself (i.e. model of the uncertainty). These design objectives have usually been referred as:

- (**D1**)-design for fixed degree of flexibility, if the aim is to achieve an optimal design/plan while ensuring feasible operation for any possible realization of the uncertain parameters

- (**D2**)-design with optimal degree of flexibility, if the trade-offs between economics and flexibility are properly explored.

Note that, from a modelling point of view, all types of uncertainty could in principle be included in either design objective. Therefore, in general, some uncertain parameters will be associated with design objective **D1**, i.e. considered as "deterministic", while some others will be treated in a "stochastic" manner (linked to design objective **D2**).

2.2.2. Combined Multiperiod/Stochastic Programming Formulation

Based on the classification of the uncertainty and design objectives presented in the previous section, and by partitioning the vector of uncertain parameters θ in two subsets θ_d

and θ_s denoting "deterministic" and "stochastic" parameters respectively, problem (2.1) can be recasted as follows:

Problem (2.3)

$$\max_{d,z} P(d, z, \theta_d, \theta_s)$$
$$s.t.\ f(d, z, \theta_d, \theta_s) \leq 0$$
$$z \in Z,\ d \in D$$
$$\theta_d \in T = \{\theta_d \mid \theta_d^L \leq \theta_d \leq \theta_d^U\},\ \ \theta_s \in J(\theta_s)$$

where f is the vector of constraints.

The vector of the "deterministic" uncertain parameters θ_d can be further described by a number of periods/scenarios, p, p=1,..,P within the set T. This results in a typical multiperiod optimization formulation as follows:

Problem (2.4)

$$\max_{d,z^p} \sum_{p=1}^{P} w^p P(d, z^p, \theta_d^p, \theta_s)$$
$$s.t.\ f(d, z^p, \theta_d^p, \theta_s) \leq 0,\ \ p = 1, ..., P$$
$$z^p \in Z,\ d \in D,\ \theta_s \in J(\theta_s)$$

where w^p denotes a weight factor of period p.

The "stochastic" uncertain parameters θ_s will be considered within a two-stage stochastic formulation satisfying design objective **D2**. (2.4) then results in the following combined multiperiod/stochastic programming formulation:

Problem (2.5)

$$\max_{d} \mathbf{E}_{\theta_s \in \mathbf{R(d)}} \sum_{p=1}^{P} w^p \bar{P}^p(d, \theta_d^p, \theta_s)$$

where: $\bar{P}^p(d, \theta_d^p, \theta_s) = \max_{z^p} P(d, z^p, \theta_d^p, \theta_s)$

$$s.t.\ f(d, z^p, \theta_d^p, \theta_s) \leq 0,\ \ p = 1, ..., P$$
$$z^p \in Z,\ d \in D,\ \theta_s \in J(\theta_s)$$

where the evaluation of the expectancy is performed within the corresponding feasible region $\mathbf{R}$(d), $\mathbf{R}$(d)= $\{\theta_s \mid \forall \theta_s \in \mathbf{R}\ \exists z^p : f(d, z^p, \theta_d^p, \theta_s) \leq 0)\ \forall p\}$.

Problem (2.5) mathematically describes a design strategy consisting of two stages. Once a design has been selected at the first (design) stage, the objective of the second (operating) stage is to determine an optimal vector of control variables z for every possible realization of the uncertainty $\theta_s \in \mathbf{R}$ and θ_d^p, $p = 1, ..., P$. Note that the overall objective of economic optimization and design feasibility is enforced at the design stage, since the selection of the design variables is based on the maximization of the expected profit evaluated inside the associated feasible region. The issue of partial feasibility (for example, partial demand satisfaction, see Wellons and Reklaitis, 1989) is not considered here; i.e. it is assumed that the inequalities $f(d, z, \theta)$ in problem (2.3) are "hard" constraints. Extensions to address these types of problems are discussed in chapter 3.

The general formulation in (2.5) captures all three types of uncertainty and both design objectives for flexibility in a unified way. Consequently, most proposed formulations for flexible design optimization can be viewed as special cases of this combined multiperiod/stochastic optimization problem; for example, multiperiod design optimization problems (Varvarezos et al., 1992) for the case when only deterministic uncertain parameters are involved, stochastic design optimization problems if stochastic uncertain parameters are only considered. An attractive feature of the formulation in (2.5) is that it preserves the block diagonal structure (in the constraints) of the conventional multiperiod optimization problems. This property will be put to advantage by properly employing a decomposition-based strategy, as will be discussed in the following sections.

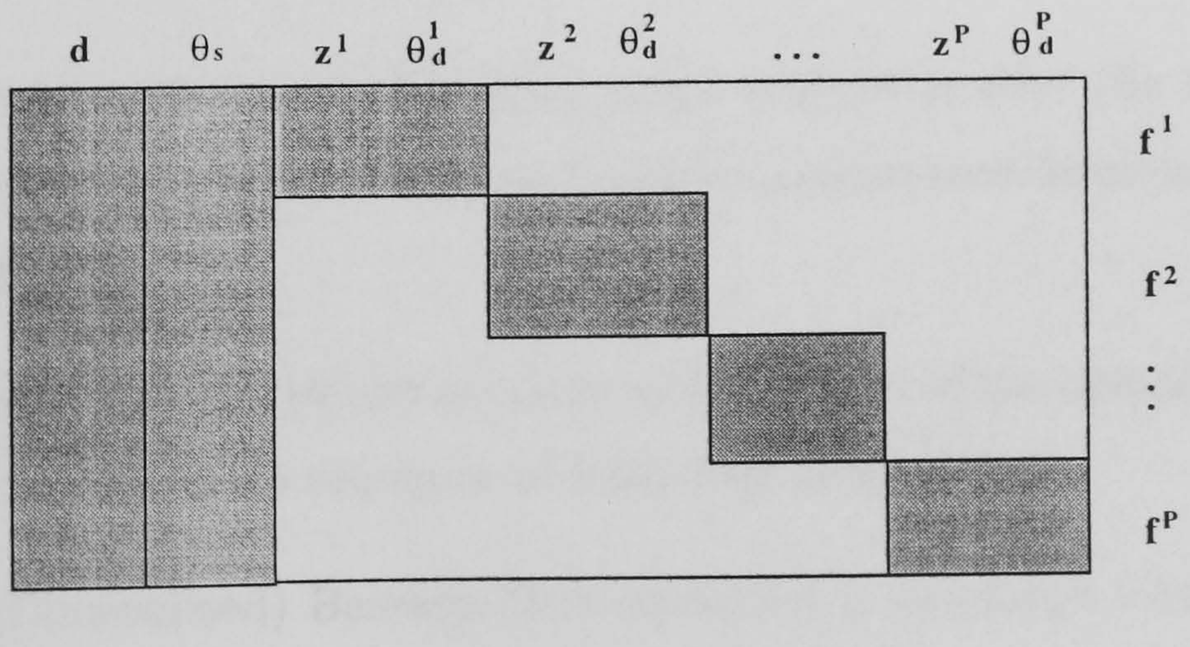


Figure 2.1: Block diagonal structure of problem (2.5)

2.3. Proposed Approach

2.3.1. Stochastic Uncertain Parameters

Before proceeding to the solution of the general (2.5) formulation, let us first examine the special case where only stochastic uncertain parameters are involved. In this case, problem (2.5) can be simplified as follows:

Problem (2.6)

$$\max_{d} \mathbf{E}_{\theta_S \in \mathbf{R}} \bar{P}(d, \theta_s)$$

$$\bar{P}(d, \theta_s) = \max_{z} P(d, z, \theta_s)$$

$$s.t.\ f(d, z, \theta_s) \leq 0$$

where $\mathbf{R}$= $\{\theta_s \mid \forall \theta_s \in \mathbf{R}\ \exists z : f(d, z, \theta_s) \leq 0)\}$.

There are two major difficulties in directly addressing problem (2.6):

(i) the evaluation of the expected profit requires integration over an (inner) optimization problem

(ii) this integration ought to be considered within the feasible region of the plant, which is unknown at the first (design) stage; furthermore, the integrands for the integration are only implicitly defined through the solution of the inner optimization problem.

To overcome the above difficulties, a solution strategy is proposed based on the following ideas:

(i) the multiple integral for the expected profit evaluation over the feasible region of the plant is approximated through a Gaussian quadrature formula with **unknown** quadrature points

(ii) the unknown quadrature points are determined as part of the optimization procedure through the solution of a sequence of feasibility subproblems

(iii) a modified (Generalized) Benders Decomposition is employed where the first-stage design variables are selected as "complicating variables".

As will be shown later, the key benefit of considering variable Gaussian quadrature points to be determined through feasibility optimization subproblems is that the boundary of the feasible region is properly identified. This, in turn, implies that the estimation of the expected profit can be effectively performed within the obtained feasible

region. Moreover, in contrast to most existing approaches, the employed modified Benders Decomposition scheme coupled with the solution of the feasibility subproblems allows for the economic optimization and design feasibility to be performed simultaneously without requiring an "a priori" discretization of the uncertainty. For convenience in the presentation, the subscripts will be omitted from the subsequent formulation.

Considering θ to follow a general probability distribution function $J(\theta)$, the expected value of the profit function P(d,z,θ) can be represented by the following multiple integral:

$$\mathbf{E}_{\theta\in\mathbf{R}}\{\max_z P(d,z,\theta)|f(d,z,\theta)\leq 0\} = \int_{\theta\in\mathbf{R}} \bar{P}(d,\theta)J(\theta)d\theta$$

$$\text{where: } \bar{P}(d,\theta) = \max_z\{P(d,z,\theta)|f(d,z,\theta)\leq 0\}$$

The above integral can then be approximated by employing a Gaussian Quadrature formula (with i=1,..,Q quadrature points) as follows:

$$\int_{\theta\in\mathbf{R}} \bar{P}(d,\theta)J(\theta)d\theta = \sum_{i=1}^{Q} w^i \bar{P}(d,\theta^i)J(\theta^i),\quad \theta^i\in\mathbf{R} \tag{2.1}$$

By considering equation 2.1, problem (2.6) can be rewritten in the following way:

Problem (2.7)

$$\max_{d,z^1,..,z^Q} \sum_{i=1}^{Q} w^i P(d,z^i,\theta^i)J(\theta^i)$$

$$s.t.\ \ f(d,z^i,\theta^i)\leq 0,\ \ i=1,..,Q$$
$$\theta^i\in\mathbf{R}$$

The difficulty of solving problem (2.7) is the determination of the feasible region **R**, i.e. the boundary of the feasible space in each direction of the uncertain parameters. For a fixed design, however, this can be achieved through the solution of the following feasibility subproblems (B1), ($B2^{q_1}$) (presented here for two uncertain parameters, see Straub and Grossmann, 1993):

Problem (B1)

$$\max_{\theta_1^U,\theta_1^L}\{\theta_1^U-\theta_1^L\}$$

$$s.t.\ \ f_1^U(d,z(.),\theta_1^U,\theta_2(.))\leq 0$$
$$f_1^L(d,z(.),\theta_1^L,\theta_2(.))\leq 0$$

where $f_1^U(f_1^L)$ denote the set of f constraints corresponding to $\theta_1^U(\theta_1^L)$; z(.), $\theta_2(.)$ denote vectors of variables associated with each set of constraints. The solution of (B1) results in the identification of the lower and upper bounds of θ_1 with which the quadrature points in θ_1-space are placed as follows:

$$\theta_1^{q_1} = 0.5[\theta_1^U(1+v_1^{q_1}) + \theta_1^L(1-v_1^{q_1})], \;\; q_1 = 1,..,Q_1 \tag{2.2}$$

where Q_1 is the number of quadrature points for θ_1 and $v_1^{q_1}$ are the parameters that correspond to the location of the quadrature points in the [-1, 1] interval (Carnahan et. al. 1969). The lower and upper bounds of θ_2 can then be obtained from the solution of the following Q_1 problems $B2^{q_1}$ for each quadrature point $q_1 = 1,..,Q_1$:

Problem ($\mathbf{B2^{q1}}$)

$$\begin{aligned} &\max_{\theta_2^{Uq_1},\theta_2^{Lq_1}} \{\theta_2^{Uq_1} - \theta_2^{Lq_1}\} \\ &s.t. \;\; f_2^{Uq_1}(d, z(.), \theta_1^{q_1}, \theta_2^{Uq_1}) \le 0 \\ &\qquad f_2^{Lq_1}(d, z(.), \theta_1^{q_1}, \theta_2^{Lq_1}) \le 0 \end{aligned}$$

The quadrature points in θ_2-space are then determined:

$$\theta_2^{q_1\,q_2} = 0.5[\theta_2^{Uq_1}(1+v_2^{q_2}) + \theta_2^{Lq_1}(1-v_2^{q_2})], \;\; q_1 = 1,..,Q_1, \;\; q_2 = 1...,Q_2 \tag{2.3}$$

If the region is convex (or 1-D convex in each parameter θ_i), the quadrature scheme will place all points inside the feasible region, thus providing a good approximation of the expected profit integral.

By including the feasibility subproblems (B1), ($B2^{q_1}$), problem (2.7) can be rewritten as follows:

Problem (2.8)

$$\max_{d, z^{q_1 q_2}} \{\frac{\theta_1^U - \theta_1^L}{2} \sum_{q_1=1}^{Q_1} w_1^{q_1} \frac{\theta_2^{Uq_1} - \theta_2^{Lq_1}}{2} \sum_{q_2=1}^{Q_2} w_2^{q_2} \; P(d, z^{q_1 q_2}, \theta_1^{q_1}, \theta_2^{q_1 q_2}) \; J(\theta_1^{q_1}, \theta_2^{q_1 q_2})\}$$
$$s.t. \; f(d, z^{q_1 q_2}, \theta_1^{q_1}, \theta_2^{q_1 q_2}) \le 0, \;\; q_1 = 1,..,Q_1, \;\; q_2 = 1,..,Q_2$$

where:

$$\left.\begin{aligned} \theta_1^U, \theta_1^L = \arg\max_{\theta_1^U,\theta_1^L} &\{\theta_1^U - \theta_1^L\} \\ s.t. \;\; f_1^U(d, z(.), \theta_1^U, \theta_2(.)) &\le 0 \\ f_1^L(d, z(.), \theta_1^L, \theta_2(.)) &\le 0 \end{aligned}\right\} \text{(B1)}$$

$$\left.\begin{array}{c} \boldsymbol{\theta_2^{Uq_1}, \theta_1^{Lq_1}} = \mathbf{arg} \max_{\theta_2^{Uq_1}, \theta_2^{Lq_1}} \{\theta_2^{Uq_1} - \theta_2^{Lq_1}\} \\ s.t.\ \ f_2^{Uq_1}(d, z(.), \theta_1^{q_1}, \theta_2^{Uq_1}) \leq 0 \\ f_2^{Lq_1}(d, z(.), \theta_1^{q_1}, \theta_2^{Lq_1}) \leq 0 \end{array}\right\} (B2^{q_1}),\ q_1 = 1, .., Q_1$$

$$\theta_1^{q_1} = 0.5[\theta_1^U(1 + v_1^{q_1}) + \theta_1^L(1 - v_1^{q_1})],\ \ q_1 = 1, .., Q_1$$

$$\theta_2^{q_1\, q_2} = 0.5[\theta_2^{Uq_1}(1 + v_2^{q_2}) + \theta_2^{Lq_1}(1 - v_2^{q_2})],\ \ q_1 = 1, .., Q_1,\ \ q_2 = 1, .., Q_2$$

Problem (2.8) is an embedded (multi-level) optimization problem, since the evaluation of the feasible region itself corresponds to the solution of the sequence of optimization problems in (B1) and $(B2^{q_1})$. Note also that since the design variables d are <u>not</u> fixed, the feasibility subproblems (B1), $(B2^{q_1})$ in problem (2.8) cannot be solved independently. To overcome these two difficulties, problem (2.8) can be first transformed to a single optimization problem by considering the optimality KKT conditions of the inner feasibility subproblems. Note that for the case of quasi-convex constraints *f*, the KKT conditions are both necessary and sufficient for global optimality. This then leads to the following **single** nonlinear optimization problem (2.9):

Problem (2.9)

$$\max_{\substack{d, z^{q_1 q_2}, \theta_1^U, \theta_1^L, \\ \theta_2^{Uq_1}, \theta_2^{Lq_1}, \theta_1^{q_1}, \theta_2^{q_1 q_2}}} \{\frac{\theta_1^U - \theta_1^L}{2} \sum_{q_1=1}^{Q_1} w_1^{q_1} \frac{\theta_2^{Uq_1} - \theta_2^{Lq_1}}{2} \sum_{q_2=1}^{Q_2} w_2^{q_2}\ P(d, z^{q_1 q_2}, \theta_1^{q_1}, \theta_2^{q_1 q_2})\ J(\theta_1^{q_1}, \theta_2^{q_1 q_2})\}$$

$$s.t.\ f(d, z^{q_1 q_2}, \theta_1^{q_1}, \theta_2^{q_1 q_2}) \leq 0,\ \ q_1 = 1, .., Q_1,\ \ q_2 = 1, .., Q_2$$

KKT Conditions of (B1):

Initial Constraints:

$$f_1^U(d, z(.), \theta_1^U, \theta_2(.)) \leq 0$$
$$f_1^L(d, z(.), \theta_1^L, \theta_2(.)) \leq 0$$

Stationary Conditions:

$$-1 + \frac{\partial f_1^U}{\partial \theta_1} \hat{\lambda}_1^U = 0,\ 1 + \frac{\partial f_1^L}{\partial \theta_1} \hat{\lambda}_1^L = 0$$
$$\frac{\partial f_1^U}{\partial \theta_2} \hat{\lambda}_1^U = 0,\ \frac{\partial f_1^L}{\partial \theta_2} \hat{\lambda}_1^L = 0$$
$$\frac{\partial f_1^U}{\partial z} \hat{\lambda}_1^U = 0,\ \frac{\partial f_1^L}{\partial z} \hat{\lambda}_1^L = 0$$

Complementarity Conditions:

$$\hat{\lambda}_1^{Ut}[f_1^U(d, z(.), \theta_1^U, \theta_2(.))] = 0$$
$$\hat{\lambda}_1^{Lt}[f_1^L(d, z(.), \theta_1^L, \theta_2(.))] = 0$$

$$\hat{\lambda}_1^U \geq 0,\ \hat{\lambda}_1^L \geq 0$$

$$
\left.\begin{array}{l}
f_2^{Uq_1}(d, z(.), \theta_1^{q_1}, \theta_2^{Uq_1}) \leq 0 \\
f_2^{Lq_1}(d, z(.), \theta_1^{q_1}, \theta_2^{Lq_1}) \leq 0
\end{array}\right\} \text{ Initial Constraints}
$$

$$
\left.\begin{array}{l}
-1 + \frac{\partial f_2^{Uq_1}}{\partial \theta_2} \hat{\lambda}_2^{Uq_1} = 0,\ 1 + \frac{\partial f_2^{Lq_1}}{\partial \theta_2} \hat{\lambda}_2^{Lq_1} = 0 \\
\frac{\partial f_2^{Uq_1}}{\partial z} \hat{\lambda}_2^{Uq_1} = 0,\ \frac{\partial f_2^{Lq_1}}{\partial z} \hat{\lambda}_2^{Lq_1} = 0
\end{array}\right\} \text{ Stationary Conditions}
$$

$$
\left.\begin{array}{l}
\hat{\lambda}_2^{Uq_1 t}[f_2^{Uq_1}(d, z(.), \theta_1^{q_1}, \theta_2^{Uq_1})] = 0 \\
\hat{\lambda}_2^{Lq_1 t}[f_2^{Lq_1}(d, z(.), \theta_1^{q_1}, \theta_2^{Lq_1})] = 0
\end{array}\right\} \text{ Complementarity Conditions}
$$

$$
\hat{\lambda}_2^{Uq_1} \geq 0,\ \hat{\lambda}_2^{Lq_1} \geq 0
$$

} KKT Conditions of $(B2^{q_1})$, $q_1 = 1, .., Q1$

$$
\theta_1^{q_1} = 0.5[\theta_1^U(1 + v_1^{q_1}) + \theta_1^L(1 - v_1^{q_1})],\ \ q_1 = 1, .., Q_1
$$

$$
\theta_2^{q_1\, q_2} = 0.5[\theta_2^{Uq_1}(1 + v_2^{q_2}) + \theta_2^{Lq_1}(1 - v_2^{q_2})],\ \ q_1 = 1, .., Q_1,\ \ q_2 = 1, .., Q_2
$$

where:

$\hat{\lambda}_1^U(\hat{\lambda}_1^L)$ are the Lagrangian multipliers of the constraints $f_1^U(f_1^L)$ in problem (B1)

$\hat{\lambda}_2^{Uq_1}(\hat{\lambda}_2^{Lq_1})$ are the Lagrangian multipliers of the constraints $f_2^{Uq_1}(f_2^{Lq_1})$ in problem $(B2^{q_1})$

Problem (2.9) cannot be directly solved since discrete decisions are involved in the complementarity conditions (defining the selection of the active sets of constraints that limit the feasible region of the design). The introduction of binary variables to represent the potential active sets of constraints transforms the (nonconvex) nonlinear problem (2.9) to the following (convex) mixed-integer nonlinear optimization problem (2.10).

Problem (2.10)

$$
\max_{\substack{d,\, z^{q_1 q_2},\, \theta_1^U,\, \theta_1^L,\\ \theta_2^{Uq_1},\, \theta_2^{Lq_1},\, \theta_1^{q_1},\, \theta_2^{q_1 q_2}}} \{\frac{\theta_1^U - \theta_1^L}{2} \sum_{q_1=1}^{Q_1} w_1^{q_1} \frac{\theta_2^{Uq_1} - \theta_2^{Lq_1}}{2} \sum_{q_2=1}^{Q_2} w_2^{q_2}\ P(d, z^{q_1 q_2}, \theta_1^{q_1}, \theta_2^{q_1 q_2})\ J(\theta_1^{q_1}, \theta_2^{q_1 q_2})\}
$$

$$
s.t.\ \ f(d, z^{q_1 q_2}, \theta_1^{q_1}, \theta_2^{q_1 q_2}) \leq 0,\ \ q_1 = 1, .., Q_1,\ \ q_2 = 1, .., Q_2
$$

$$
\begin{aligned}
& f_1^U(d, z(.), \theta_1^U, \theta_2(.)) + s_1^U = 0 \\
& f_1^L(d, z(.), \theta_1^L, \theta_2(.)) + s_1^L = 0 \\
& -1 + \tfrac{\partial f_1^U}{\partial \theta_1} \hat{\lambda}_1^U = 0,\ 1 + \tfrac{\partial f_1^L}{\partial \theta_1} \hat{\lambda}_1^L = 0 \\
& \tfrac{\partial f_1^U}{\partial \theta_2} \hat{\lambda}_1^U = 0,\ \tfrac{\partial f_1^L}{\partial \theta_2} \hat{\lambda}_1^L = 0 \\
& \tfrac{\partial f_1^U}{\partial z} \hat{\lambda}_1^U = 0,\ \tfrac{\partial f_1^L}{\partial z} \hat{\lambda}_1^L = 0 \\
& \hat{\lambda}_1^U - M y_1^U \leq 0 \\
& s_1^U - M(1 - y_1^U) \leq 0 \\
& \hat{\lambda}_1^L - M y_1^L \leq 0 \\
& s_1^L - M(1 - y_1^L) \leq 0 \\
& \textstyle\sum y_1^U \leq n_z + 1,\ \sum y_1^L \leq n_z + 1 \\
& \hat{\lambda}_1^U, \hat{\lambda}_1^L \geq 0,\ s_1^U, s_1^L \geq 0,\ y_1^U, y_1^L = \{0, 1\}
\end{aligned}
$$

$$
\begin{aligned}
& f_2^{Uq_1}(d, z(.), \theta_1^{q_1}, \theta_2^{Uq_1}) + s_2^{Uq_1} = 0 \\
& f_2^{Lq_1}(d, z(.), \theta_1^{q_1}, \theta_2^{Lq_1}) + s_2^{Lq_1} = 0 \\
& -1 + \tfrac{\partial f_2^{Uq_1}}{\partial \theta_2} \hat{\lambda}_2^{Uq_1} = 0,\ 1 + \tfrac{\partial f_2^{Lq_1}}{\partial \theta_2} \hat{\lambda}_2^{Lq_1} = 0 \\
& \tfrac{\partial f_2^{Uq_1}}{\partial z} \hat{\lambda}_2^{Uq_1} = 0,\ \tfrac{\partial f_2^{Lq_1}}{\partial z} \hat{\lambda}_2^{Lq_1} = 0 \\
& \hat{\lambda}_2^{Uq_1} - M y_2^{Uq_1} \leq 0 \\
& s_2^{Uq_1} - M(1 - y_2^{Uq_1}) \leq 0 \\
& \hat{\lambda}_2^{Lq_1} - M y_2^{Lq_1} \leq 0 \\
& s_2^{Lq_1} - M(1 - y_2^{Lq_1}) \leq 0 \\
& \textstyle\sum y_2^{Uq_1} \leq n_z + 1,\ \sum y_2^{Lq_1} \leq n_z + 1 \\
& \hat{\lambda}_2^{Uq_1}, \hat{\lambda}_2^{Lq_1} \geq 0,\ s_2^{Uq_1}, s_2^{Lq_1} \geq 0,\ y_2^{Uq_1}, y_2^{Lq_1} = \{0, 1\} \\
& \theta_1^{q_1} = 0.5[\theta_1^U(1 + v_1^{q_1}) + \theta_1^L(1 - v_1^{q_1})],\ \ q_1 = 1, .., Q_1 \\
& \theta_2^{q_1\ q_2} = 0.5[\theta_2^{Uq_1}(1 + v_2^{q_2}) + \theta_2^{Lq_1}(1 - v_2^{q_2})],\ \ q_1 = 1, .., Q_1,\ \ q_2 = 1, .., Q_2
\end{aligned}
$$

where:

$s_1^U(s_1^L)$	are the slacks of the constraints $f_1^U(f_1^L)$ in problem (B1)
$s_2^{Uq_1}(s_2^{Lq_1})$	are the slacks of the constraints $f_2^{Uq_1}(f_2^{Lq_1})$ in problem $(B2^{q_1})$
$y_1^U, y_1^L, y_2^{Uq_1}, y_2^{Lq_1}$	binary variables representing active constraints of problems (B1), $(B2^{q_1})$, respectively
n_z	is the length of vector of control variables

As will be shown in the sequel, the direct solution of the MINLP problem in (2.10) is not really required, since by fixing the vector of design variables d, problem (2.10) essentially collapses into a sequence of nonlinear optimization problems with the discrete decisions simultaneously obtained. This naturally suggests a decomposition approach as follows.

By fixing the design variables d, the feasibility problems (B1) and $(B2^{q_1})$ can be solved independently leading to the evaluation of the boundary of the feasible region. Then, the quadrature points $(\theta_1^{q_1}, \theta_2^{q_1\,q_2})$ are properly defined from equations 2.2, 2.3, and problem (2.7) can be solved to evaluate the expected profit. Note that problem (2.7) can be further decomposed into the following $Q_1 \times Q_2$ optimization problems (at each quadrature node i, i=1,..,$Q_1 \times Q_2$):

$$\max_{z^i} \{P(d, z^i, \theta^i) \mid f(d, z^i, \theta^i) \leq 0\} \qquad (PQ)$$

The solution of problem (2.7) (or its equivalent set of subproblems (PQ)) yields a value of the expected profit term, which is a valid lower bound to the objective function of the overall maximization problem in (2.9) since the design variables are held fixed.

An upper bound can also be obtained following the general Benders Decomposition principles by constructing a suitable master problem. This construction relies on a dual approximation requiring the values of the Lagrange multipliers of the constraints of problem (2.10) for fixed design variables (primal problem). By exploiting the special structure of the model (2.10), the required Lagrange multipliers can be obtained from the already available dual information from the solution of (B1), $(B2^{q_1})$ and (PQ) subproblems (by additionally applying analytically calculated corrected factors) as follows.

First note that the solution of the feasibility subproblems (B1), $(B2^{q_1})$, for fixed values of the design variables d, results in the direct identification of the active (and inactive) constraints for each subproblem. Consequently, the stationary conditions in (2.10) correspond to a square system of equations whereas the complementarity conditions are trivially satisfied (see Appendix A.1). Therefore, for fixed d, problem (2.10) can be recasted in the following way:

Problem (2.11)

$$EP(d) = \max_{\substack{z^{q_1 q_2}, \theta_1^U, \theta_1^L, \theta_2^{Uq_1}, \\ \theta_2^{Lq_1}, \theta_1^{q_1}, \theta_2^{q_1 q_2}}} \{\frac{\theta_1^U - \theta_1^L}{2} \sum_{q_1=1}^{Q_1} w_1^{q_1} \frac{\theta_2^{Uq_1} - \theta_2^{Lq_1}}{2} \sum_{q_2=1}^{Q_2} w_2^{q_2}\ P(d, z^{q_1 q_2}, \theta_1^{q_1}, \theta_2^{q_1 q_2})\ J(\theta_1^{q_1}, \theta_2^{q_1 q_2})\}$$

$$s.t.\ f(d, z^{q_1 q_2}, \theta_1^{q_1}, \theta_2^{q_1 q_2}) \leq 0, \quad q_1 = 1,..,Q_1, \quad q_2 = 1,..,Q_2$$

$$\begin{aligned}
&f_{1A}^{U}(d, z(.), \theta_1^{U}, \theta_2(.)) = 0 \\
&f_{1A}^{L}(d, z(.), \theta_1^{L}, \theta_2(.)) = 0 \\
&f_{1I}^{U}(d, z(.), \theta_1^{U}, \theta_2(.)) < 0 \\
&f_{1I}^{L}(d, z(.), \theta_1^{L}, \theta_2(.)) < 0
\end{aligned}$$

$$\left.\begin{aligned}
&f_{2A}^{Uq_1}(d, z(.), \theta_1^{q_1}, \theta_2^{Uq_1}) = 0 \\
&f_{2A}^{Lq_1}(d, z(.), \theta_1^{q_1}, \theta_2^{Lq_1}) = 0 \\
&f_{2I}^{Uq_1}(d, z(.), \theta_1^{q_1}, \theta_2^{Uq_1}) < 0 \\
&f_{2I}^{Lq_1}(d, z(.), \theta_1^{q_1}, \theta_2^{Lq_1}) < 0
\end{aligned}\right\} \quad q_1 = 1,..,Q1$$

$$\begin{aligned}
&\theta_1^{q_1} = 0.5[\theta_1^{U}(1 + v_1^{q_1}) + \theta_1^{L}(1 - v_1^{q_1})], \quad q_1 = 1,..,Q_1 \\
&\theta_2^{q_1\, q_2} = 0.5[\theta_2^{Uq_1}(1 + v_2^{q_2}) + \theta_2^{Lq_1}(1 - v_2^{q_2})], \quad q_1 = 1,..,Q_1, \quad q_2 = 1,..,Q_2
\end{aligned}$$

where :

f_{1A}^{U}, f_{1A}^{L}	the active constraints of problem (B1)
f_{1I}^{U}, f_{1I}^{L}	the inactive constraints of problem (B1)
$f_{2A}^{Uq_1}, f_{2A}^{Lq_1}$	the active constraints of problem $(B2^{q_1})$
$f_{2I}^{Uq_1}, f_{2I}^{Lq_1}$	the inactive constraints of problem $(B2^{q_1})$

The construction of the Lagrangian L^1 requires the Lagrangian multipliers of (2.11):

$$\begin{aligned}
L^1 = EP(d) &- \sum_{q_1=1}^{Q1} \sum_{q_2=1}^{Q2} \eta^{q_1 q_2} f(d, z^{q_1 q_2}, \theta_1^{q_1}, \theta_2^{q_1 q_2}) \\
&- \lambda_1^{U} f_1^{U}(d, z(.), \theta_1^{U}, \theta_2(.)) \\
&- \lambda_1^{L} f_1^{L}(d, z(.), \theta_1^{L}, \theta_2(.)) \\
&- \sum_{q_1=1}^{Q1} \lambda_2^{Uq_1} f_2^{Uq_1}(d, z(.), \theta_1^{q_1}, \theta_2^{Uq_1}) \\
&- \sum_{q_1=1}^{Q1} \lambda_2^{Lq_1} f_2^{Lq_1}(d, z(.), \theta_1^{q_1}, \theta_2^{Lq_1})
\end{aligned}$$

$$- \sum_{q_1=1}^{Q1} \mu_1^{q_1} \{\theta_1^{q_1} - 0.5[\theta_1^U(1+v_1^{q_1}) + \theta_1^L(1-v_1^{q_1})]\}$$
$$- \sum_{q_1=1}^{Q1}\sum_{q_2=1}^{Q2} \mu_2^{q_1 q_2} \{\theta_2^{q_1 q_2} - 0.5[\theta_2^{Uq_1}(1+v_2^{q_2}) + \theta_2^{Lq_1}(1-v_2^{q_2})]\} \quad (2.4)$$

The required multipliers $\eta^{q_1 q_2}, \lambda_1^U, \lambda_1^L, \lambda_2^{Uq_1}, \lambda_2^{Lq_1}, \mu_1^{q_1}, \mu_2^{q_1 q_2}$ can be determined by applying appropriate correction factors to the Lagrangian multipliers obtained from the solution of (B1), ($B2^{q_1}$) and (PQ) subproblems. These correction factors can be calculated analytically by comparing the KKT conditions of problem (2.11) with the KKT conditions of problems (B1), ($B2^{q_1}$) and (PQ), respectively (see Appendix A.2 for the analytical derivations). Hence, for problem (B1) the corrected multipliers for the constraints are:

$$\lambda_1^U = CF_1^U \hat{\lambda}_1^U, \ \lambda_1^L = CF_1^L \hat{\lambda}_1^L \quad (2.5)$$

where:

$$CF_1^U = CF_1 - \sum_{q_1=1}^{Q1} \mu_1^{q_1} \{(-0.5)(1+v_1^{q_1})\} \quad (2.6)$$

$$CF_1^L = CF_1 + \sum_{q_1=1}^{Q1} \mu_1^{q_1} \{(-0.5)(1-v_1^{q_1})\} \quad (2.7)$$

$$CF_1 = \frac{1}{2}\sum_{q_1=1}^{Q_1} w_1^{q_1} \frac{\theta_2^{Uq_1} - \theta_2^{Lq_1}}{2} \sum_{q_2=1}^{Q_2} w_2^{q_2} \ P(d, z^{q_1 q_2}, \theta_1^{q_1}, \theta_2^{q_1 q_2}) \ J(\theta_1^{q_1}, \theta_2^{q_1 q_2}) \quad (2.8)$$

$$\mu_1^{q_1} = \frac{\theta_1^U - \theta_1^L}{2} w_1^{q_1} \frac{\theta_2^{Uq_1} - \theta_2^{Lq_1}}{2} \sum_{q_2=1}^{Q_2} w_2^{q_2} \ \frac{\partial PJ}{\partial \theta_1^{q_1}} - \lambda_2^{Uq_1} \frac{\partial f_2^{Uq_1}}{\partial \theta_1^{q_1}} - \lambda_2^{Lq_1} \frac{\partial f_2^{Lq_1}}{\partial \theta_1^{q_1}}$$
$$- \sum_{q_2=1}^{Q_2} \eta^{q_1 q_2} \frac{\partial f}{\partial \theta_1^{q_1}} \quad (2.9)$$

Similarly, by comparing the KKT conditions of problems ($B2^{q_1}$) and (2.11) the following corrected multipliers are obtained:

$$\lambda_2^{Uq_1} = CF_2^{Uq_1} \hat{\lambda}_2^{Uq_1}, \ \lambda_2^{Lq_1} = CF_2^{Lq_1} \hat{\lambda}_2^{Lq_1} \quad (2.10)$$

where:

$$CF_2^{Uq_1} = CF_2^{q_1} - \sum_{q_2=1}^{Q2} \mu_2^{q_1 q_2} \{(-0.5)(1+v_2^{q_2})\} \quad (2.11)$$

$$CF_2^{Lq_1} = CF_2^{q_1} + \sum_{q_2=1}^{Q2} \mu_2^{q_1 q_2} \{(-0.5)(1-v_2^{q_2})\} \quad (2.12)$$

$$CF_2^{q_1} = \frac{1}{2}\frac{\theta_1^U - \theta_1^L}{2} w_1^{q_1} \sum_{q_2=1}^{Q_2} w_2^{q_2} \ P(d, z^{q_1 q_2}, \theta_1^{q_1}, \theta_2^{q_1 q_2}) \ J(\theta_1^{q_1}, \theta_2^{q_1 q_2}) \quad (2.13)$$

$$\mu_2^{q_1 q_2} = \frac{\theta_1^U - \theta_1^L}{2} w_1^{q_1} \frac{\theta_2^{Uq_1} - \theta_2^{Lq_1}}{2} w_2^{q_2} \ \frac{\partial PJ}{\partial \theta_2^{q_1 q_2}} - \eta^{q_1 q_2} \frac{\partial f}{\partial \theta_2^{q_1 q_2}} \quad (2.14)$$

Finally, the corrected multipliers for problems (PQ) are:

$$\eta^{q_1 q_2} = CF^{q_1 q_2} \hat{\eta}^{q_1 q_2} \tag{2.15}$$

where:

$$CF^{q_1 q_2} = \frac{\theta_1^U - \theta_1^L}{2} w_1^{q_1} \frac{\theta_2^{U q_1} - \theta_2^{L q_1}}{2} w_2^{q_2} \; J(\theta_1^{q_1}, \theta_2^{q_1 q_2}) \tag{2.16}$$

Based on equations 2.5-2.16 the required corrected multipliers of the Lagrangian in 2.4 are determined through the following steps:

Step 1. Solve problems (B1), $(B2^{q_1})$, (PQ) to obtain the multipliers $\hat{\lambda}_1^U, \hat{\lambda}_1^L, \hat{\lambda}_2^{U q_1}, \hat{\lambda}_2^{L q_1}, \hat{\eta}^{q_1 q_2}$.

Step 2. Calculate $CF^{q_1 q_2}$ from equation 2.16 and determine $\eta^{q_1 q_2}$ from equation 2.15.

Step 3. Calculate $\mu_2^{q_1 q_2}$ through 2.14, determine $CF_2^{U q_1}, CF_2^{L q_1}$ through 2.11, 2.12, respectively and calculate the corrected multipliers $\lambda_2^{U q_1}, \lambda_2^{L q_1}$ from 2.10.

Step 4. Calculate $\mu_1^{q_1}$ from 2.9, determine CF_1^U, CF_1^L through 2.6, 2.7 respectively and calculate the corrected multipliers λ_1^U, λ_1^L from 2.5.

Note, that the multipliers $\lambda_1^U, \lambda_1^L, \lambda_2^{U q_1}, \lambda_2^{L q_1}$ can take either positive or negative values since they correspond to either inequalities (inactive constraints) or equalities (active constraints) of problem (2.11), whereas $\eta^{q_1 q_2}$ are always positive (see Appendix A.3).

Given different values of the design variables d^k, k=1,..K, the following master problem can then be constructed in terms of the design variables (d), involving the Lagrangian cut for each one of k iterations; its solution provides a valid upper bound and returns a new set of design variables d.

Problem (2.12)

$$EP_U^K = \max_{\mu_B, d} \; \mu_B$$

$$s.t. \; \mu_B \leq \frac{\theta_1^{Uk} - \theta_1^{Lk}}{2} \sum_{q_1=1}^{Q_1} w_1^{q_1} \frac{\theta_2^{U q_1 k} - \theta_2^{L q_1 k}}{2} \sum_{q_2=1}^{Q_2} w_2^{q_2} \; P(d, z^{q_1 q_2 k}, \theta_1^{q_1 k}, \theta_2^{q_1 q_2 k}) \; J(\theta_1^{q_1 k}, \theta_2^{q_1 q_2 k})$$

$$- \sum_{q_1=1}^{Q_1} \sum_{q_2=1}^{Q_2} \eta^{q_1 q_2 k} f(d, z^{q_1 q_2 k}, \theta_1^{q_1 k}, \theta_2^{q_1 q_2 k})$$

$$- \lambda_1^{Uk} f_1^U(d, z^k(.), \theta_1^{Uk}, \theta_2^k(.)) - \lambda_1^{Lk} f_1^L(d, z(.)^k, \theta_1^L, \theta_2^k(.))$$

$$-\sum_{q_1=1}^{Q_1} \lambda_2^{Uq_1k} f_2^{Uq_1}(d, z^{q_1k}(.), \theta_1^{q_1k}, \theta_2^{Uq_1k})$$
$$-\sum_{q_1=1}^{Q_1} \lambda_2^{Lq_1k} f_2^{Lq_1}(d, z^{q_1k}(.), \theta_1^{q_1k}, \theta_2^{Lq_1k}), \qquad k = 1, .., K$$

where: μ_B a scalar variable

EP_U^K the predicted upper bound

$\eta^{q_1q_2k}$ the corrected multipliers for the constraints of problems (PQ) for design d^k

$\lambda_1^{Uk}, \lambda_1^{Lk}$ the corrected multipliers for the constraints of problem (B1) for design d^k

$\lambda_2^{Uq_1k}, \lambda_2^{Lq_1k}$ the corrected multipliers for the constraints of problems ($B2^{q_1}$) for design d^k

Note that EP_U^K is guaranteed to be a valid upper bound if the inequality constraints f are convex in (d, z, θ) and the expected profit EP is a concave function (Geoffrion 1972).

DESIGN UNDER UNCERTAINTY ALGORITHM

The steps of the proposed decomposition-based algorithm for process design models under uncertainty (problem 2.6) can then be summarized as follows (see also Figure 2.2):

Step 1: Select an initial design d^1. Set the lower bound $EP_L = -\infty$, K=1 and select a tolerance ϵ.

Step 2: Solve the feasibility subproblems (B1), ($B2^{q_1}$) to obtain the boundary of the feasible region and the corresponding Lagrangian multipliers.

Step 3: At each quadrature point $(\theta_1^{q_1}, \theta_2^{q_1q_2})$ solve problem (PQ) to evaluate the optimal value of profit and obtain the corresponding Lagrangian multipliers.

Step 4: Calculate the expected profit (EP) using the Gaussian Quadrature formula; update the lower bound, $EP_L = \max\{EP, EP_L\}$.

Step 5a: Calculate the corrected multipliers $\lambda_1^U, \lambda_1^L, \lambda_2^{Uq_1}, \lambda_2^{Lq_1}, \eta^{q_1q_2}$ following equations 2.5-2.16 and the steps described earlier.

Step 5b: Solve the master problem (2.12) to obtain a new design d^{K+1} and an upper bound EP_U^K.

Step 6: If $EP_U^K \leq EP_L + \epsilon$, stop; the optimal solution corresponds to design d^K with expected profit EP_L. Otherwise, set K=K+1 and return to Step 2.

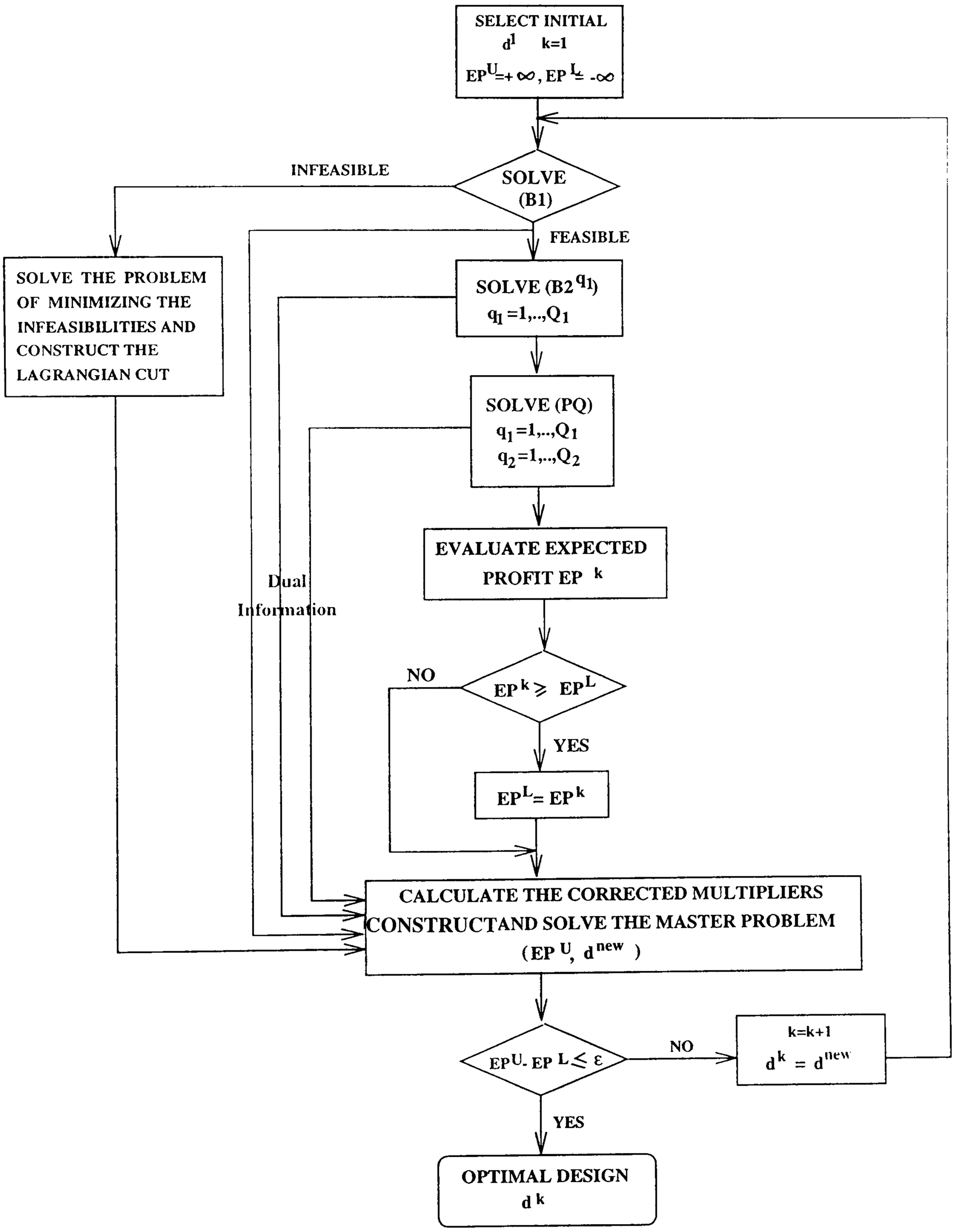


Figure 2.2: Design under Uncertainty Algorithm - problem (2.6)

In Step 2 it has been assumed that problems (B1), ($B2^{q_1}$) are feasible, i.e. d^k has a nonempty feasible region. If this is not the case, the form of the master problem must be modified to include infeasibility cuts derived from the Lagrangian functions of a corresponding problem that minimizes the infeasibilities of constraints in problem (2.11) (see Geoffrion, 1972).

This iterative algorithmic procedure, which is guaranteed to converge to a global optimum in a finite number of iterations for the case of convex constraints and concave objective function, results in the determination of an optimal design with the maximum expected profit. The algorithm does not require postulation of "a priori" values for the uncertain parameters, nor does it rely on any distributional form assumption of the uncertainty. The evaluation of the expected profit is performed within the simultaneously obtained feasible region; the algorithm does not directly address partial feasibility considerations, however, one can envisage the extension of this approach to account for this important issue (since it might be possible to establish a sensible penalty measure for partially feasible operation given that the feasible region of the design is obtained, see for example chapter 3). In contrast to most previous attempts (Pistikopoulos and Grossmann, 1988b, 1989b, Straub and Grossmann, 1992) a distinct advantage of the new algorithm is that profit optimization and design feasibility are **simultaneously** performed, thus obtaining a design with an optimal level of feasibility/flexibility.

The computational penalty for these theoretical advances is, however, quite high: a large number of, although of much smaller size, optimization subproblems have to be solved per iteration for the evaluation of the feasible region and expected profit (problems (B1), ($B2^{q_1}$) and (PQ), respectively). This number depends on the number of quadrature points for the Gaussian Quadrature approximation and increases exponentially with the number of uncertain parameters. Nevertheless, the algorithm has a highly parallel structure, since most optimization tasks can be performed independently. This is a key factor that must be fully exploited to enhance computational performance for such an approach to be useful in practice (Acevedo et al. 1995).

The number of quadrature points directly depends on the desired accuracy for the evaluation of the integration to approximate the expected profit term of problem (2.6); while this may be problem dependent, our experience indicates, as also discussed in section 4, that typically 5-7 quadrature points (at each direction of the uncertain parameter) are

sufficient for the integration.

If the number of uncertain parameters is large (>10), parallelization of the algorithm may not be sufficient to address the problem of increased computational requirement by itself; here, additional methodologies such as statistical techniques to reduce the number of uncertain parameters based on their relative importance and/or the consideration of fixed quadrature grid for some of the parameters may also be worth exploring.

The assumption of convex models is another critical issue. Although, such a decomposition based approach can be, in principle, applied to non-convex problems, it is well established (Floudas and Visweswaran, 1990, Sahinidis and Grossmann 1991) that local or even suboptimal solutions may well be encountered. Furthermore, for the non-convex case, the employed quadrature scheme may not be accurate enough since the placement of infeasible quadrature points can not be easily avoided. The recent developments, however, of global optimization algorithms, which are decomposition-based (GOP algorithm; Floudas and Visweswaran, 1990,1993, Visweswaran and Floudas, 1990,1993) provide enough hope for also addressing special classes of non-convex design under uncertainty problems (see also Visweswaran et al. 1995).

As will be shown in the next section, the proposed algorithm can be extended to address the general problem (2.5) by exploiting its special block diagonal structure. Moreover, it offers a platform for addressing a variety of process engineering problems under uncertainty:

- process synthesis & design applications similar to the problems considered in section 2.4,
- multiproduct/multipurpose batch plant design problems which will be discussed in Chapter 3,
- planning and capacity expansion models which will be discussed in Chapter 4,
- optimization models for reliability, maintenance and safety of the type discussed in Pistikopoulos and Thomaidis (1992,1994).

2.3.2. Extended Algorithmic Procedure

Figure 2.1 shows the block diagonal structure of model (2.5) with the design variables d and uncertainty θ_s being the "connecting" variables. By fixing the vector of design

variables d at $\bar{d}$, the solution of the following feasibility subproblems (in θ_s subspace)

$$\max_{z^{pU}, z^{pL}, \theta_s^U, \theta_s^L,} \{\theta_s^U - \theta_s^L\}$$

$$\text{s.t.} \quad f(\bar{d}, z^{pL}, \theta_d^p, \theta_s^L) \leq 0 \ \ \forall p$$

$$f(\bar{d}, z^{pU}, \theta_d^p, \theta_s^U) \leq 0 \ \ \forall p$$

$$\theta_s^{min} \leq \theta_s^L \leq \theta_s \leq \theta_s^U \leq \theta_s^{max}$$

results in the determination of the corresponding feasible region (of design $\bar{d}$), with which quadrature points for θ_s can be appropriately defined by equations 2.2, 2.3. At the end of this step, the expected profit optimization problem exhibits the expanded block diagonal structure of Figure 2.3, implying that each subproblem can be solved independently:

$$\max_{z^{qp}} P^{qp}(\bar{d}, z^{qp}, \theta_d^p, \theta_s^q)$$
$$\text{s.t.} \quad f(\bar{d}, z^{qp}, \theta_d^p, \theta_s^q) \leq 0$$

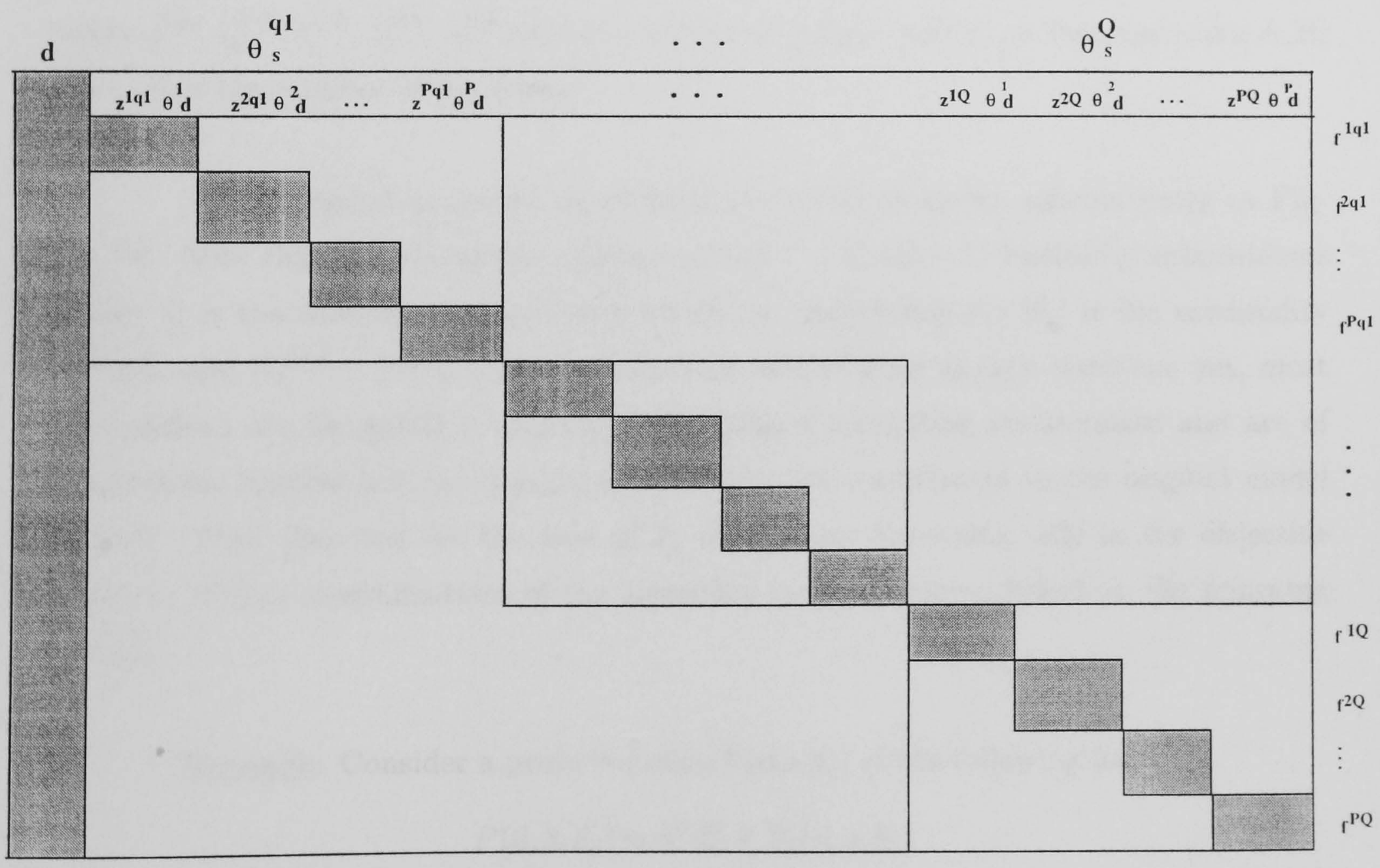


Figure 2.3: Expanded block diagonal structure of profit optimization subproblem

The evaluation of the expectancy, which is a valid lower bound of (2.5), then results as:

$$EP^k(d) = \sum_{Q \times P} w^{qp} P^{qp}(\bar{d}, z^{qp}, \theta_d^p, \theta_s^{qp}) J(\theta_s^{qp})$$

From the dual information obtained from the solution of the feasibility and profit subproblems, and the application of the general correction factors of Appendix A.2, the following master problem is constructed, yielding an upper bound to the solution of (2.5) and a new set of design variables d.

$$EP^{UB} = \max_{d,\mu} \mu$$

$$\text{s.t. } \mu \leq EP^k(d) - \sum_{Q \times P} \eta^{kqp} [f(d, z^{kqp}, \theta_d^p, \theta_s^{kqp}))]$$

$$-\sum_{i=2}^{|\theta_s|} \{ \sum_{Q=\{q_1..q_{i-1}\}} \lambda_i^{U,k} f^U(\cdot) + \lambda_i^{L,k} f^L(\cdot) \}$$

$$-\lambda_1^{U,k} f^U(\cdot) - \lambda_1^{L,k} f^L(\cdot) \qquad k = 1, .., K$$

where $\eta^{kqp}, \lambda_i^{U,k}, \lambda_i^{L,k}, \lambda_1^{U,k}, \lambda_1^{L,k}$ are the corrected Lagrange multipliers (see Appendix A.2); k=1,..,K is the number of iterations.

The expanded proposed algorithmic procedure is shown schematically in Figure 2.4. Note that it involves the solution of $(Q^{|\theta_s|} - 1)/(Q - 1)$ feasibility subproblems (where Q is the number of quadrature points per uncertainty θ_s; $|\theta_s|$ is the cardinality of θ_s) and $(Q^{|\theta_s|} \times P^{|\theta_d|})$ profit optimization subproblems at each iteration; yet, most subproblems can be solved in a parallel/distributed computing environment and are of considerable smaller size (in number of variables) when compared to the original model in (2.5). Note also that for the case of θ_s uncertainty appearing only in the objective function, further simplifications of the algorithm can be achieved based on the following remark:

Remark: Consider a profit function P(d,z,θ_s) of the following form:

$$P(d, z, \theta_s) = b^T \theta_s'' + P_0(d, z, \theta_s')$$

Then:

$$E_{\theta_s \in \mathbf{R}(d)} \{\max_z P(d, z, \theta_s)\} = \int_{\theta_s'} \max_z [P_0(d, z, \theta_s')] J(\theta_s') d\theta_s' + b^T E\{\theta_s''\} \int_{\theta_s'} J(\theta_s') d\theta_s'$$

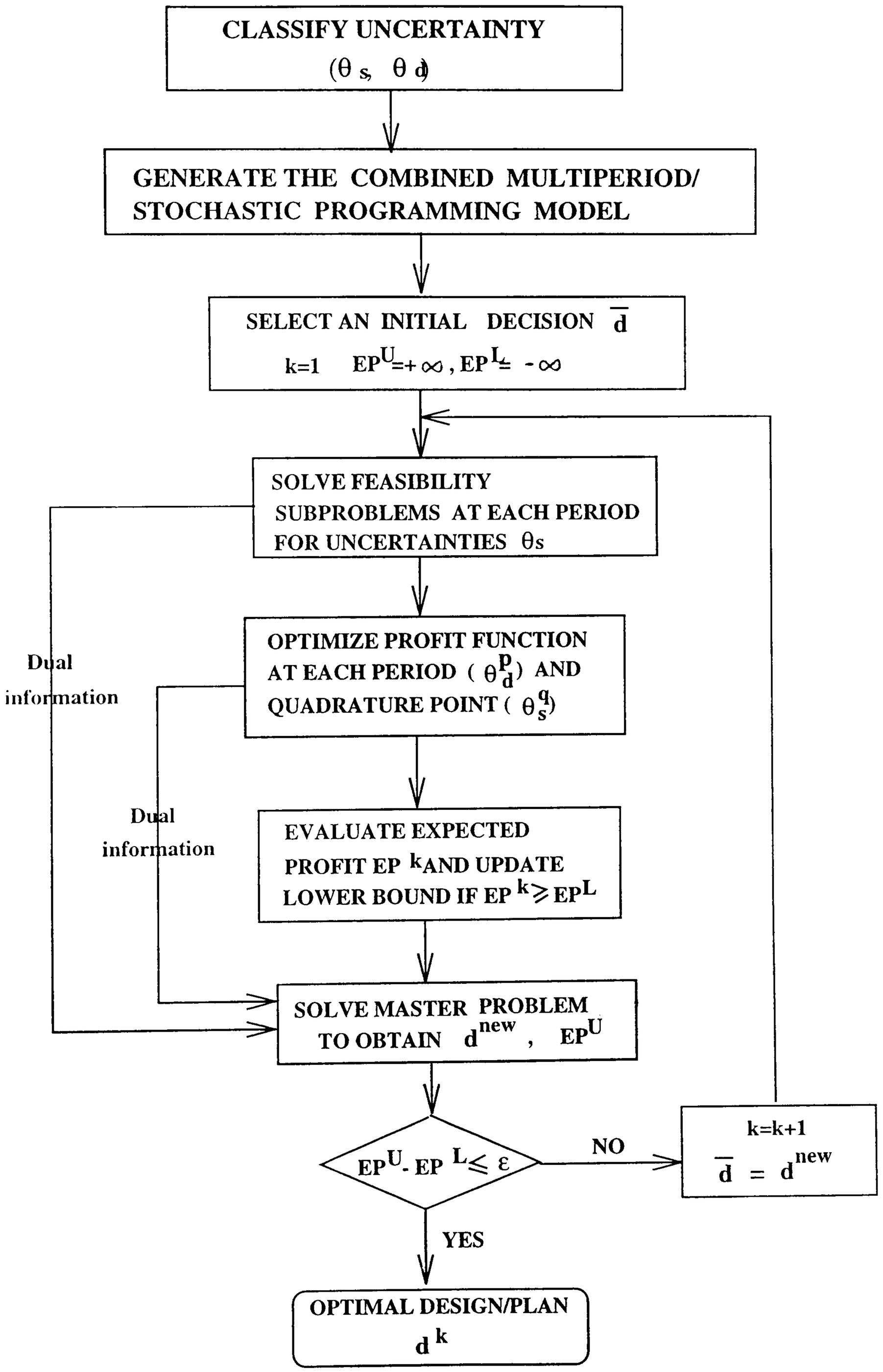


Figure 2.4: Unified Algorithm of Combined Multiperiod/stochastic Programming Problem

where $\theta_s = (\theta'_s \bigcup \theta''_s)$. The proof is shown in Appendix A.4.

The next section describes the application of the proposed algorithms to process synthesis and design example problems.

2.4. Applications

In this section, the proposed algorithmic developments are applied to five example problems. The purpose of the first example, a small linear retrofit design model involving two or three uncertain parameters, is to illustrate the steps of the proposed algorithmic procedure and to discuss the computations involved. The second example problem corresponds to a small convex mixed integer nonlinear model; it serves to demonstrate the capability of the new algorithm to handle (0,1) binary (structural) variables. The third example involves a process synthesis/planning application where decisions should be made concerning the optimal production plan; the fourth example examines the problem of selecting the optimal separation scheme for process stream (F1), whereas the final example considers the problem of designing a benzene chlorination plant.

Example 1: A linear retrofit model

(a) two uncertain parameters

The retrofit design example considered in Pistikopoulos and Grossmann (1988b) is examined here. The specifications of a design are represented by the following linear inequalities:

$$f_1 = z - \theta_1 + 0.5\theta_2 + d_1 - 3d_2 \leq 0$$
$$f_2 = -z - \theta_1/3 - \theta_2 + d_2 + 1/3 \leq 0$$
$$f_3 = z + \theta_1 - \theta_2 - d_1 - 1 \leq 0$$

These inequalities involve one control variable z, two design variables d_1, d_2 and two uncertain parameters θ_1, θ_2 which are both described by a normal distribution function, N(2,2). Hence, with a level of confidence 70 %, the expected parameter deviations are $\Delta\theta_1^+ = \Delta\theta_1^- = \Delta\theta_2^+ = \Delta\theta_2^- = 2$; the values of the existing design variables are $d_1^E = 3, d_2^E = 1$. The investment cost for the redesign is given by a linear function: $c(\Delta d) = 10\Delta d_1 + 10\Delta d_2$, and the revenue function is: r(z)=10z. Thus, the profit function is linear of the following form: $P = 10z - 10\Delta d_1 - 10\Delta d_2$.

Applying the steps of the proposed approach, the following results are obtained:

Step 1: An initial redesign is selected: $(\Delta d_1, \Delta d_2)$ =(1.5, 3.5); $EP_L = -\infty$, k=1 and $\epsilon = 0.1$.

Step 2: The solution of the feasibility problem (B1) leads to the following bounds of θ_1: $0 \leq \theta_1 \leq 4$. Considering 5 quadrature points for θ_1 and solving $(B2^{q_1})$ at each of these points the results shown in Table 2.1 are obtained (see also Figure 2.5).

q_1	1	2	3	4	5
$\theta_1^{q_1}$	0.188	0.923	2.000	3.077	3.812
$\theta_2^{Lq_1}$	0.000	0.000	0.333	0.692	0.937
$\theta_2^{Uq_1}$	4	4	4	4	4

Table 2.1: Bounds for θ_2 at $\theta_1^{q_1}$ of initial design

Step 3: Considering 5 quadrature points for θ_2 and solving problem (PQ) at each of these points the results shown in Table 2.2 are obtained.

q_2 / q_1	1	2	3	4	5
1	5.00	12.35	23.12	26.49	22.81
2	-2.35	5.00	15.77	26.54	30.17
3	-10.05	-3.21	6.67	16.54	23.28
4	-17.29	-11.21	-2.31	6.6	12.68
5	-22.32	-16.68	-8.44	-0.19	5.44

Table 2.2: Optimal profit at the quadrature points (5x5 grid)

Step 4: The expected profit is evaluated through a Gaussian Quadrature formula yielding a value of -25.56 units; the lower bound is updated, $EP_L = -25.56$.

Step 5a,5b: After the evaluation of the corrected multipliers the master problem is formulated as follows:

$$\begin{aligned} EP_U^k = \max_{\mu_B, \Delta d_1, \Delta d_2} \ & \mu_B \\ s.t. \ & \mu_B \leq 18.46 - 5.01\Delta d_1 - 10.43\Delta d_2 \\ & 0 \leq \Delta d_1 \leq 4 \\ & 0 \leq \Delta d_2 \leq 4 \end{aligned}$$

The solution of the master problem yields the following redesign $(\Delta d_1, \Delta d_2) = (0, 0)$ and an upper bound of EP_U^1=18.46 units.

Step 6: Since the stopping criterion is not satisfied $EP_U^1 = 18.46 > EP_L$ =-25.56, set k=k+1 and return to Step 2.

The proposed approach requires 6 iterations to reach the optimal solution within a tolerance of 0.01 for the lower and upper bounds. The optimal solution corresponds

BIBL. LONDIN. UNIV.

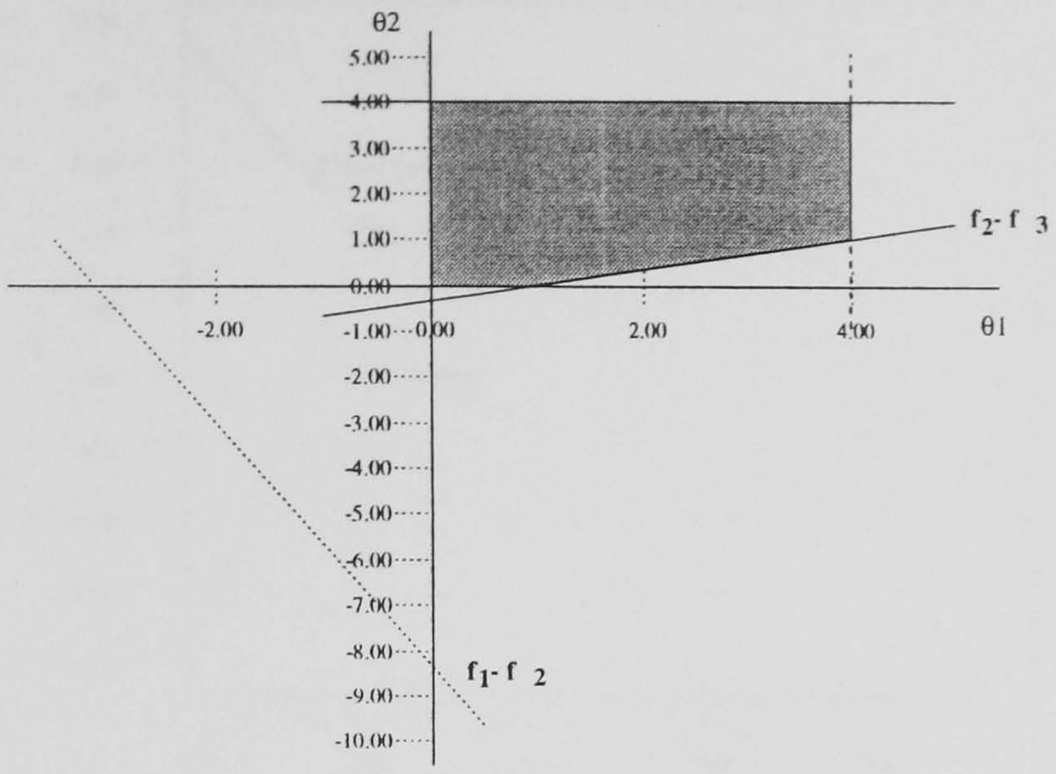


Figure 2.5: Feasible region of the initial design - Example 1

to the design changes $(\Delta d_1, \Delta d_2)$= (0, 0.462). This redesign has an expected profit of 4.28 units within a corresponding feasible region (see Figure 2.6) defined by the following bounds: for θ_1, $0 \leq \theta_1 \leq 4$, and for each quadrature point $\theta_1^{q_1}$ by bounds for θ_2 as shown in Table 2.3.

q_1	1	2	3	4	5
$\theta_1^{q_1}$	0.188	0.923	2.000	3.077	3.812
$\theta_2^{Lq_1}$	0.29	0.00	0.00	0.00	0.172
$\theta_2^{Uq_1}$	4	4	4	4	4

Table 2.3: Bounds for θ_2 at $\theta_1^{q_1}$ of optimal design

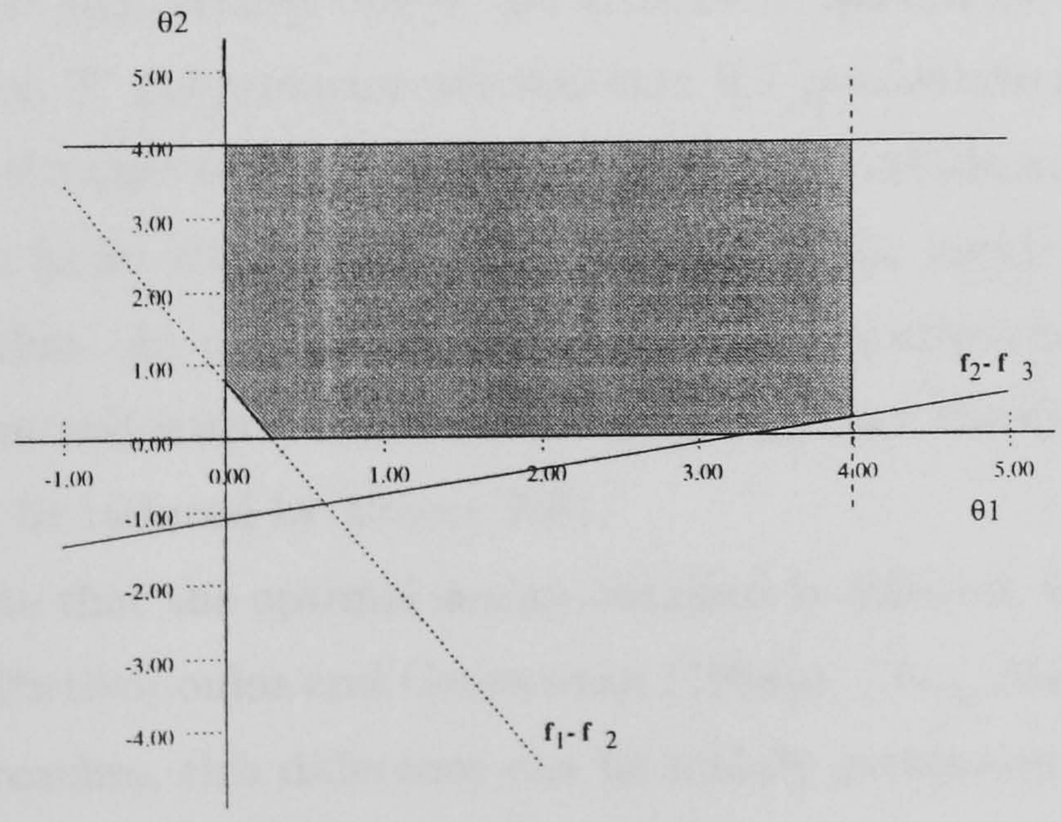


Figure 2.6: Feasible region of the optimal design - Example 1

The progress of the convergence of the algorithm is shown in Figure 2.7. Using

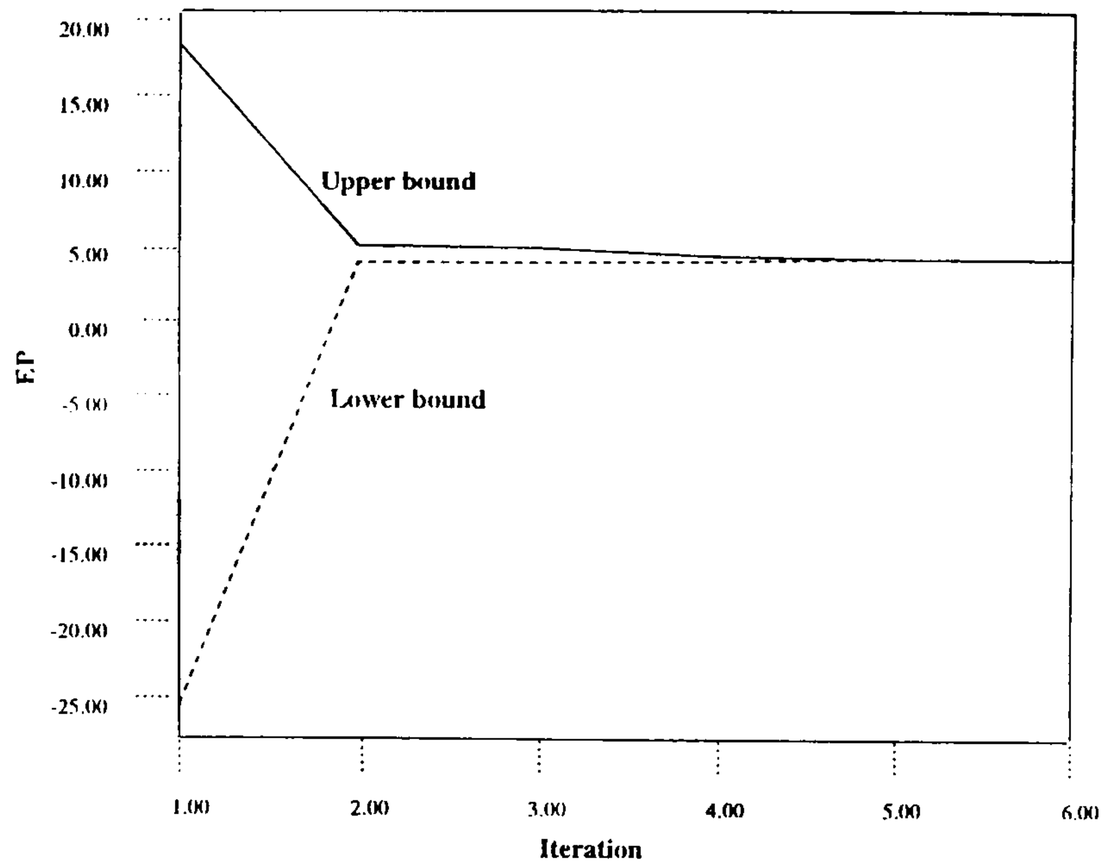


Figure 2.7: Convergence of the algorithm - Example 1

GAMS/MINOS for the solution of the linear subproblems and master problem it requires a total of approximately 34.8 CPU s on SPARC IPX (5.8 CPU s for each iteration with approximately 5.5 CPU s spent at the solution of the subproblems and 0.3 CPU s at the solution of the master problem). The effect of considering different numbersof quadrature points for each θ direction is illustrated in Table 2.4. Starting from the same initial point, the number of iterations required does not change significantly. This is expected, since the convergence of the algorithm mainly depends on the values of the upper and lower bounds obtained based on the approximation of the objective function, whereas the number of quadrature points affects the quality of the numerical approximation of the multiple integral of the expected profit. On the other hand, the computational time needed per iteration increases significantly due to the increase in the number of subproblems that have to be solved (e.g. 57 subproblems per iteration if 7 quadrature points are considered compared to 31 for the case of 5 quadrature points). Computational considerations need further investigation in an attempt to take advantage of the highly parallel structure of the proposed algorithm. At the limit, if the independent optimization tasks were solved on parallel processors and with a linear speed-up factor, then the CPU time required for each iteration could be reduced by almost 70%.

Finally, note that the optimal design obtained is different to the one obtained by the approach of Pistikopoulos and Grossmann (1988b), $(\Delta d_1, \Delta d_2) = (0, 0.335)$. Comparing the two approaches, this difference can be mainly attributed to the following reasons:

(i) the approach of Pistikopoulos and Grossmann (1988b) is based on an iterative procedure, where first the designs corresponding to minimum retrofit investment cost

Quadrature points in each θ direction	Inner Subproblems	CPU time per iteration	Number of iterations
5	31	5.8	6
7	57	8	7
9	91	15	7

Table 2.4: Results for different number of quadrature points - Example 1

are obtained and then the expected revenue is estimated and optimized; in contrast, this new algorithm performs directly the maximization of the expected profit by balancing investment cost and revenue.

(ii) in Pistikopoulos and Grossmann (1988b), the evaluation of the expected profit term was performed within the area confined by the definition of the scalar flexibility index of Swaney and Grossmann (1985); in contrast here the expected profit term is evaluated within the actual feasible region of the design (approximated by the Gaussian Integration formula), thus providing a better approximation of its value.

(b) three uncertain parameters

A variation of the model in case (a) is considered here involving three uncertain parameters with probability distributional data as shown in Table 2.5.

$$f_1 = z - \theta_1 + 0.5\theta_2 + d_1 - 3d_2 + 2\theta_3 - 8 \leq 0$$
$$f_2 = -z - \theta_1/3 - \theta_2 + d_2 - \theta_3/3 + 8/3 \leq 0$$
$$f_3 = z + \theta_1 - \theta_2 - d_1 + \theta_3 - 4 \leq 0$$

Uncertain parameter	Distribution function	Mean value	Positive deviation	Negative deviation
θ_1	N(2, 0.5)	2	2	2
θ_2	N(2, 0.5)	2	2	2
θ_3	N(2, 0.5)	2	2	2

Table 2.5: Data for uncertain parameters - Example 1

By implementing the algorithm from the same initial redesign, convergence is achieved after 6 iterations. The optimal design changes in this case are $(\Delta d_1, \Delta d_2)$=

(0.69, 0.0) with an expected profit equal to 24.42 units. Note that the required computational effort increases significantly (a total of 300 CPU s) mainly due to the large number of subproblems that have to be solved per iteration (156 optimization subproblems for the case of 5 quadrature points compared to 31 for the case of 2 uncertain parameters). These computational requirements intensify the need for a parallel implementation especially in view of the fact that this large number of optimization subproblems can be in fact solved independently.

Example 2: A convex mixed integer nonlinear model

Consider the following model:

$$EP = \max_{y_1,y_2,d_1,d_2} E_\theta\{\max_{z_1,z_2,z_3}\{200z_3 - 12z_1 - 10z_2\}\} - (5d_1 + 9d_2) - (20y_1 + 30y_2)$$

subject to:

$$2z_3 + 1.6\theta_1 - 1.6z_1 - 2.14z_2 \leq 0$$

$$1.7z_1 + z_2^2 - 0.62\theta_2 \leq 0$$

$$2.61z_1 - d_1 \leq 0$$

$$3.14z_2 - d_2 \leq 0$$

$$2y_1 \leq d_1 \leq 5y_1$$

$$2y_2 \leq d_2 \leq 5y_2$$

$$y_1 + y_2 \geq 1$$

$$y_1, y_2 = \{0, 1\},\ z_1, z_2 \geq 0,\ z_3 \geq 1.3$$

where EP is the expected profit; y_1, y_2 are (0,1) binary structural variables; d_1, d_2 continuous design variables; z_1, z_2, z_3 control variables; θ_1, θ_2 uncertain parameters with distribution functions as shown in Table 2.6. Note that the model is convex in z and linear in d and θ; it also involves (0,1) variables and therefore corresponds to a convex mixed integer nonlinear program.

Uncertain parameter	Distribution function	Mean value	Positive deviation	Negative deviation
θ_1	N(1.6, 0.25)	1.6	1	1
θ_2	N(5, 1)	5	4	4

Table 2.6: Data for uncertain parameters - Example 2

The proposed algorithm can be readily applied to this type of mixed integer de-

sign models by considering as complicating variables both the (0,1) binary and continuous design variables:

Step 1: An initial structure and design is selected : $(y_1, y_2) = (1,0)$; $(d_1, d_2) = (3.5,0)$ $EP_L = -\infty$, k=1 and $\epsilon = 0.1$.

Step 2: The solution of the feasibility problems (B1),$(B2^{q_1})$ leads to the identification of the feasible region as shown in Figure 2.8.

Step 3-4: Considering 8 quadrature points for θ_2, the expected profit is evaluated through the Gaussian Quadrature formula yielding a value of 68.34 units; the lower bound is updated, $EP_L = 68.34$.

Step 5a,5b: After the evaluation of the corrected multipliers the master problem is formulated as follows:

$$
\begin{aligned}
EP_U^k = \max_{\mu_B, y_1, y_2, d_1, d_2} \ & \mu_B \\
s.t. \ & \mu_B \leq -334.75 - 20y_1 - 30y_2 + 120.88d_1 + 142.39d_2 \\
& 2y_1 \leq d_1 \leq 5y_1 \\
& 2y_2 \leq d_2 \leq 5y_2 \\
& y_1 + y_2 \geq 1
\end{aligned}
$$

The solution of the master MILP problem yields the following values for the (0,1) and continuous design variables:$(y_1, y_2) = (1, 1)$, $(d_1, d_2) = (5, 5)$ and an upper bound of EP_U^1=931.6 units.

Step 6: Since the stopping criterion is not satisfied EP_U^1=931.6 > EP_L=68.34, set k=k+1 and return to Step 2.

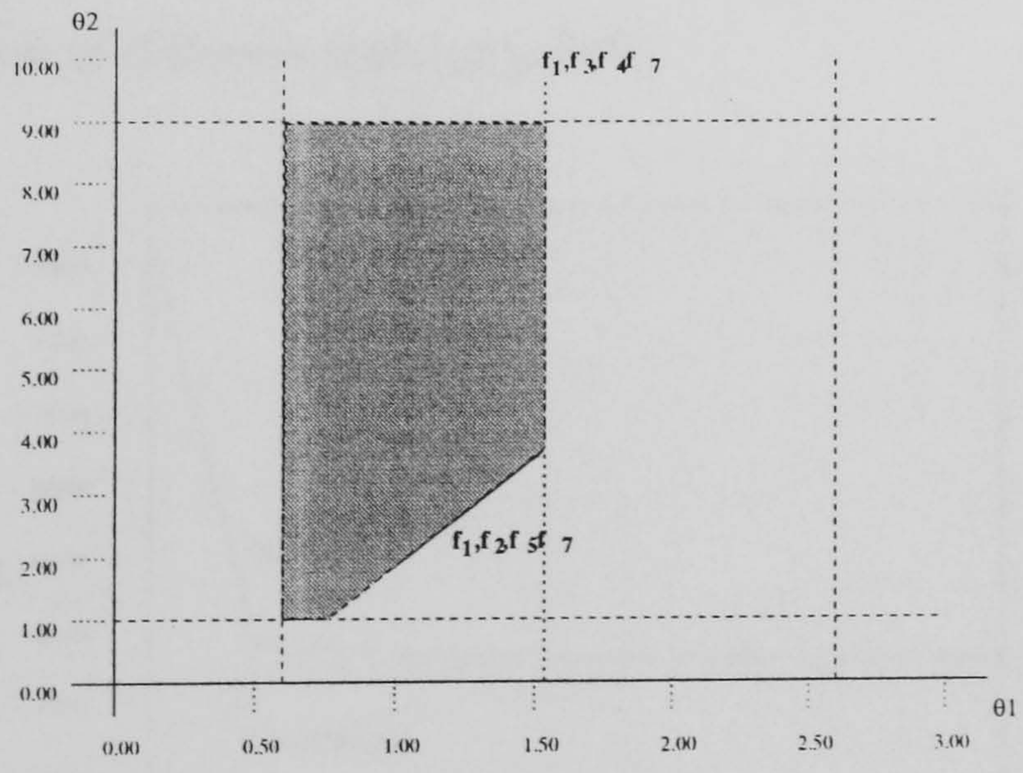


Figure 2.8: Feasible region of the initial design - Example 2

The proposed approach requires 9 iterations to reach the optimal solution within a tolerance of 0.03 for the lower and upper bounds. The optimal solution is the plant that corresponds to the following values of the structural and design variables $(y_1, y_2) = (1, 1)$, $(d_1, d_2) = (4.6, 3.9)$. This plant has an expected profit of 354.3 units within its

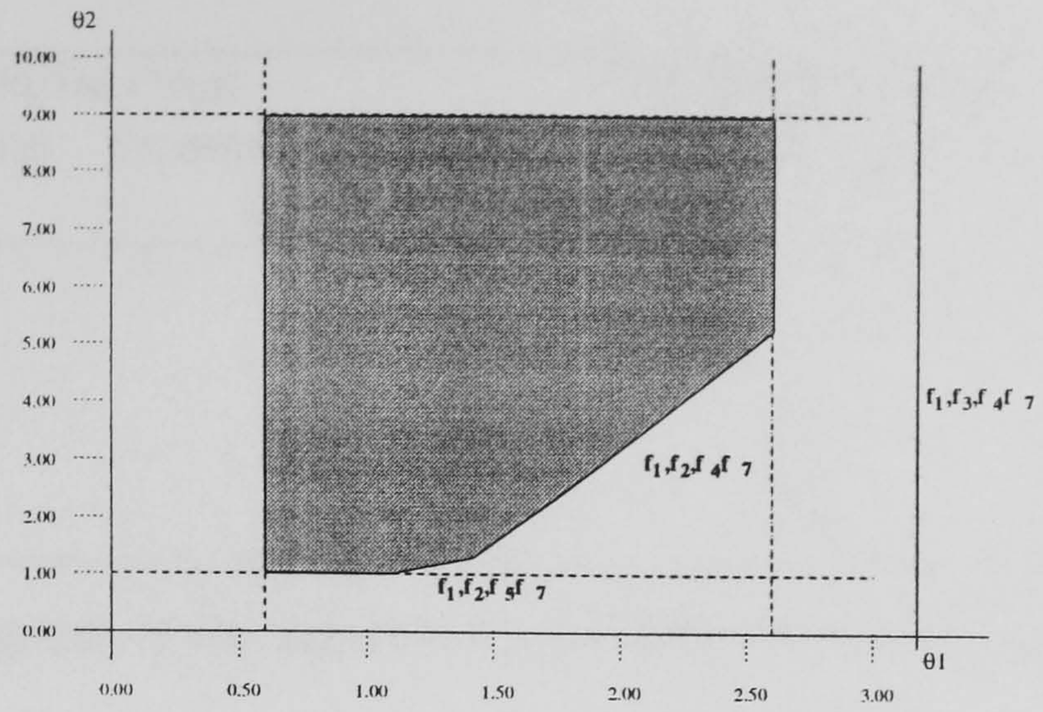


Figure 2.9: Feasible region of the optimal design - Example 2

corresponding feasible region as depicted in Figure 2.9.

The progress of the convergence of the algorithm is shown in Figure 2.10. Using GAMS/MINOS for the solution of the nonlinear subproblems and GAMS/SCICONIC for the solution of MILP master problem it requires a total of approximately 49.5 CPU s on SPARC 2 (5.5 CPU s for each iteration with approximately 5.1 CPU s spent at the solution of the subproblems and 0.4 CPU s at the solution of the master problem). The effect of the consideration of different starting points on the performance of the algorithm is shown in Table 2.7; note that for this example, the performance of the algorithm is not sensitive to the selection of different starting points.

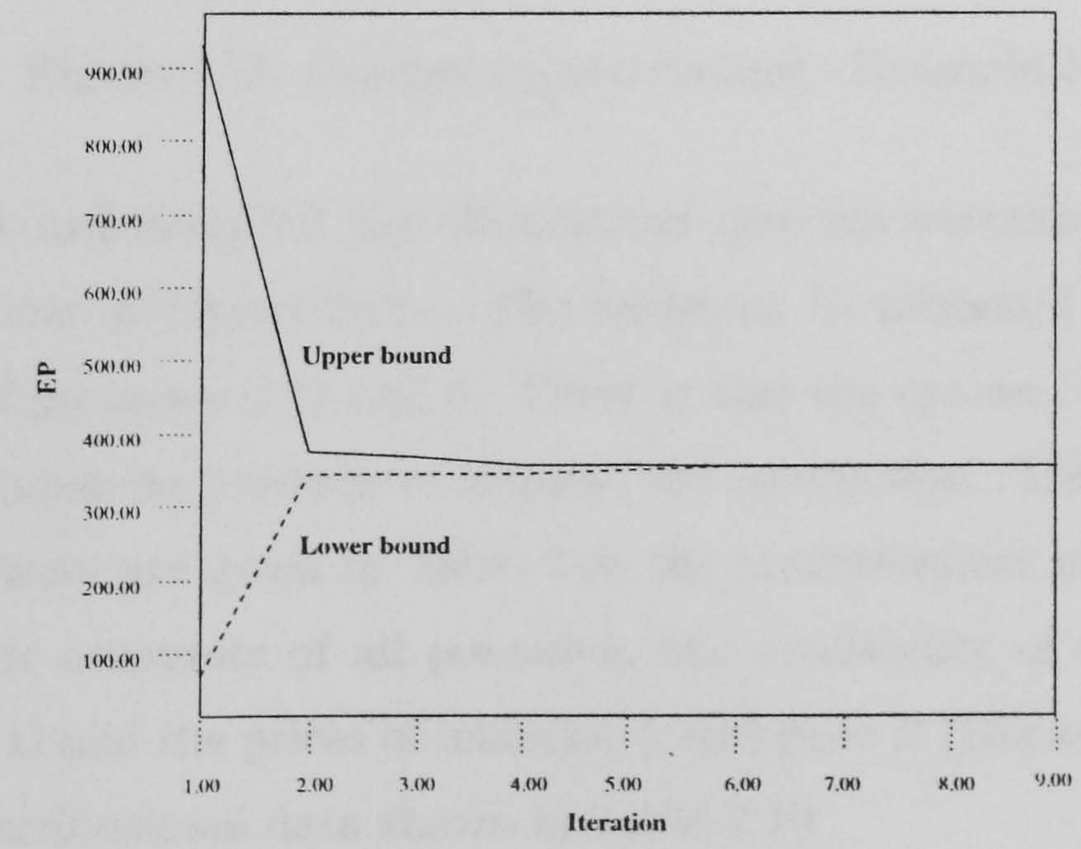


Figure 2.10: Convergence of the algorithm - Example 2

Initial Point		Computation time	Number
Design Variables (d_1, d_2)	Structure Variables (y_1, y_2)	CPU s per iteration	of iterations
(3.5,0)	(1,0)	5.5	9
(5,0)	(1,0)	5.5	10
(0,3.5)	(0,1)	5.5	10
(0,5)	(0,1)	5.5	9
(5,5)	(1,1)	5.5	9

Table 2.7: Convergence of the algorithm from different starting points - Example 2

Example 3: A Process Synthesis/Planning Model

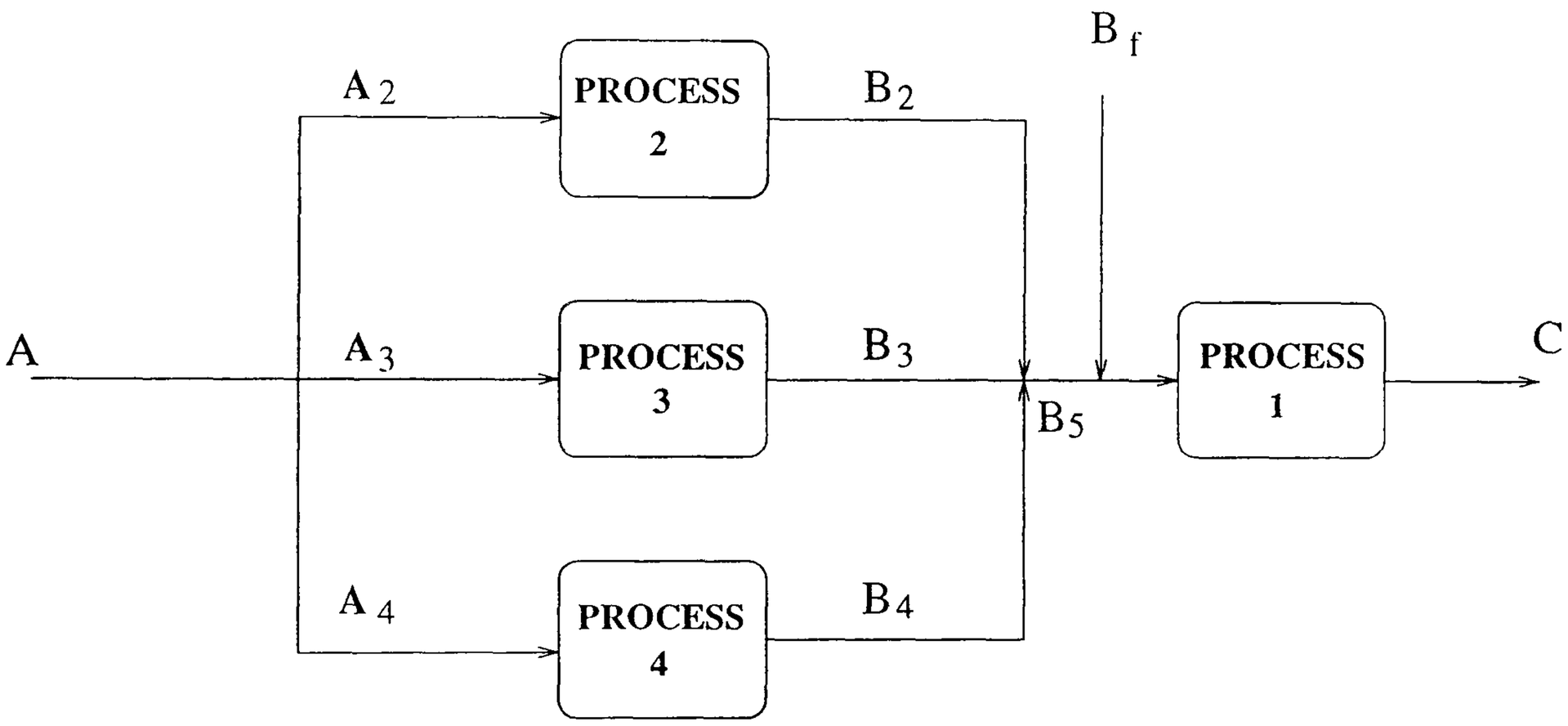


Figure 2.11: Process superstructure - Example 3

A network indicating all the alternatives (process superstructure) for the production of C is shown in Figure 2.11 . The feedstock to process 1 is produced by one or a combination of processes 2, 3 and 4. There is also the option of buying a restricted amount of the intermediate product to increase the production. The economic data and the equilibria constants are given in Table 2.8; the mathematical model is given in Table 2.9. The kinetic constants of all processes, the availability of raw material A, the demand of product C and the prices of material A and pure B (Bf) are considered to vary according to the distributional data shown in Table 2.10.

Five quadrature points were used for the integration; the algorithm took three iterations to converge to the optimal solution involving all three processes. The progress

Process	Production Constant (2.12)	Fixed cost Constant (FC)
Process 1		100
Process 2	18	80
Process 3	20	130
Process 4	15	150

Table 2.8: Data for Example 3

Material Balances	$A_2 + A_3 + A_4 = A$
	$B_2 + B_3 + B_4 = B_5$
Process conversions	$C = 0.9(B_f + B_5)$
	$B_2 = MP_2 \ln(1 + A_2/k_2)$
	$B_3 = MP_3 \ln(1 + A_3/k_3)$
	$B_4 = MP_4 \ln(1 + A_4/k_4)$
Demand Limitation	$C \leq \theta_1$
Availability Limitations	$B_f \leq 15$
	$A \leq \theta_2$
Production Limitations	$A_2 \leq 25y_2$
	$A_3 \leq 20y_3$
	$A_4 \leq 20y_4$
Objective Function	Profit $= 550C - (250A + 300B_f) -$
	$[(FC_1 + 15(B_f + B_5)) - (FC_2y_2 + 5A_2) -$
	$(FC_3y_3 + 15A_3) - (FC_4y_4 + 5A_4)]$
A_2, A_3, A_4	the utilization of raw material at processes 2,3, 4, respectively
B_2, B_3, B_4	the production of intermediate product B at processes 2,3,4, respectively
C	the production of final product
B_f	the amount of material B purchased
y_2, y_3, y_4	(0,1) binary structural variables representing the existence (or not) of units 2, 3 and 4

Table 2.9: Mathematical model of Example 3

Uncertain parameter	Distribution function	Mean value	Positive deviation	Negative deviation
Demand of C (θ_1)	N(17.5, 2.5)	17.5	7.5	7.5
Availability of A (θ_2)	N(27.5, 2.5)	27.5	7.5	7.5
Cost of A (θ_3)	N(250, 10)	250	30	30
Cost of B (θ_4)	N(300, 15)	300	45	45

Kinetic Constants	Periods/scenarios							
	1	2	3	4	5	6	7	8
$k_2(\theta_5)$	19	19	20	20	20	21	21	21
$k_3(\theta_6)$	20	21	21	22	22	22	21	20
$k_4(\theta_7)$	25	26	25	26	27	27	26	26
Weights	0.1	0.15	0.15	0.15	0.1	0.1	0.15	0.1

Table 2.10: Data for uncertain parameters - Example 3

of the convergence of the proposed algorithmic procedure is shown in Figure 2.12. A total of 250 CPU s on SPARC IPX was required using GAMS/MINOS for the solution of the nonlinear subproblems (83 CPU s per iteration) and GAMS/SCICONIC for the solution of the MILP master subproblem (0.15 CPU s per iteration), respectively.

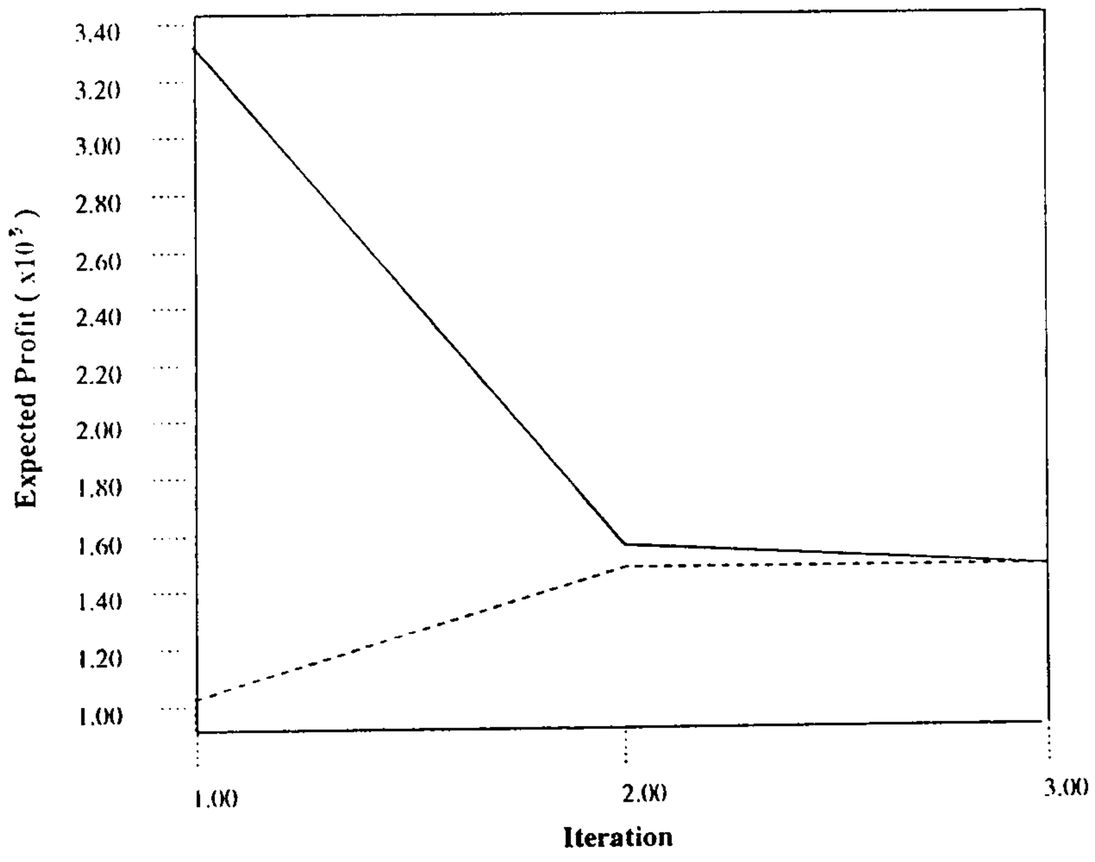


Figure 2.12: Convergence of the algorithm - Example 3

Example 4: Separation Process Synthesis

A modified version of the separation system considered in Kocis (1988) is examined here (see Figure 2.13). The problem consists in selecting the optimal separation scheme to be used to separate a process stream (F1) of two components (A and B) into two product streams (P1 and P2) for which purity specifications have been set to a minimum

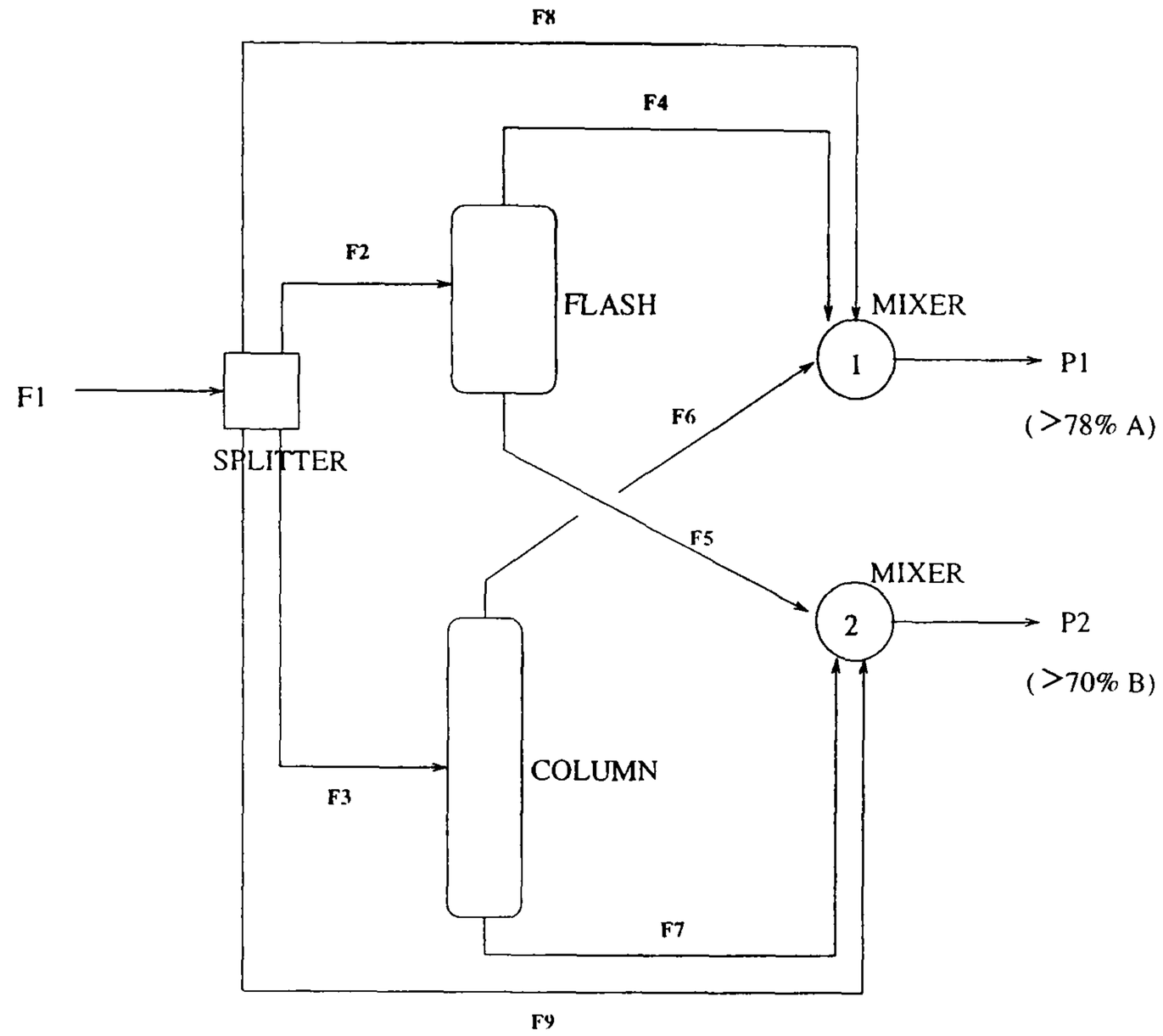


Figure 2.13: Process Superstructure - Example 4

of 78% of A in product P1 and a minimum of 70% of B in product P2. Five uncertain parameters are considered here: the input flow of A in the feedstream ($F1_A$), the separation constant for B in the flash separator (kb), the prices of the products and the cost of raw material, all described by the normal distribution functions of Table 2.12.

For this separation, a distillation column and a flash drum are considered to form the superstructure shown in Figure 2.13 where three different alternatives are embedded: flash separation, distillation, or flash separation and distillation in parallel. As seen in Figure 2.13 feed stream F1 is split into four streams (F2,F3,F8, and F9). F2 and F3 are the inputs to the flash and to the distillation column, while F8 and F9 bypass the separation units and are blended with the top and the bottom streams from the flash and distillation column, respectively to form products P1 and P2.

Mathematical Model

- Splitter mass balances

$$F2_A = S_1 F1_A$$
$$F2_B = S_1(F1 - F1_A)$$

$$F8_A = S_2 F1_A$$
$$F8_B = S_2(F1 - F1_A)$$
$$F9_A = S_3 F1_A$$
$$F9_B = S_3(F1 - F1_A)$$
$$F3_A = F1 - F2_A - F3_A - F8_A$$
$$F3_B = (F1 - F1_A) - F2_B - F3_B - F8_B$$

where S_1, S_2, S_3 are the split factors; $F1_A, F2_A$, $F3_A$, $F8_A, F9_A$ are the flowrates of component A at streams F1,F2,F3,F8,F9, respectively; whereas $F1_B, F2_B$, $F3_B$, $F8_B, F9_B$ are the flowrates of component B at the same streams.

- Flash mass balances

$$F4_A = 0.75 F2_A$$
$$F4_B = (1 - kb) F2_B$$
$$F5_A = 0.25 F2_A$$
$$F5_B = kb F2_B$$

where $F4_A, F5_A$ are the flowrates of component A at streams F4 and F5, respectively; whereas $F4_B, F5_B$ are the flowrates of component B at the same streams, and kb is the separation constant for B in the flash.

- Distillation Column mass balances

$$F6_A = 0.825 F3_A$$
$$F6_B = 0.125 F3_B$$
$$F7_A = 0.175 F3_A$$
$$F7_B = 0.875 F3_B$$

where $F6_A, F7_A$ are the flowrates of component A at streams F4 and F5, respectively, and $F6_B, F7_B$ are the flowrates of component B at the same streams.

- Mixers mass balances

$$P1_A = F4_A + F6_A + F8_A$$
$$P1_B = F4_B + F6_B + F8_B$$
$$P2_A = F5_A + F7_A + F9_A$$
$$P2_B = F5_B + F7_B + F9_B$$

where $P1_A, P2_A$ are the flowrates of component A at products P1 and P2, respectively; whereas $P1_B, P2_B$ are the flowrates of component B at these products.

- Product Purity requirements

$$P1_A \geq 3.5P1_B$$

$$P2_B \geq 2.5P2_A$$

- Design Equations

$$D_F^2 \geq \frac{1.27M(F4_A + F4_B)}{45v\rho_v}$$

$$D_C^2 \geq \frac{1.27M(F3_A + F3_B)}{35v\rho_v}$$

where D_F, D_C are the diameters of flash and column, respectively; M is the molecular weight of the feed; ρ_v is the vapour density of the feed and v is the velocity of vapour phase in the drums given by:

$$v = 0.064\sqrt{(\rho_l - \rho_v)/\rho_v}$$

where ρ_l is the liquid density of the feed.

- Size Restrictions

$$2.2y_C \leq D_C \leq 6y_C$$

$$2.2y_F \leq D_F \leq 5.5y_F$$

where y_C, y_F are binary variables corresponding to the selection of column or flash, respectively.

- Objective function

$$\begin{aligned} \text{Profit} \quad = \quad & (45P1_A + 40P2_B) - 8F1 - \\ & [(20y_F + 2D_F^2) + 0.2(F2_A + F2_B)] - \\ & [(50y_C + D_C^2(0.3NP + 2)) + 2.5(F3_A + F3_B)] \end{aligned}$$

where the first term corresponds to revenue from product sales, the second term represents purchase cost for F1 and the two other terms correspond to costs for the flash separator and distillation column. Problem constants are given in Table 2.11.

The above model is a MINLP problem where nonlinearities appear in the objective function in the capital cost of units and in the design equations due to the presence of the terms D_C^2, D_F^2 and also in the splitter and flash mass balances since splitter fractions are variables and the separation constant of flash k_b as well as the flowrate of component A at feed stream are considered as uncertain parameters. The introduction of the auxiliary

Parameters	Values
F1 (Feed flowrate)	33
M (Molecular Weight)	92
ρ_l (Liquid Density)	883
ρ_v (Vapour Density)	3
NP (Number of plates in column)	20

Table 2.11: Data for Example 4

Uncertain parameter	Distribution function	Mean value	Positive deviation	Negative deviation
$F1_A$	N(15, 0.667)	15	17	13
kb	N(0.84, 0.1)	0.84	0.88	0.8
Price of A	N(75, 1.25)	75	80	70
Price of B	N(55, 1.25)	55	60	50
Cost of feed	N(8, 0.5)	8	10	6

Table 2.12: Data for uncertain parameters - Example 4

variables $d_C = D_C^2$ leads to the convexification of the capital cost and design equations with respect to design variables D_F, D_C. However, nonconvexities still remain due to the splitter and flash mass balances since $F1_A, k_b$ are considered as uncertain parameters and consequently are optimization variables of the feasibility subproblems.

The proposed approach is applied by considering the binary structure variables y_C, y_F and the continuous design variables D_C, D_F as complicating variables and the splitter fractions S_1, S_2, S_3 as control variables. Starting from a structure consisting of both units ($d_F = 20, d_C = 10$) and using 5 quadrature points, the algorithm takes 8 iterations to converge to an optimal structure where both units are present with diameters 4.4m and 2.9m for the flash and the column, respectively, with expected annual profit of \$1,609,897. The algorithm requires also 8 to 9 iterations to converge to the same optimal solution from different starting points. Using GAMS/MINOS for the solution of the NLP subproblems and ZOOM for the solution of master MILP problem, the computational times on Sparc10 are approximately 0.4 CPUs for the feasibility and profit maximization subproblems and 0.9 CPUs for master problem.

Example 5: Reaction-Separation System

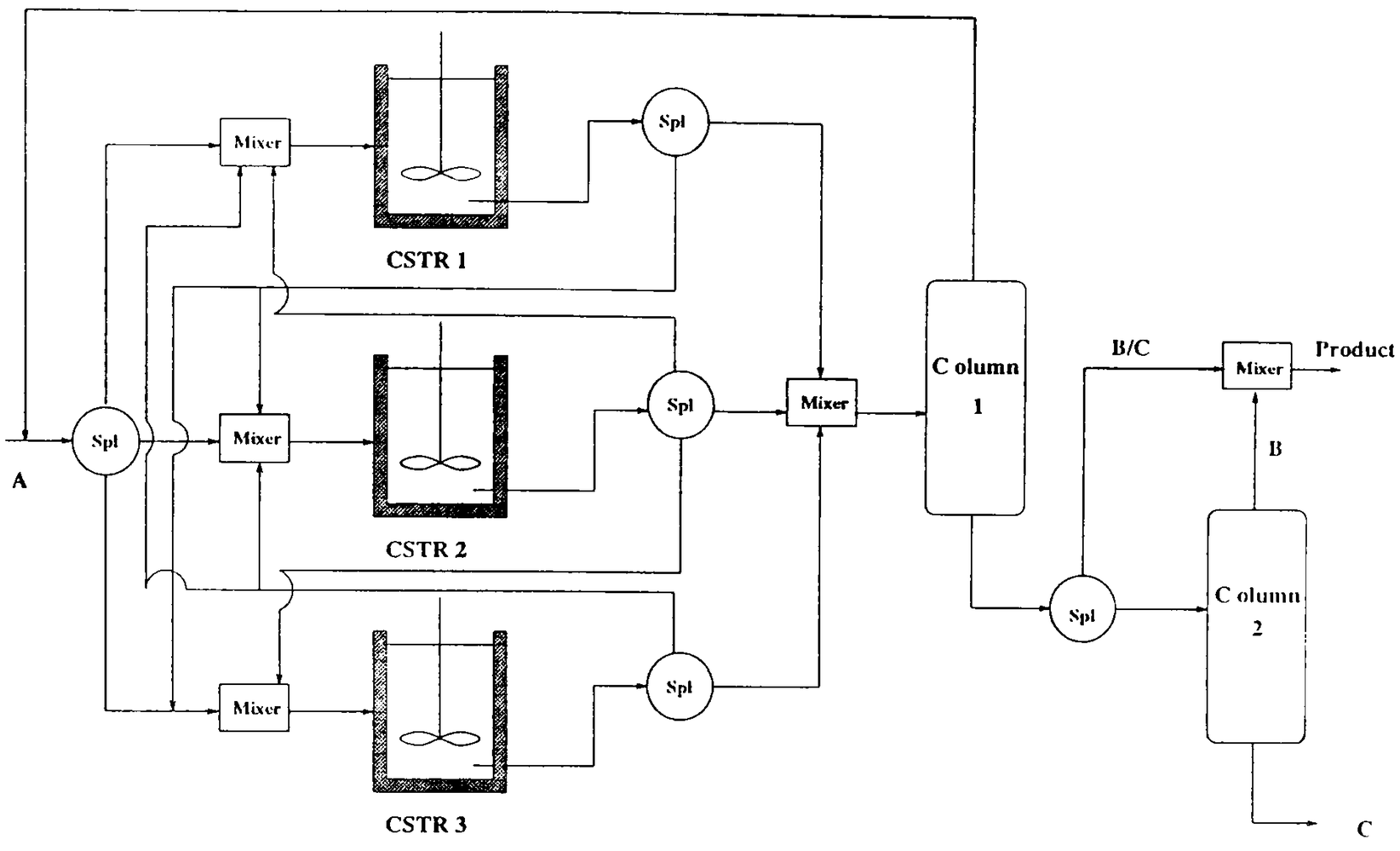


Figure 2.14: Benzene chlorination process

A benzene chlorination process is examined here, consisting of two consecutive first-order irreversible reactions, where benzene (A) is consecutively transformed into monochlorobenzene (B) and dichlorobenzene (C). As shown in Figure 2.14, the process involves a reaction section, where three CSTRs can be potentially used in any possible combination (full connectivity), and a separation section involving two distillation columns - in the first column unreacted benzene is separated and recycled with the bottom stream of mono- and di- chlorobenzene separated in a second column according to purity requirements (see Kokossis and Floudas, 1991 for the complete mathematical model). Product demand and quality (in terms of chlorobenzene molar fraction) are considered as uncertain parameters following normal probability distribution functions, N(55,1.67) and N(0.985, 0.00167), respectively.

First-stage decisions comprise plant configuration and unit capacities i.e. how many reactors are required, the actual reactor network, whether a second distillation unit is required and volumes of reactors. Second-stage decisions mainly involve operating variables, split fractions, etc. The proposed algorithmic procedure requires 6 iterations and 16.3 CPU s per iteration in SPARC 10 to converge in an optimal solution with an expected profit of 6.99 $\times 10^4$ \$/year involving the installation of all three reactors in series with corresponding capacities of 9.6, 3.5 and 3.5 m^3 followed by two distillation columns for chlorobenzene separation. Although no claim can be made for this case regarding

global optimality, the reported solution is the best obtained from different starting points. Figure 2.15 illustrates the EP as a function of total reactor capacity with the maximum corresponding to the optimal plant of $18m^3$ reactor capacity.

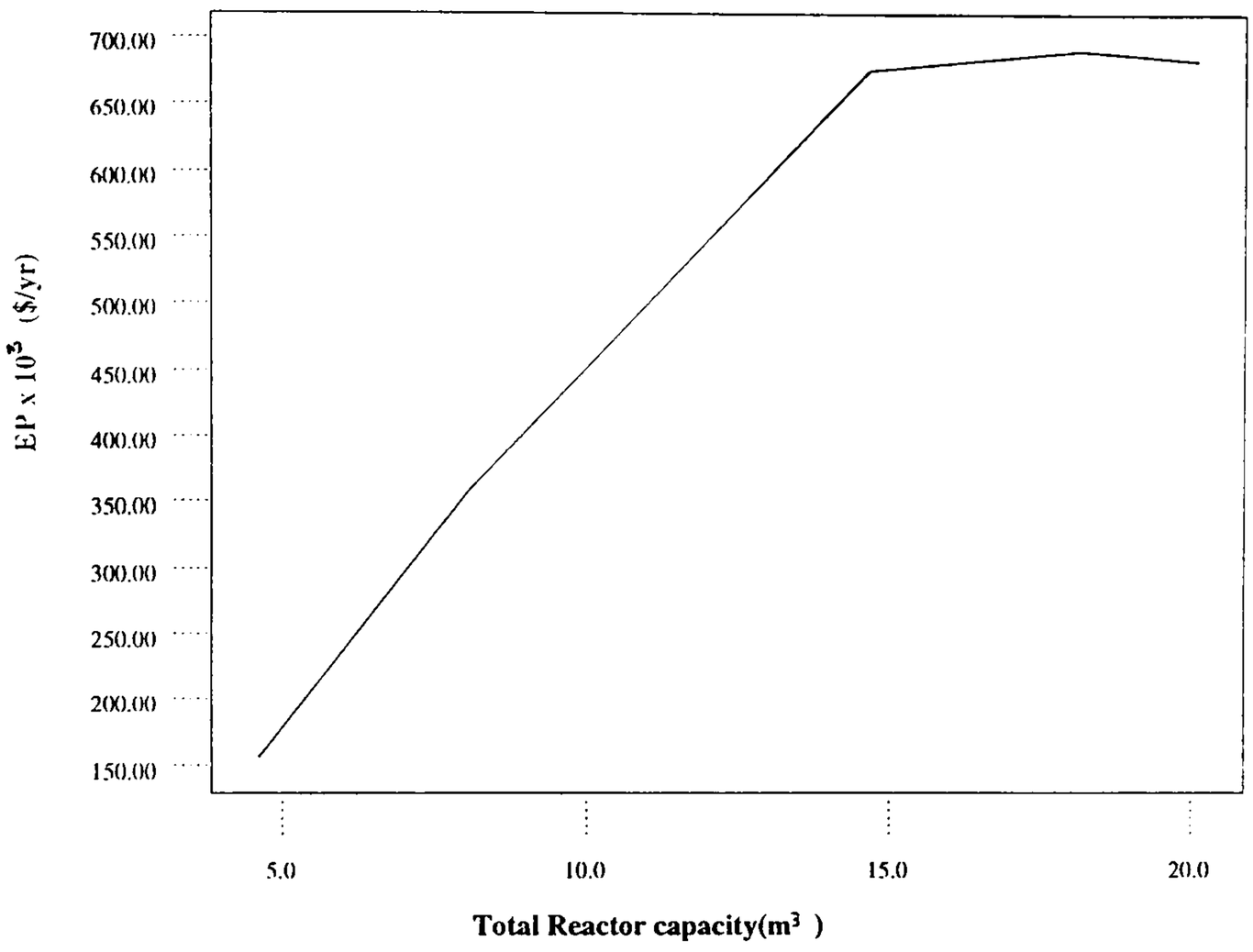


Figure 2.15: Expected profit vs. Reactor capacity - Example 5

The same problem is then solved considering also the kinetic constants as uncertain parameters varying within the ranges: $k_1 \in [0.453, 0.458]hr^{-1}$, $k_2 \in [0.053, 0.056]hr^{-1}$. A multiperiod formulation is considered for these parameters assuming 5 periods resulting in a model of 492 variables and 482 constraints. The application of the proposed approach requires 5 iterations to converge to an optimal plant involving 2 reactors of 8.4 and $8.1m^3$, respectively and only one distillation column with an expected profit of 6.99×10^4 \$/year. An average of 2.3 CPUs is required for the feasibility and profit maximization subproblems and 2.6 to 3.8 CPU s for the master problem.

2.5. Summary

In this chapter modelling issues regarding process engineering problems under uncertainty were discussed. In particular, the different types of uncertainty have been identified and embodied within a combined multiperiod/stochastic optimization framework. A decomposition-based algorithm has also been presented that properly exploits the structure of the optimization model resulting in an optimal design with maximum expected profit and optimum degree of flexibility. A key feature of the proposed approach is that

feasibility is performed simultaneously with economic optimality; the approach also features a highly parallel structure that can be further exploited to enhance computational performance. Five example problems from the area of process synthesis and design under uncertainty have been presented to illustrate the potential of the proposed algorithmic procedure.

Chapter 3

Batch Plant Design and Operations under Uncertainty

This chapter addresses the problem of including aspects of uncertainty in process parameters and product demands at the design stage of multiproduct/multipurpose batch plants. It is shown that based on the special structure of the problem, feasibility properties can be derived enabling transformation of the two-stage stochastic problem to a single model in which the structure of the corresponding deterministic model is fully preserved. Efficient global optimization procedures are then proposed for the case of continuous and discrete equipment sizes. The versatility of the proposed unified framework is demonstrated with a battery of example problems covering most batch plant design and scheduling formulations previously suggested in the open literature.

3.1. Introduction

While significant developments have been made in the design and scheduling of multiproduct/multipurpose batch plants (see Reklaitis, 1990, and Rippin, 1993, for extensive reviews), the problem of "flexibility and uncertainty" (Rippin, 1993) in batch processing has received much less attention; yet, its practical relevance is obvious considering the incomplete information about the chemical/physical steps involved, the high degree of uncertainty regarding recipe parameters, resource and equipment availabilities, product demands and product market trends as well as the need to process multiple products in the same facility. In this chapter, a unified framework is presented to address the problem of dealing with uncertainty at the design of batch plants. In the rest of this section a brief literature review is made on both deterministic and stochastic approaches of batch plant design.

3.1.1. Deterministic Design Problem

Among the works that have appeared in the literature, Grossmann and Sargent (1979) have presented a mixed integer nonlinear programming formulation to address the problem of multiproduct batch plant design operating with single product campaign (SPC). Birewar and Grossmann (1989) considered the incorporation of scheduling with mixed product campaigns. A mixed integer linear programming reformulation of the above models presented by Voudouris and Grossmann (1992) was based on the consideration of discrete equipment sizes.

Most of the early works on the design of multipurpose batch plants (Suhami and Mah, 1982; Vaselenak et al., 1987; Faqir and Karimi, 1989) considered plants operating in SPC and single production routes. Faqir and Karimi (1990) presented a MINLP formulation for the more realistic case of multiple production routes. Voudouris and Grossmann (1992) used the discrete equipment sizes to reformulate the problem as a MILP program. A more complete formulation with different assignments of equipments to tasks developed by Papageorgaki and Reklaitis (1990). Finally, Shah and Pantelides (1991) considered the effect of intermediate storage in order to decouple the production of different products into stages.

3.1.2. Batch Plant Design Problem under Uncertainty

Despite the fact that perfect models are rare in practical applications, the direct solution of the nominal (deterministic) optimization problems is the most frequent approach in industrial applications in which case the parameters are chosen at or near their mean values over the modelling runs. Among the academic research contributions to deal with the problem of designing batch plants under uncertainty is the work of Reinhart and Rippin (1986,1987) and the subsequent extensions of Fichtner et al. (1990), who presented a number of model variants and solution procedures (scenario-based, penalty functions, two-stage approach) for the problem of multiproduct batch plant design with uncertain demands assuming one piece of equipment per stage. Wellons and Reklaitis (1989) also investigated the flexibility of multiproduct batch plants. They considered staged plant expansion over time to account for uncertainty in product demand; they also suggested a distinction between "hard" and "soft" constraints, introducing penalty terms for the latter type. Assuming as uncertain the time it takes for each product to reach the target product demand, they derived analytical expressions of expected profit objective. Straub

and Grossmann (1992) considered uncertainties in both product demands and equipment availability, and presented a framework to maximize an expected profit by considering separately economic optimality and design feasibility. Shah and Pantelides (1992) presented a scenario-based approach for the design of multipurpose batch plants considering different schedules for different set of production requirements. Rotstein et al. (1994) presented a MILP formulation for the evaluation of a lower bound of stochastic flexibility of multipurpose batch plants based on the assumption of independent uncertain parameters (appearing only at the RHS of the constraint set). Subrahmanyam et al. (1994) have addressed the problem of design and operations of batch processes under demand uncertainty employing a scenario-based approach based on a discrete representation of uncertain demands with known probabilities. They incorporate scheduling problem within a decomposition solution approach as a subsequent stage solved after the design problem. However, they did not fully exploit the plant flexibility since (i) design optimization and scheduling determination are performed independently, (ii) they did not account for different schedules with respect to uncertain parameter realizations, and (iii) the set of scenarios considered and the corresponding probabilities of occurrence are assumed to be known a priori (i.e. trade-offs between feasibility and economic optimality are not considered).

The objective here is to establish a unified framework to deal with uncertainty in the design and operations of batch plants. Uncertainty in process parameters and product demands is considered based on which a two-stage stochastic programming formulation is proposed. The proposed general formulation featuring a relaxation of the feasibility requirement with respect to uncertain demand conceptually allows economic optimality and plant feasibility to be performed simultaneously. It is shown that the exploitation of the special structure of the problem enables the transformation of the initial two-stage (embedded) stochastic formulation to a single optimization problem, which can be efficiently solved for the cases of discrete and continuous equipment sizes.

The rest of the chapter is organised as follows. First, in the next section a general two-stage stochastic programming formulation is proposed to capture the consideration of both process uncertainties and demand variations, the main features of the stochastic design problem are presented and the key properties are established that transforms the original two-stage problem to a single optimization model. Then in section 3.3 a global optimization approach is proposed for the case of continuous equipment sizes, whereas in section 3.4 a MILP reformulation is presented based on the assumption of discrete

equipment sizes. Finally, section 3.5 presents various applications of the proposed unified approach to design of multiproduct/multipurpose batch plants under uncertainty.

3.2. A Conceptual Mathematical Formulation

We consider multiproduct/multipurpose batch plant design models involving uncertainty in (i) processing times and size factors, reflecting process variability and model inaccuracy, and (ii) product demands, reflecting changing market conditions and/or variations of forecasted customer orders. The design objective is then to:

Obtain an optimal design and corresponding operating plan for the manufacturing (over time) of the various products, by ensuring (i) feasible batch plant operation for any possible realization of the processing times and size factors variations, and (ii) optimal demand order satisfaction, in order to maximize an expected profit criterion.

Such a design objective is more general than simply requiring feasibility for a number of postulated scenarios, used to describe the various elements of uncertainty. In fact, as will be shown later, scenario-based formulations can be obtained as special cases of the problem as posed above.

In order to mathematically represent the proposed design objective, three additional modelling features are considered:

(i) expected profit will be evaluated within the feasible operating region of the batch plant - this will ensure a balanced consideration of economic potential and design feasibility (Pistikopoulos and Ierapetritou, 1995)

(ii) demand constraints will be partially relaxed and a penalty term will be included in the objective function - the former will ensure best utilization of available resources where the latter is needed to monitor the extent of demand satisfaction (see also Wellons and Reklaitis, 1992)

(iii) processing times and size factors are described via a compact parameter set defined by appropriate lower and upper bounds; demand orders are given by a vector of (forecasted) probability distribution functions.

Based on the above considerations and the design objective, the following general

mathematical formulation is proposed (for ease in the presentation the case of multiproduct batch plant operating in a single product campaign mode is first considered here; the extension to other operational modes is shown later in the subsequent sections):

Problem (3.1)

$$\max_{V_j,N_j} E_{\theta\in R(V_j,N_j)} \sum_p w^p \max_{Q_i^p} \sum_i p_i Q_i^p - \delta \sum_j N_j a_j V_j^{\beta_j}$$
$$-\gamma E_{\theta\in R(V_j,N_j)} \sum_p w^p \max_{Q_i^p} (\sum_i p_i \theta_i - \sum_i p_i Q_i^p)$$

$$s.t. \quad \sum_i \frac{Q_i^p T_{Li}^p}{B_i} \leq H \; ; \; \forall p$$

$$T_{Li}^p \geq (\frac{t_{ij}^p}{N_j}) \; ; \; \forall i,j,p$$

$$B_i \leq \frac{V_j}{S_{ij}^p} \; ; \; \forall i,j,p$$

$$Q_i^p \leq \theta_i \; ; \; \forall i,p$$

$$\theta_i \in R(V_j, N_j)$$

where p=1,..,P is the set of scenarios used to describe the variation of process parameters t_{ij}, S_{ij}; θ is the vector of uncertain product demands (see also nomenclature); $R(V_j, N_j)$ is the feasible region of the design (V_j, N_j) i.e. $R(V_j, N_j) = \{\theta \mid \forall\theta \in R \exists Q_i, T_{Li}$ which satisfy the constraints of problem (3.1)$\}$.

Problem (3.1) mathematically describes a design strategy consisting of two stages. At the first stage the objective is to select the volume and the number of batch equipments per stage that maximize an expected profit, whereas at the second stage the optimal production policy (Q_i) and/or schedule is determined for each realization of the uncertainty θ_i and S_{ij}^p, t_{ij}^p. Long-term demand variations via capacity expansion options (as in Wellons and Reklaitis, 1992), can also be included in problem (3.1) as discussed in Appendix B.1.

Other strategies that have appeared in the open literature with regard to demand consideration are the following (see Figure 3.1 for graphic representation):

- $Q_i = \theta_i, \theta_i \in R(V_j, N_j)$ representing the decision maker's choice to meet always the demand within plant's feasible region (see Pistikopoulos and Ierapetritou, 1995)

- $Q_i = \theta_i, \theta_i \in T(\theta_i)$ (scenario approach) representing the DM requirement of demand satisfaction within a specified range T defined by appropriate lower and upper bounds (see Subrahmanyam et al. 1994)

It is interesting to note that, as illustrated in Figure 3.2, the proposed approach captures the whole family of model instances regarding the demand satisfaction depending on the values of the penalty coefficient γ as it is shown in Figure 3.2. In particular, as the value of γ increases implying a more severe penalization of partial order fulfilment, the result of decision strategy in (3.1) moves towards the direction of complete demand satisfaction which coincides with the result of scenario-based approach. It can be proved (see Appendix B.2) that there exists a critical value of γ for which problem (3.1) is equivalent to the multiperiod formulation with $\theta_i \in T(\theta_i)$. Note also that the priority of demand satisfaction among the different products is controlled by the relative values of the ratio T_{Li}/B_i representing the required batch production time for product i as well as the relative values of product prices p_i.

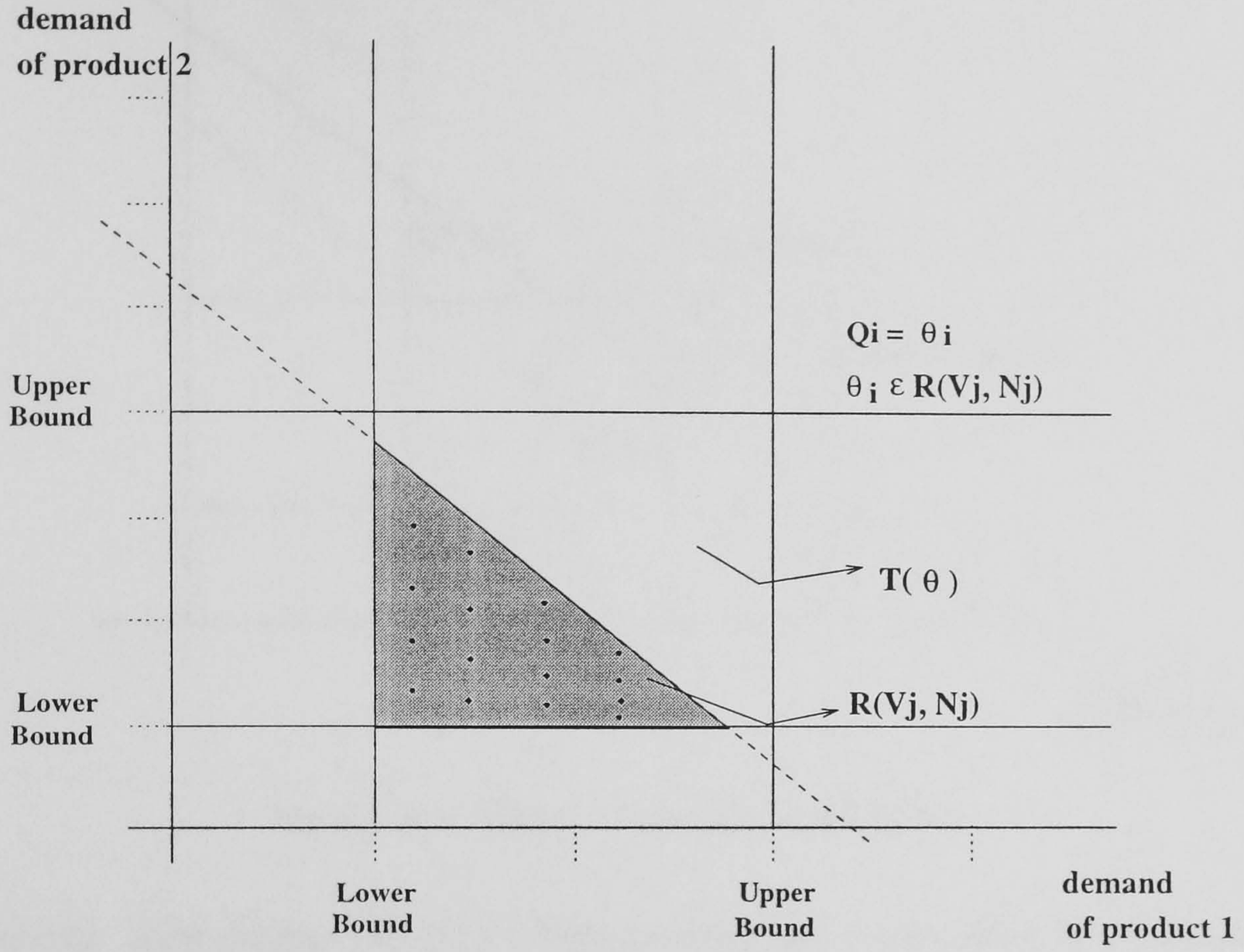
However, problem (3.1) cannot be directly solved since it involves the evaluation of the expected profit within the unknown at the design stage feasible region of the plant and moreover it requires an integration (expectation evaluation) over an optimization problem (maximization of revenue with respect to production variables). These difficulties can be overcome based on the following ideas:

(i) The multiple integral for the expected revenue evaluation over the feasible region of the design is approximated through a Gaussian quadrature formula (with q=1,..,Q quadrature points) as follows:

$$\int_{\theta \in \mathbf{R}} \sum_{p=1}^{P} w^p \sum_{i=1}^{N} p_i \bar{Q}_i^k J(\theta) d\theta = \sum_{\theta^q \in \mathbf{R}} w^q J^q \sum_{p=1}^{P} w^p \sum_{i=1}^{N} p_i \bar{Q}_i^{qp} \tag{3.1}$$

where $\bar{Q}_i$ are the arguments of the inner optimization subproblem (profit estimation): w^q are the weights corresponding to each quadrature point; J^q is the probability of each point. Note that through this transformation the location of the quadrature points is still unknown.

(ii) The relaxation of the demand constraints $Q_i^p \leq \theta_i$ gives rise to the following feasibility property:



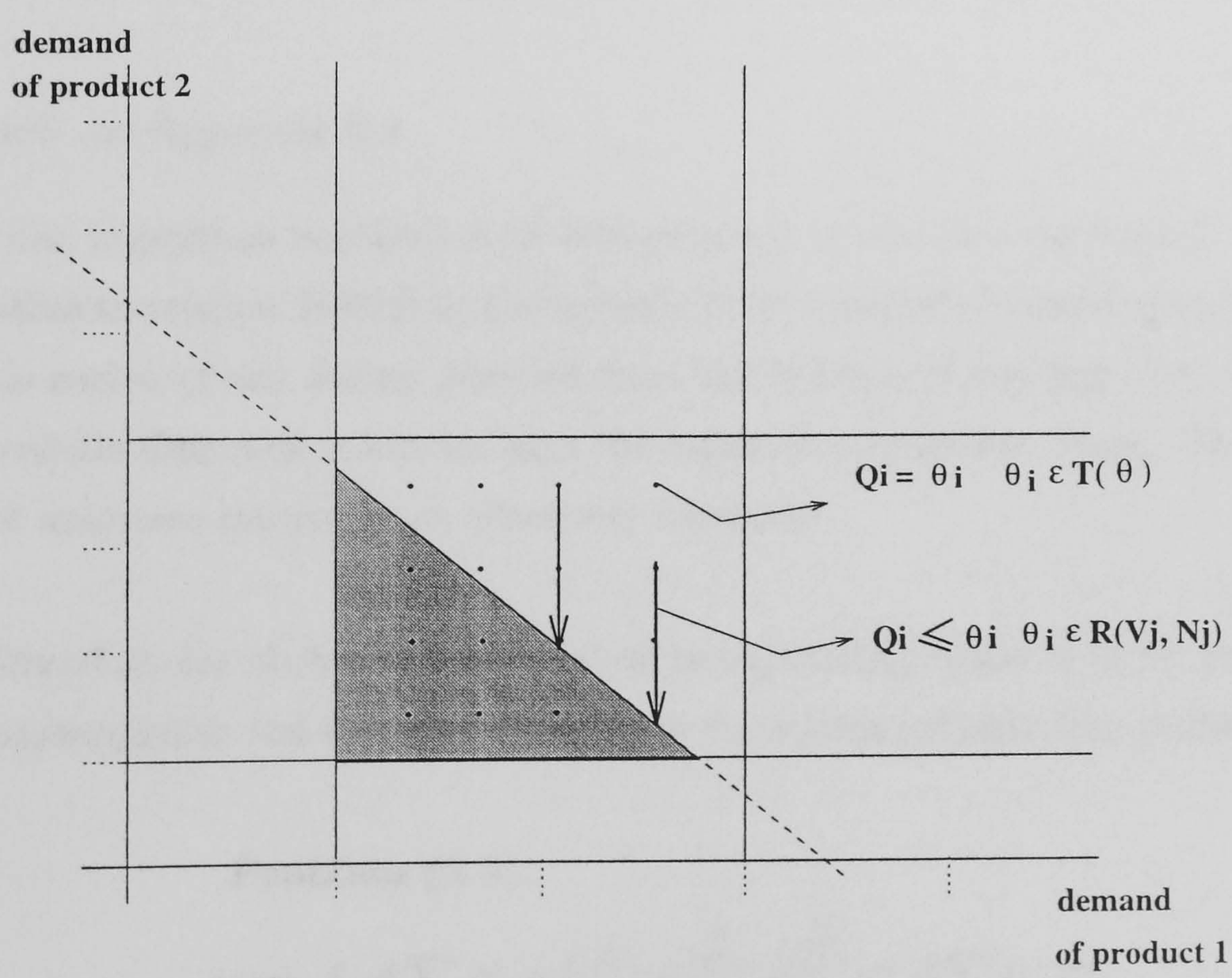


Figure 3.1: Different demand constraints

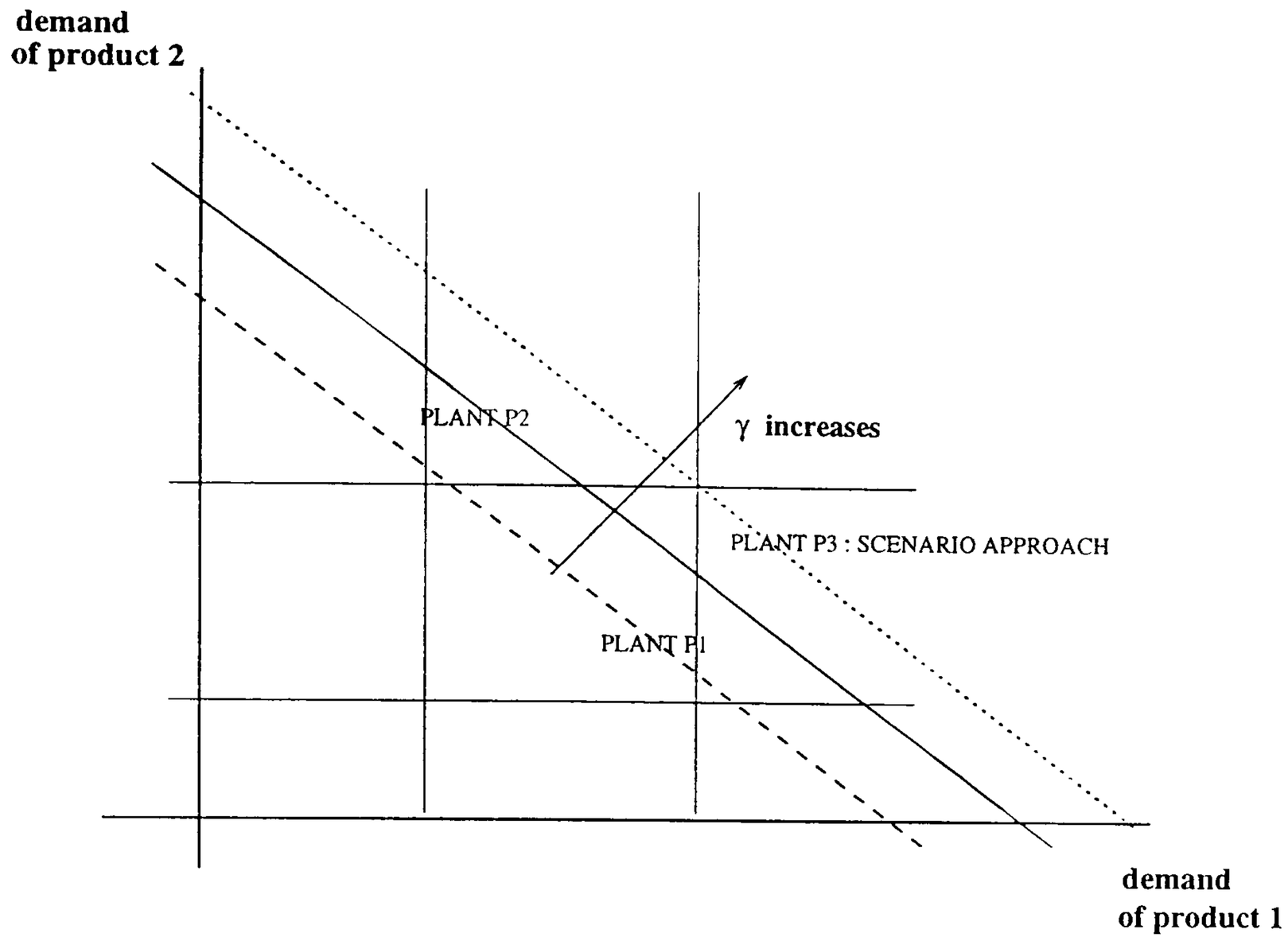


Figure 3.2: Effect of penalty coefficient γ

Property- Any design (V_j, N_j) which satisfies the constraints of problem (3.1) for fixed product demands θ_i, is feasible for the whole parameter range, $\mathrm{T}(\theta)$.

Proof- see Appendix B.3.

The important implication of this property is that the integration can be performed within the region defined by the bounds of the uncertain demand parameters, since the feasible region of any design depicted from the solution of problem (3.1) in the space of the uncertain demands coincides with the uncertain parameter range. Therefore, the obstacle of unknown integrands is effectively overcome.

Based on the above property and by incorporating equation (3.1), problem (3.1) can be transformed to the following single level equivalent optimization problem (3.2):

Problem (3.2)

$$\max_{V_j, N_j, Q_i^{qp}} \{-\delta \sum_j N_j \alpha_j V_j^{\beta_j}) + \sum_{p=1}^{P} w^p \sum_{q=1}^{Q} w^q J^q \sum_i P_i Q_i^{qp}$$
$$-\gamma \sum_{p=1}^{P} w^p \sum_{q=1}^{Q} w^q J^q (\sum_i p_i \theta_i^q - \sum_i p_i Q_i^{qp})\}$$

$$\text{subject to:} \quad B_i \leq \frac{V_j}{S_{ij}^p} \; ; \; \forall i, j, p$$

$$T_{Li}^p \geq \frac{t_{ij}^p}{N_j} \; ; \; \forall i, j, p$$

$$\sum_i \frac{Q_i^{qp}}{B_i} T_{Li}^p \leq H \; ; \; \forall q, p$$

$$Q_i^{qp} \leq \theta_i^q \; ; \; \forall i, q, p$$

$$V_j^{LO} \leq V_j \leq V_j^{UP}, \;\; \theta_i^q \in T(\theta), \;\; \gamma \geq 0$$

Tables 3.1, 3.2, 3.3 present the single level equivalent formulations of different batch plant design formulations in the presence of uncertainty appeared in the open literature, several of which involving explicit scheduling models concerning plant operation (for example multiple product campaign with zero wait (ZW) or unlimited intermediate storage (UIS)). Note that schedule patterns are considered to change with respect to demand realizations in order to achieve the best utilization of the proposed plant (see also the discussion in example 7).

Note that in problem (3.2) the location of quadrature points within the plant's feasible region is fully determined from the optimization procedure. In this way, the postulation of arbitrary scenarios is effectively avoided; instead, the number and location of scenarios (integration points) will only depend on the degree of integration accuracy required.

Nevertheless, problem (3.2) still corresponds to a non-convex nonlinear mixed integer optimization problem due to the presence of the non-convex objective function (investment cost) and the horizon constraint. In the following sections we propose global optimization solution approaches for problem (3.2) for the cases of continuous and discrete equipment sizes.

STOCHASTIC MULTIPRODUCT BATCH PLANT DESIGN FORMULATION			
SINGLE PRODUCT CAMPAIGN		MULTIPLE PRODUCT CAMPAIGN	
		Zero Wait Policy (ZW)	Unlimited Intermediate Storage (UIS)
V_j continuous	V_j discrete	V_j continuous	V_j discrete
$\max \sum_q w^q \sum_p w^p \sum_i p_i Q_i^{qp} - \delta \sum_j N_j a_j V_j^{\beta_j} - \gamma \sum_q w^q \sum_p w^p (\sum_i p_i D_i^q - \sum_i p_i Q_i^{qp})$	$\max \sum_q w^q \sum_p w^p \sum_i p_i Q_i^{qp} - \delta \sum_j \sum_s \sum_n n a_j v_{js}^{\beta_j} y_{jsn} - \gamma \sum_q w^q \sum_p w^p (\sum_i p_i D_i^q - \sum_i p_i Q_i^{qp})$	$\max \sum_q w^q \sum_p w^p \sum_i p_i Q_i^{qp} - \delta \sum_j a_j V_j^{\beta_j} - \gamma \sum_q w^q \sum_p w^p (\sum_i p_i D_i^q - \sum_i p_i Q_i^{qp})$	$\max \sum_q w^q \sum_p w^p \sum_i p_i Q_i^{qp} - \delta \sum_j \sum_s \sum_n n a_j v_{js}^{\beta_j} y_{jsn} - \gamma \sum_q w^q \sum_p w^p (\sum_i p_i D_i^q - \sum_i p_i Q_i^{qp})$
subject to:	subject to :	subject to :	subject to :
$V_j \geq B_i S_{ij}^p$	$n_i^{qp} \geq \sum_s \sum_n \frac{Q_i^q S_{ij}^p}{v_{js}} y_{jsn}$	$V_j \geq B_i S_{ij}^p$	$n_i^{qp} \geq \sum_s \sum_n \frac{Q_i^{qp} S_{ij}^p}{v_{js}} y_{jsn}$
$T_{Li}^p \geq \frac{t_{ij}^p}{N_j}$	$T_i^{qp} \geq \sum_s \sum_n (\frac{t_{ij}^p}{n}) w_{ijsn}^{qp}$	$n_i^{qp} = \frac{Q_i^{qp}}{B_i}$	$\sum_s \sum_n y_{jsn} = 1$
$\sum_i \frac{Q_i^{qp} T_{Li}^p}{B_i} \leq H$	$n_i^{qp} = \sum_s \sum_n w_{ijsn}^{qp}$	$n_i^{qp} = \sum_k NP_{ik}^{qp}$	$n_i^{qq} = \sum_k NP_{ik}^{qp}$
$Q_i^{qp} \leq D_i^q$	$w_{ijsn}^{qp} \leq U_{ijsn}^{qp} y_{jsn}$	$n_k^{qp} = \sum_i NP_{ik}^{qp}$	$n_k^{qp} = \sum_i NP_{ik}^{qp}$
	$\sum_s \sum_n y_{jsn} = 1$	$NP_{ii}^{qp} \leq n_i^{qp} - 1$	$NP_{ii}^{qp} \leq n_i^{qp} - 1$
	$\sum_i T_i^{qp} \leq H$	$\sum_i (n_i^{qp} t_{ij}^p + \sum_k NP_{ik}^{qp} SL_{ikj}) \leq H$	$\sum_i (n_i^{qp} t_{ij}^p + \sum_k NP_{ik}^{qp} SL_{ikj}) \leq H \sum_s \sum_n n y_{jsn}$
	$Q_i^{qp} \leq D_i^q$	$Q_i^{qp} \leq D_i^q$	$Q_i^{qp} \leq D_i^q$

Table 3.1: Stochastic Models for Multiproduct Batch Plant Design

STOCHASTIC MULTIPURPOSE BATCH PLANT DESIGN FORMULATION

SINGLE PRODUCTION ROUTES		MULTIPLE PRODUCTION ROUTES	
V_j continuous	V_j discrete	V_j continuous	V_j discrete
$\max \sum_q w^q \sum_p w^p \sum_i p_i Q_i^{qp} -$	$\max \sum_q w^q \sum_p w^p \sum_i p_i Q_i^{qp} -$	$\max \sum_q w^q \sum_p w^p \sum_i p_i Q_i^{qp} -$	$\max \sum_q w^q \sum_p w^p \sum_i p_i Q_i^{qp} -$
$\delta \sum_j N_j a_j V_j^{\beta_j} -$	$\delta \sum_j \sum_s \sum_n n a_j v_{js}^{\beta_j} y_{jsn} -$	$\delta \sum_j N_j a_j V_j^{\beta_j} -$	$\delta \sum_j \sum_s \sum_n n a_j v_{js}^{\beta_j} y_{jsn} -$
$\gamma \sum_q w^q \sum_p w^p (\sum_i p_i D_i^q - \sum_i p_i Q_i^{qp})$	$\gamma \sum_q w^q \sum_p w^p (\sum_i p_i D_i^q - \sum_i p_i Q_i^{qp})$	$\gamma \sum_q w^q \sum_p w^p (\sum_i p_i D_i^q - \sum_i p_i Q_i^{qp})$	$\gamma \sum_q w^q \sum_p w^p (\sum_i p_i D_i^q - \sum_i p_i Q_i^{qp})$
subject to:	subject to :	subject to :	subject to :
$V_j \geq B_i S_{ij}^p$	$n_i^{qp} \geq \sum_s \sum_n \frac{Q_i^{qp} S_{ij}^p}{v_{js}} y_{jsn}$	$\tau_r^{qp} \geq \frac{q_r^{qp} S_{ij}^p T_{Lr}^p}{V_j}$	$\tau_r^{qp} \geq \sum_s \frac{q_r^{qp} S_{ij}^p T_{Lr}^p}{V_j}$
$T_{Li}^p \geq \frac{t_{ij}^p}{N_j}$	$T_i^{qp} \geq \sum_s \sum_n (\frac{t_{ij}^p}{n}) w_{ijsn}^{qp}$	$\sum_{r \in ER_i} q_r^{qp} \geq Q_i^{qp}$	$\sum_s y_{js} = 1$
$T_i^{qp} B_i = T_{Li}^p Q_i^{qp}$	$n_i^{qp} = \sum_s \sum_n w_{ijsn}^{qp}$	$\sum_h \alpha_{hr} \theta_h^{qp} \geq \tau_r^{qp}$	$\sum_{r \in ER_i} q_r^{qp} \geq Q_i^{qp}$
$\sum_h \alpha_{hi} \theta_h^{qp} \geq T_i^{qp}$	$w_{ijsn}^{qp} \leq U_{ijsn}^{qp} y_{jsn}$	$\sum_h \theta_h^{qp} \leq H$	$\sum_h \alpha_{hr} \theta_h^{qp} \geq \tau_r^{qp}$
$\sum_h \theta_h^{qp} \leq H$	$\sum_s \sum_n y_{jsn} = 1$	$Q_i^{qp} \leq D_i^q$	$\sum_h \theta_h^{qp} \leq H$
$Q_i^{qp} \leq D_i^q$	$\sum_h \alpha_{hi} \theta_h^{qp} \geq T_i^{qp}$		$Q_i^{qp} \leq D_i^q$
	$\sum_i T_i^{qp} \leq H$		
	$Q_i^{qp} \leq D_i^q$		

Table 3.2: Stochastic Models for Multipurpose Batch Plant Design

STOCHASTIC MULTIPURPOSE BATCH PLANT DESIGN FORMULATION

Optimal Design and Campaign Planning	Optimal Design with Detailed Scheduling Constraints
$\max \sum_q w^q \sum_s w^s \sum_p p_p R_p^{qs} - \delta C_j E_j$	$\max \sum_q w^q \sum_p w^p \sum_s p_s (S_{sT}^{qp} - S_{s0}^{qp}) - \delta C_j E_j$
$- \gamma \sum_q w^q \sum_s w^s (\sum_p p_p D_p^q - \sum_p p_p R_p^{qs})$	$- \gamma \sum_q w^q \sum_p w^p [\sum_s p_s D_s^q - \sum_s p_s (S_{sT}^{qp} - S_{s0}^{qp})]$
subject to:	subject to :
Allocation constraints	Allocation constraints
$\sum_{i \in \Omega_{jk}} U_{jki}^{qs} \leq E_j$	$\sum_{i \in I_j} \sum_{\theta=0}^{p_i - 1} W_{ijt-\theta}^{qp} \leq E_j$
$y_{kk'}^{qs} + y_{k'k}^{qs} \geq \sum_{i \in \Omega_{jk}} U_{jki}^{qs} + \sum_{i \in \Omega_{jk'}} U_{jk'i}^{qs} - 1$	Unit capacity constraints
Timing constraints	$B_{ijt}^{qp} \leq V_i$
$t_k^{inqs} \geq t_{k'}^{fqs} + y_{kk'}^{qs} \tau_{kk'} - (1 - y_{kk'}^{qs}) H$	$B_{ijt}^{qp} \leq W_{ijt}^{qp} V_i^{max}$
Material balances	Material balances
$R_p^{qs} \leq \frac{\phi_{ik}}{T_k^s} \sum_{j \in \Lambda_{ik}} \hat{U}_{jki}^{qs} V_j$	$S_{st}^{qp} = S_{st-1}^{qp} - \sum_{i \in T_s} \sum_{j \in K_i} \rho_{is}^p B_{ijt}^{qp} + \sum_{i \in \bar{T}_s} \sum_{j \in K_i} \bar{\rho}_{is}^p B_{ijt-p_{is}}^{qp}$
$\hat{U}_{jki}^{qs} \leq t_k^{fqs} - t_k^{inqs}$	Storage capacity constraints
$\hat{U}_{jki}^{qs} \leq H U_{jki}^{qs}$	$S_{st}^{qp} \leq C_s$
Production requirements	Production requirements
$R_p^{qs} \leq D_p^q$	$S_{sT}^{qp} - S_{s0}^{qp} \leq \frac{T}{H} D_s^q$

Table 3.3: Stochastic Models for Multipurpose Batch Plant Design

3.3. Continuous equipment sizes

For the case of continuous equipment sizes, the following exponential transformations can be introduced (Kocis and Grossmann, 1988):

$$V_j = \exp(v_j), B_i = \exp(b_i), T_{Li} = \exp(t_{Li}), N_j = \exp(n_j),$$

$$n_j = \sum_r y_{jr} \ln(r); \sum_r y_{jr} = 1; y_{jr} = \{0,1\}; r = 1,..,N_j$$

where v_j, b_i, t_{Li}, y_{jr} are the new transformed variables. Unlike the pure deterministic case, however, in which the reformulation leads to a convex MINLP problem, in this case the consideration of the uncertain demands still preserves non-convexities of the following form:

$$\sum_i Q_i \exp(t_{Li} - b_i) \leq H,$$

since Q_i are optimization variables. This calls for global optimization solution approach.

For the case of multiproduct batch plants operating in single product campaign, it will be shown that the resulting stochastic formulation can be effectively solved to global optimality by the GOP algorithm proposed by Floudas and Visweswaran (1990, 1993). Moreover, as it will be briefly discussed the different formulations shown in Tables 3.1, 3.2, 3.3 for the case of continuous equipment sizes can be treated in a similar way.

The multiproduct batch plant design formulation (3.2) after the exponential transformations of Kocis and Grossmann, corresponds to the following single nonlinear optimization problem involving nonconvexities in the horizon constraint:

Problem (3.3)

$$\max_{\substack{v_j, b_i, y_{jr} \\ t_{Li}, Q_i^q}} \{-\delta \sum_{j=1}^{M} \alpha_j \exp(\sum_r y_{jr} \ln(r) + \beta_j v_j) + \sum_{q=1}^{Q} w^q J^q \{\sum_{i=1}^{N} p_i Q_i^q\}$$

$$-\gamma \sum_{q=1}^{Q} w^q J^q \{\sum_{i=1}^{N} p_i \theta_i^q - \sum_{i=1}^{N} p_i Q_i^q\}\}$$

$$\text{subject to: } v_j \geq \ln(S_{ij}) + b_i \; ; \; i = 1,..,N, \; j = 1,..,M$$

$$t_{Li} \geq \ln(t_{ij}) - \textstyle\sum_r y_{jr} \ln(r) \; ; \; i = 1,..,N, \; j = 1,..,M$$

$$\sum_{i=1}^{N} Q_i^q \exp(t_{Li} - b_i) \leq H$$

$$Q_i^q \leq \theta_i^q \; ; \; i = 1,..,N, \; q = 1,..,Q$$

$$\ln(V_j^{LO}) \leq v_j \leq \ln(V_j^{UP})$$

$$y_{jr} = \{0,1\}, \; \theta_i^q \in T(\theta), \; \gamma \geq 0$$

Based on the following variable partition:

$$y = \{v_j, b_i, y_{jr}, t_{Li}\}, \; x = \{Q_i^q\}, \; j = 1,..,M, \; i = 1,..,N, \; q = 1,..,Q$$

with which problem (3.3) satisfies conditions (**A**) of the GOP algorithm (Floudas and Visweswaran, 1990), since both the objective and the constraints are convex in $\{v_j, b_i, y_{jr}, t_{Li}\}$ for every fixed Q_i^q and linear in Q_i^q for each fixed $\{v_j, b_i, y_{jr}, t_{Li}\}$. Similar partitions are suggested for the different formulation appeared in the open literature (see Tables 3.1, 3.2, 3.3) for the case of continuous equipment sizes. In particular, for the case of multiple product operation mode of multiproduct batch plant $y = \{v_j, b_i, y_{jr}, t_{Li}\}$, $x = \{Q_i^q, \theta_h^q\}$, whereas for multipurpose batch plants with single production route $y = \{v_j, b_i\}$, $x = \{Q_i^q, \theta_h^q, \tau_r^q\}$ and with multiple production routes $y = \{v_j, b_i\}$, $x = \{Q_i^q, n_i^q, NP_{ik}^q\}$.

Although GOP can in principle be applied for the solution of problem (3.3) to global optimality, it requires prohibitively high computational cost ($2^{N \times Q}$ subproblems per iteration). However, as it will be shown in the sequel by exploiting the special structure of the batch plant design model in (3.4), the number of relaxed dual subproblems that have to be solved per iteration can be reduced by orders of magnitude (scaling only to the number of products).

Properties of multiproduct batch plant design problem

Projecting on $y = \{v_j, b_i, y_{jr}, t_{Li}\}$, the following linear primal problem is obtained at the kth iteration:

Problem (3.4)

$$\min_{Q_i^q} \{\delta \sum_{j=1}^{M} \alpha_j \exp(\sum_r y_{jr}^k \ln(r) + \beta_j v_j^k) - \sum_{q=1}^{Q} w^q J^q \{\sum_{i=1}^{N} p_i Q_i^q\}\}$$

$$s.t. \sum_{i=1}^{N} Q_i^q \exp(t_{Li}^k - b_i^k) \leq H,\ q = 1,..,Q$$
$$Q_i^q \leq \theta_i^q,\ q = 1,..,Q$$
$$-Q_i^q \leq 0,\ q = 1,..,Q$$

The solution to problem (3.4) provides the optimal multiplier vectors $\mu^k, \lambda_1^k, \lambda_2^k$ (corresponding to the original inequality constraints) and an upper bound to the global solution of problem (3.3). The Lagrangian can then be formulated as:

$$\begin{aligned} L(v_j, b_i, Q_i^q, \mu^k, \lambda_1^{qk}, \lambda_2^{qk}) \quad = \quad & \delta \sum_{j=1}^{M} \alpha_j \exp(\sum_r y_{jr} \ln(r) + \beta_j v_j) - \sum_{q=1}^{Q} w^q J^q \{\sum_{i=1}^{N} p_i Q_i^q\}\} \\ & + \sum_{q=1}^{Q} \mu^{qk} (\sum_{i=1}^{N} Q_i^q \exp(t_{Li} - b_i) - H) + \sum_{q=1}^{Q} \lambda_1^{qk} (Q_i^q - \theta_i^q) \\ & + \sum_{q=1}^{Q} \lambda_2^{qk} (-Q_i^q) \end{aligned} \tag{3.2}$$

From the KKT conditions of the primal problem (3.4):

$$-w^q J^q p_i = -\mu^{qk} \exp(t_{Li}^k - b_i^k) - \lambda_1^{qk} + \lambda_2^{qk} \tag{3.3}$$

Substituting equation (3.3) in (3.2) yields:

$$\begin{aligned} L(v_j, b_i, Q_i^q, \mu^{qk}, \lambda_1^{qk}, \lambda_2^{qk}) = \delta \sum_{j=1}^{M} \alpha_j \exp(\sum_r y_{jr} \ln(r) + \beta_j v_j) \\ + \sum_{q=1}^{Q} \mu^{qk} \{\sum_{i=1}^{N} Q_i^q [\exp(t_{Li} - b_i) - \exp(t_{Li}^k - b_i^k)]\} \\ - \sum_{q=1}^{Q} \mu^{qk} H - \sum_{q=1}^{Q} \lambda_1^{qk} (\theta_i^q) \end{aligned}$$

Hence, the qualifying constraints (gradients of the Lagrange function with respect to the "connected" variables Q_i^q) to be added along with the Lagrange function in the relaxed dual problem take the following form:

$$\mu^{qk}[\exp(t_{Li} - b_i) - \exp(t_{Li}^k - b_i^k)] \leq 0 \quad \text{if} \quad Q_i^q = \theta_i^q$$
$$\mu^{qk}[\exp(t_{Li} - b_i) - \exp(t_{Li}^k - b_i^k)] \geq 0 \quad \text{if} \quad Q_i^q = 0$$

Since, however, $\mu^{qk} \geq 0\ \forall q = 1,..,Q$ all the qualifying constraints are of the form:

$$\left.\begin{aligned} \exp(t_{Li} - b_i) - \exp(t_{Li}^k - b_i^k) \leq 0 \ \text{ if } \ T_{Li}/B_i \geq T_{Li}^k/B_i^k \\ \exp(t_{Li} - b_i) - \exp(t_{Li}^k - b_i^k) \geq 0 \ \text{ if } \ T_{Li}/B_i \leq T_{Li}^k/B_i^k \end{aligned}\right\} \tag{3.4}$$

The major implication of the qualifying constraints in(3.4)is that instead of solving $2^{N\times Q}$ relaxed dual (RD) problems, it is now sufficient to solve only 2^N subproblems, which is a reduction of at least twenty orders of magnitude (2^{25}) even for two uncertain parameters with five quadrature points each! In fact, it is this major reduction which enables the efficient implementation of the GOP algorithm in this case.

Furthermore, since the gradient of the Lagrange function with respect to Q_i^q (qualifying constraints) is not a function of $Q_i^q, i = 1,..,N, q = 1,..,Q$, two other properties of the GOP algorithm (Visweswaran and Floudas, 1993) can be used to further reduce the number of relaxed dual problems at each iteration, as follows:

(i) If at the kth iteration the qualifying constraint for product i is ≤ 0 (or ≥ 0) for every other product, i.e. $\mu^{qk}[\exp(t_{Li} - b_i) - \exp(t_{Li}^k - b_i^k)] \leq 0$ (or ≥ 0) $\forall i = 1,..,N$, which implies that $T_{Li}/B_i \geq T_{Li}^k/B_i^k$ (or $T_{Li}/B_i \leq T_{Li}^k/B_i^k$) $\forall i = 1,..,N$ - this is true when T_{Li}^k/B_i^k corresponds to lower (or upper) bound of T_{Li}/B_i, and consequently the solution of the relaxed dual with the following qualifying constraints: $\mu^{qk}[\exp(t_{Li} - b_i) - \exp(t_{Li}^k - b_i^k)] \geq 0$ (or ≤ 0) can be effectively avoided.

(ii) If at the kth iteration the qualifying constraint of product i $\mu^{qk}[\exp(t_{Li} - b_i) - \exp(t_{Li} - b_i^k)] = 0\ \forall i = 1,..,N$ that is satisfied when $\mu^{qk} = 0$, $\forall q = 1,..,Q$, then it is sufficient to solve only one RD problem at either the lower or upper bounds of Q_i^q variables.

The algorithmic procedure is shown graphically in Figure 3.3. In section 3.5 Example 2 is used to illustrate the results from the implementation of the global optimization algorithm for the solution of batch plant design problem.

3.4. Discrete equipment sizes

For the case of discrete equipment sizes, nonconvexities can be effectively avoided based on the following reformulation (Voudouris and Grossmann, 1992):

$$\frac{1}{V_j} = \sum_s \frac{y_{js}}{v_{js}}$$

$$\sum_s y_{js} = 1$$

$$y_{js} = \begin{cases} 1 & \text{if unit at stage j has size s} \\ 0 & \text{otherwise} \end{cases}$$

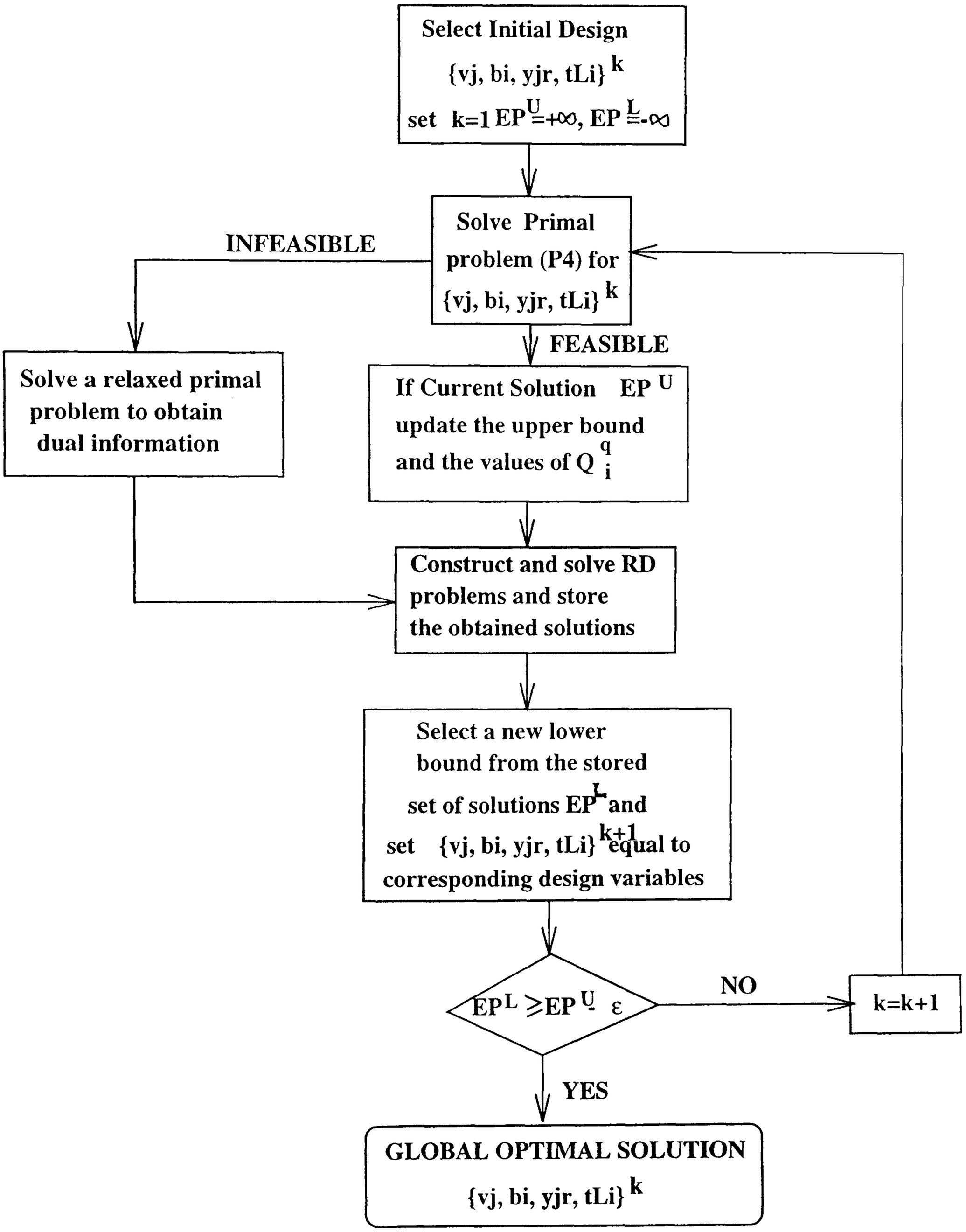


Figure 3.3: Global Optimization Algorithm

where V_j is restricted to take values from the set $SV_j = \{v_{j1}, ..., v_{js}\}$. In this way problem (3.2) can be rewritten as follows:

Problem (3.5)

$$\max_{V_j, N_j} \sum_q w^q \sum_p w^p \sum_i p_i Q_i^{qp} - \delta \sum_j \sum_s \sum_n n a_j v_{js}^{\beta_j} y_{jsn}$$
$$-\gamma \sum w^q \sum w^p (\sum p_i D_i^q - \sum p_i Q_i^{qp})$$
$$q \qquad p \qquad i \qquad i$$

$$s.t. \;\; n_i^{qp} \geq \sum_s \sum_n \frac{Q_i^{qp} S_{ij}^p}{v_{js}} y_{jsn} \;;\; \forall i, j, p, q$$

$$T_i^{qp} \geq \sum_s \sum_n (\frac{t_{ij}^p}{n}) w_{ijsn}^{qp} \;;\; \forall i, j, p, q$$

$$n_i^{qp} = \sum_s \sum_n w_{ijsn}^{qp} \;;\; \forall i, j, p, q$$

$$w_{ijsn}^{qp} \leq U_{ijsn} y_{jsn} \;;\; \forall i, j, s, n, p, q$$

$$\sum_i T_i^{qp} \leq H \;;\; \forall q, p$$

$$Q_i^{qp} \leq \theta_i^q \;;\; \forall i, q, p$$

Problem (3.5) is a mixed integer linear programming problem and conventional MILP tools (such as SCICONIC, CPLEX) can be used for its solution. Note that in this case the structure of the deterministic formulation is fully preserved despite the use of general continuous probability distribution forms for the description of uncertain product demands! As shown in Tables 3.1, 3.2, 3.3 similar stochastic models have been obtained for various design and scheduling formulations appeared in the open literature.

3.5. Examples

In this section a variety of examples that illustrate the features of the approach described in the previous sections batch plant design and scheduling in the presence of process parameter variations (processing times and size factors) and demand fluctuations will be presented.

First for the case of continuous equipment sizes an illustrative multiproduct batch plant example is presented to give more insight in the nature of the problem. Then a multiproduct batch plant of two products and three stages is considered to motivate the need of global optimization solution procedure for the case of continuous equipment sizes and to illustrate the effects of considering different formulations with regard to demand constraint as well as the effect of penalty term in the objective function. Assuming discrete equipment sizes the same example is used to account for long-term demand variations on a capacity expansion basis and to consider uncertain processing times and size factors through a multiperiod formulation. Finally, the incorporation of more involved scheduling formulations describing multiple product campaign operation with zero wait (ZW) or unlimited intermediate storage (UIS) are also examined. The following example of six stages and four products is used to present some computational aspects regarding the application of the modified GOP algorithm for the case of continuous equipment sizes. Discrete equipment sizes are assumed for the rest of the examples which describe multipurpose batch plants based on the different formulations presented in Tables 3.1, 3.2, 3.3 in order to illustrate the significant benefits of the proper consideration of uncertainty at the design stage.

Example 1

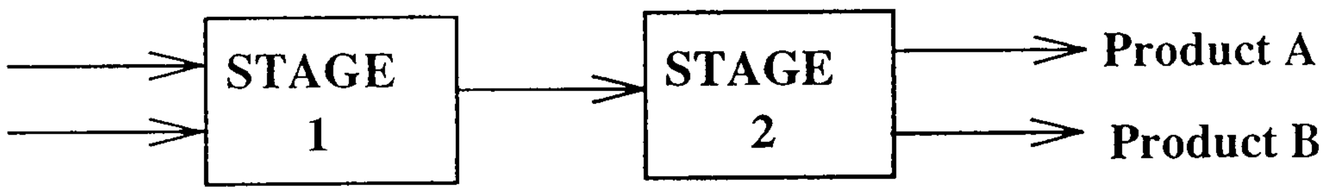


Figure 3.4: Batch Plant - Example 1

(a) Size factors			(b) Processing times		
	Stage			Stage	
Product	1	2	Product	1	2
1	2	4	1	8	20
2	4	5	2	10	12
(c) Investment cost coefficients			(d) Prices of products		
Stage j	α_j	β_j	Product	p_i	
1	5	0.6	1	10.0	
2	5	0.6	2	12.0	
Time horizon H=1200 h					

Table 3.4: Data for example 1

In order to gain some further insight on the nature of the problem of designing batch plants, consider the production of two products, 1 and 2, in two stages (as shown in Figure 3.4) with a single equipment per stage (a single product campaign is assumed, with no intermediate storage). Data regarding size factors, processing times and equipment cost are given in Table 3.4.

Assume that there is a demand for products 1 and 2 of 2000 and 1800 units, respectively. Consider a specific design d_1 with (V_1, V_2)=(100,160). Then:

$$B_1 = \min\{\frac{V_1}{S_{11}}, \frac{V_2}{S_{12}}\} = 40$$

$$B_2 = \min\{\frac{V_1}{S_{21}}, \frac{V_2}{S_{22}}\} = 25$$

with which the horizon constraint

$$\frac{Q_1}{B_1}T_{L1} + \frac{Q_2}{B_2}T_{L2} \leq H$$

is violated for Q_1=2000, Q_2=1800 (see also Figure 3.5); thus, the suggested design can not fully accommodate the demands for products 1 and 2. However, with the cost data of Table 3.4, the solution of the following problem:

$$\max_{Q_1,Q_2} P_1Q_1 + P_2Q_2$$

$$\text{subject to:} \quad \frac{Q_1}{40}20 + \frac{Q_2}{25}12 \leq 1200$$
$$Q_1 \leq D_1$$
$$Q_2 \leq D_2$$

results in $Q_1^* = 672, Q_2^* = 1800$ with a maximum revenue of 28320 units; i.e. by relaxing the requirement to produce at least as much as demanded, a different production plan was obtained which deviates from the target demand of (2000, 1800) because of the insufficient design capability. The "loss" incurred can be measured by the following penalty term:

$$(P_1D_1 + P_2D_2) - (P_1Q_1^* + P_2Q_2^*) = 41600 - 28320 = 13280 \text{ units}$$

If a different design $d_2 = (V_1, V_2)$=(200,360) is considered with larger volumes (and thus larger investment cost), as is also shown in Figure 3.5, it can accommodate both demands with maximum revenue of 20800 units (zero losses); therefore, there are trade-offs between investment cost and revenues (including "losses" due to design insufficiency) which can be explored through the following formulation:

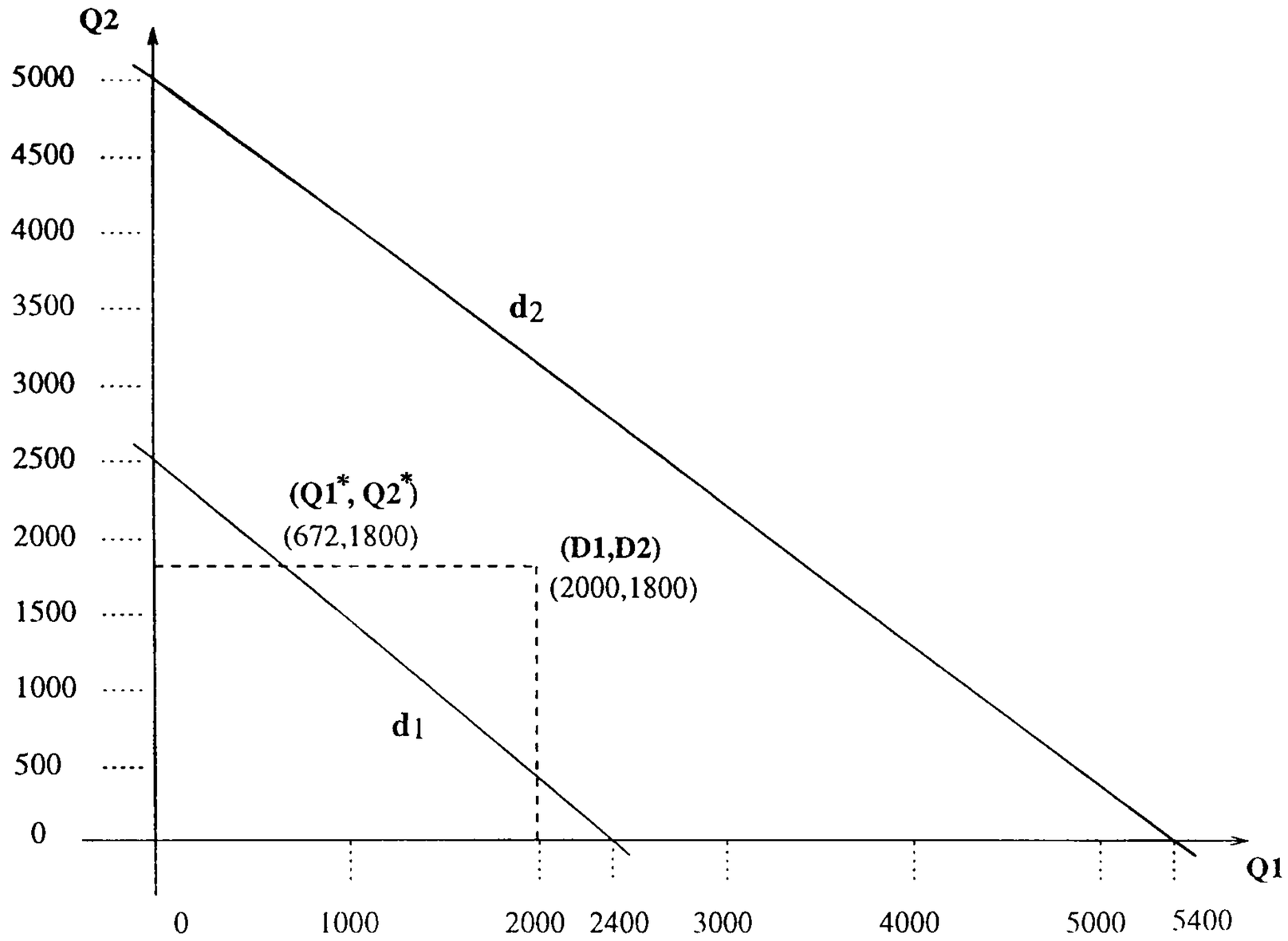


Figure 3.5: Feasible region (in production space) for two alternative batch plants - Example 1

$$\max_{V_j,\ Q_i} \{\underbrace{P_1Q_1 + P_2Q_2}_{Revenue} - \underbrace{\sum_{j=1}^{2}\alpha_j V_j^{\beta_j}}_{Investment\ Cost} - \underbrace{\gamma[(P_1D_1 + P_2D_2) - (P_1Q_1 + P_2Q_2)]}_{Penalty\ term}\}$$

subject to:

$$\left.\begin{array}{l} \dfrac{Q_1}{B_1}T_{L1} + \dfrac{Q_B}{B_B}T_{L2} \le H \end{array}\right\} \text{Horizon Constraint}$$

$$\left.\begin{array}{l} Q_1 \le D_1 \\ Q_2 \le D_2 \end{array}\right\} \text{Demand Constraints}$$

$$\left.\begin{array}{l} B_1 = \min\{\dfrac{V_1}{S_{11}}, \dfrac{V_2}{S_{12}}\} \\ B_2 = \min\{\dfrac{V_1}{S_{21}}, \dfrac{V_2}{S_{22}}\} \end{array}\right\} \text{Batch size Constraints}$$

$$\left.\begin{array}{l} T_{L1} = \max\{t_{11}, t_{12}\} \\ T_{L2} = \max\{t_{21}, t_{22}\} \end{array}\right\} \text{Cycle time Constraints}$$

where γ is a penalty coefficient. The solution of the above formulation (with γ=0) yields the optimal design $d^* = (V_1, V_2) = (162.7, 239.2)$ with profit equal to 320 units which

properly balance investment cost and plant revenues (see Table 3.5).

Demand		Design		Revenue	Investment	Expected	Flexibility
D_1	D_2	V_1	V_2		Cost	Profit	
2500	2300	206.9	300.0	526	275.7	356.3	0.78
2200	2000	180.9	263.1	460	254.7	363.9	0.14
2000	1800	162.7	239.2	416	239.8	362.3	0.017
1500	1300	118.4	178.2	306	199.7	275.6	0.0

Table 3.5: Uncertain demand consideration - Example 1

However, as shown in Table 3.5 there are also trade-offs between plant flexibility and economic optimality. The requirement of accommodating larger demand values leads to more profitable but also more expensive batch plants. Designing for a specific value of demand (problem (3.1)) cannot accommodate this task. In order to balance properly the trade-offs between economic optimality and plant flexibility problem formulation (3.2) should be adopted which results in a plant (V_1, V_2)=(180.9,263.1) with the maximum expected profit equal to 364 units at the optimal level of flexibility (0.14) (see Figure 3.6). Notice that this plant has larger flexibility and larger expected profit comparing to the design obtained at the nominal demand values (V_1, V_2)=(162.7,239.2).

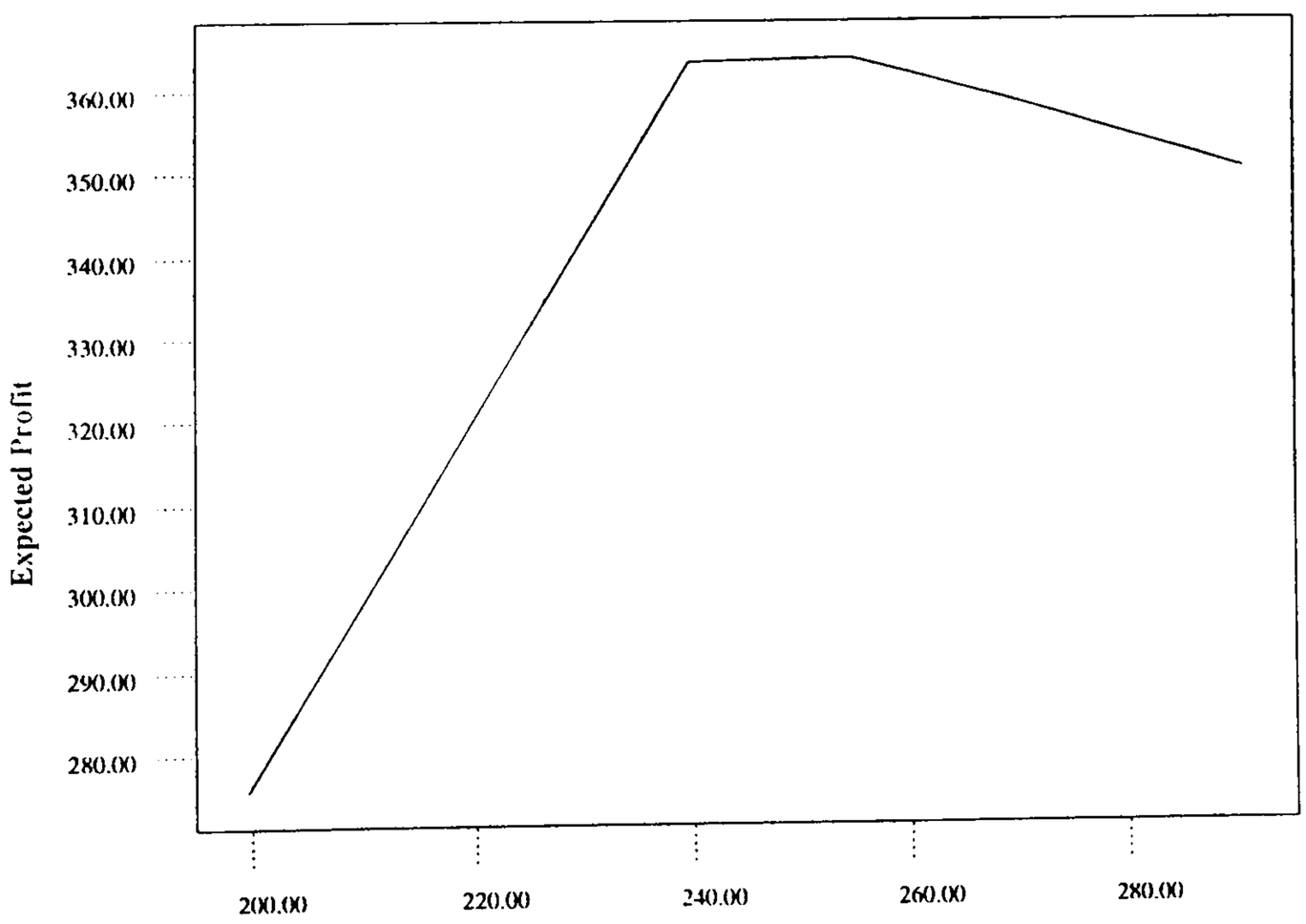


Figure 3.6: Expected Profit vs Capital Cost - Example 1

In order to illustrate the effect of different formulations with regard to demand

constraint, problem (3.2) is solved by considering the demand satisfaction as hard constraint and also by employing a scenario approach representing total demand satisfaction. It should be noticed that both the optimal plants obtained $(V_1, V_2) = (198.3, 295.9)$ and $(V_1, V_2) = (226.8, 327.4)$ respectively, involve larger equipment sizes and consequently can accommodate larger demand variations as shown in Figure 3.7. However, the proposed formulation based on the relaxation of demand constraint and the incorporation of a penalty term in the objective function to penalize the partial order fulfillment results in proper balance of the above trade-offs. As shown in Table 3.6 as the value of penalty coefficient γ increases corresponding to more severe penalization we move towards the complete demand satisfaction which coincides with the result of scenario-based approach.

γ values	Optimal Plant (V_1, V_2)
0	(180.9, 263.1)
1	(169.8, 281.3)
10	(170.7, 280.2)
100	(200.1, 292.4)
1000	(194.4, 299.5)
10000	(205.7, 320.8)
100000	(226.8, 327.4)

Table 3.6: Results of example 1

For the case of discrete equipment sizes within the set $\{150, 200, 250\}$ the solution of problem (3.6) with $\gamma = 0$ yields the plant $(V_1, V_2) = (250, 250)$ with expected profit 344 units, a plant very close to the one obtained when continuous sizes are considered.

Periods	Product	t_{ij}		S_{ij}	
		Stage 1	Stage 2	Stage 1	Stage 2
1	1	8	20	1.5	3.5
	2	10	12	3.5	4.5
2	1	7	19	2	4
	2	9	11	4	5
3	1	9	21	2.5	4.5
	2	11	13	4.5	5.5

Table 3.7: Uncertain process parameters - Example 1

Finally, processing times and size factors are considered as uncertain parameters

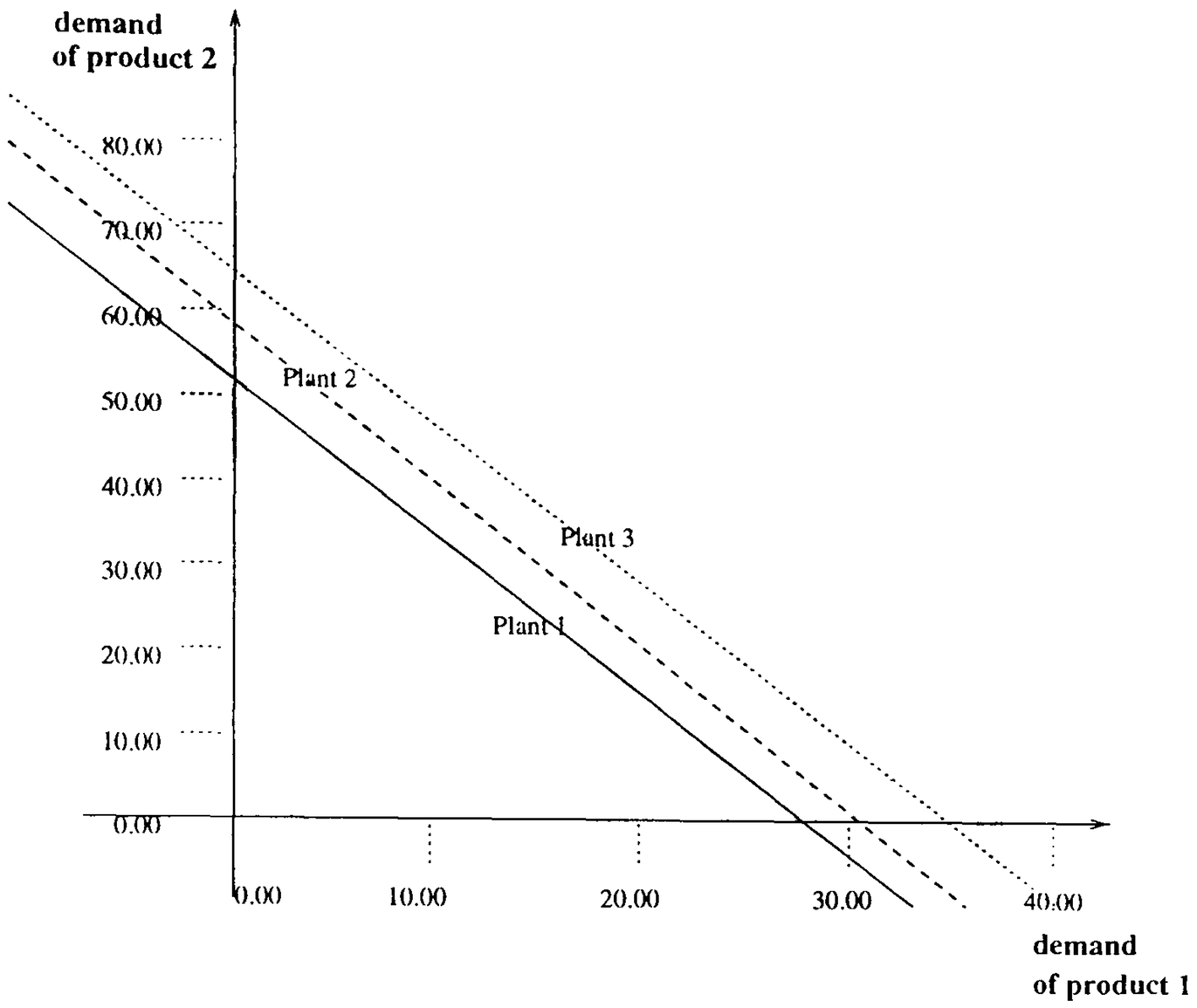


Figure 3.7: Results from different formulations - Example 1

through a multiperiod formulation with three time periods as shown in Table 3.7 resulting in a more conservative optimal design of $(V_1, V_2) = (219.2, 312.5)$ since larger processing times and size factors correspond to less effective equipment utilization.

Example 2

The batch plant problem presented in section 1.2 is solved here using the modified GOP algorithm. The results are summarized in Table 3.8.

The following points should be highlighted: (a) orders of magnitude reductions of the required relaxed dual problems are achieved by applying the derived properties, (b) convergence of the algorithm does not depend on different starting points, (c) the effect of penalty coefficient γ: the larger the value of γ the more "conservative" the design, (d) the slow convergence of the algorithm to yield highly accurate results (with an optimality stopping criterion of $\epsilon = 2 \times 10^{-4}$, the algorithm takes almost twice as many iterations compared to the solution with $\epsilon = 0.016$), (e) increasing the number of quadrature points per θ does not increase the number of problems that have to be solved per iteration, e.g. for a 9×9 grid again the maximum number of relaxed dual problems per iteration is 4; yet, since the primal problem (3.3) is of much larger size in this case, its CPU solution time increases (0.25 s versus 0.1 s required for the 5×5 grid).

γ=0					
	Number of RD		Upper Bound	Lower Bound	Design (V_1, V_2, V_3)
	Without properties	With properties			
iteration 1	2^{50}	1	146.7	-1394.5	(500, 500, 500)
iteration 2	2^{50}	1	146.7	-569.2	(883.7, 1325.5, 1767.4)
iteration 3	2^{50}	4 (2^2)	20.2	-323	(500, 1703.4, 937.8)

Optimal Design		
(1800, 2700, 3600)	ϵ=0.016	8 iterations
	ϵ=0.0002	14 iterations

Different penalty values				Different Starting points		
	Optimal Design			Starting Design	Number of	CPU s per
γ value	V_1	V_2	V_3	(V_1, V_2, V_3)	iterations	iteration
γ=0	1800	2700	3600	(1000, 1000, 1000)	13	0.8
γ=4	1907	2861	3815	(4500, 4500, 4500)	14	0.8
γ=8	1972	2958	3944	(500, 500, 500)	15	0.8

Table 3.8: Results of Global Optimization Algorithm - Example 2

Example 3

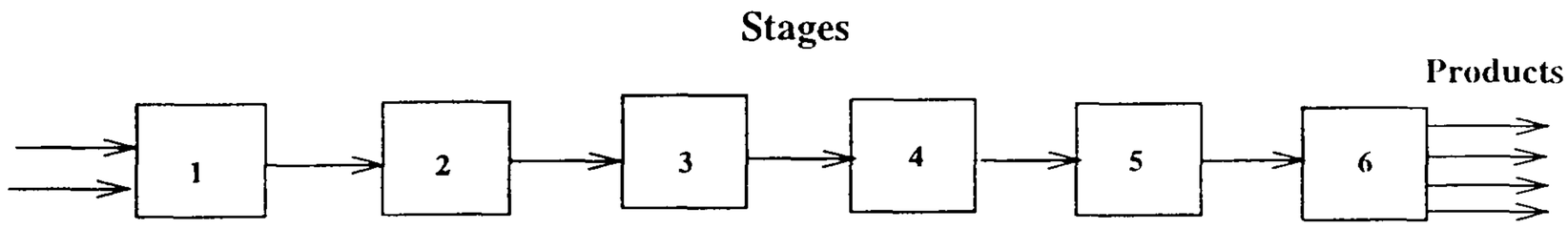


Figure 3.8: Batch Plant - Example 3

Consider the six-stage, four-product batch plan shown in Figure 3.8, where the demands of the four products are considered uncertain with the following normal distribution functions N(150, 10), N(150, 8), N(180, 9) and N(160, 10). Data are shown in Table 3.9. Model (3.2) consists of 625 (for 5 quadrature points in each uncertain parameter direction) nonconvex horizon constraints, 780 bounding constraints for the actual production of each product and 24 batch size constraints. Starting from a design $(V_1, V_2, V_3, V_4, V_5, V_6)$= (2500, 2500, 2500, 2500, 2500, 2500), the algorithm requires 37 iterations to reach the global optimum design $(V_1, V_2, V_3, V_4, V_5, V_6)$= (3918.9, 1917.8, 2547.3, 3251.4, 2988.2, 2139.1), EP=26000 units, with relative tolerance of 0.003 (although it requires only 8 iterations to converge within ϵ=0.006). In each iteration a maximum of 2^4=16 relaxed dual (NLP) problems are solved and one primal LP problem. Using GAMS/MINOS for the solution of NLP and LP problems, the computational time re-

quired per iteration is approximately 97 s CPU time in SPARCstation 10.

	(a) Size factors						(b) Processing times						(c) Prices of products
	Stage						Stage						
Product	1	2	3	4	5	6	1	2	3	4	5	6	p_i
1	8.0	2.0	5.2	4.9	6.1	4.2	7	8.3	6	7	6.5	8	3.5
2	0.7	0.8	0.9	3.8	2.1	2.5	6.8	5	6	4.8	5.5	5.8	4.0
3	0.7	2.6	1.6	3.4	3.2	2.9	4	5.9	5	6	5.5	4.5	3.0
4	4.7	2.3	1.6	2.7	1.2	2.5	2.4	3	3.5	2.5	3	2.8	2.0
(d) Investment cost coefficients $a_j = 10$, $\beta_j = 0.6$, j=1,..,4													

Table 3.9: Data for Example 3

Example 4

For the case of multipurpose batch plants with single product campaigns and single production routes the example given in Vaselenak et al. 1987 and Voudouris and Grossmann 1992 has been used. This problem considers the production of 5 products in 5 stages where two parallel units are allowed. The demand of products 1 and 2 are considered uncertain following normal probability distribution functions N(200,10) and N(150,10) respectively.

Considering discrete equipment sizes taking values from the set 500,1000,1500,2000, the deterministic problem results in the selection of one unit per stage of size 1500 with capital cost 3.1E+4 which can meet demand within the region 160 $\leq$ demand of product 1 $\leq$ 200, 110 $\leq$ demand of product 2 $\leq$ 150. The size of the model (see Table 3.2) is 303 continuous and 40 binary variables and 499 constraints. The solution was obtained using GAMS/CPLEX in 12 CPU s in a Sparc10.

The stochastic model on the other hand, involves 1851 continuous and 40 binary variables and 3359 constraints and requires 126 CPU s solution time. The optimal plant corresponds to the selection of one equipment per stage of size 2000 with larger capital cost 3.6E+4 which however can accommodate the whole range of demand variations 160 $\leq$ demand of product 1 $\leq$ 240, 110 $\leq$ demand of product 2 $\leq$ 190. Notice that although the size of the model has greatly increased, the number of binary variables remains the same since it corresponds to the selection of the plant configuration. Also exploiting the special structure of the problem which enables the parallel solution of most of the optimization

tasks involved (parallel evaluation of profit maximization at each integration point) computational performance can be significantly reduced.

Example 5

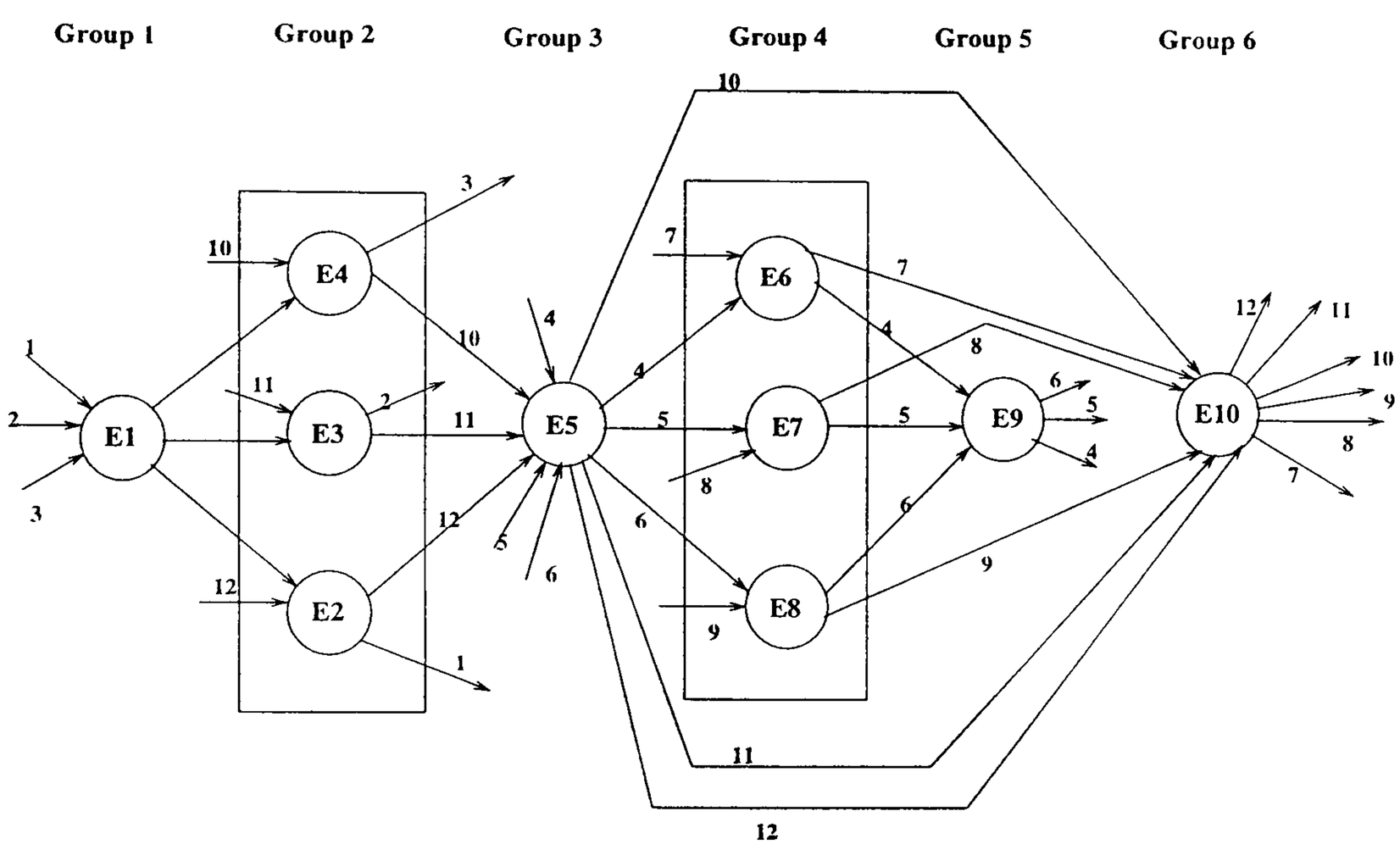


Figure 3.9: Plant layout for Example 5

For the case of multipurpose batch plants with multiple production routes the example given in Faqir and Karimi 1990 and Voudouris and Grossmann 1992 has been used (Table 3.2). The data for this problem are given in Table 3.10 whereas the production routes are shown in the plant layout in Figure 3.9. Horizon constraints are given in Table 3.11. Demand of products A and B are considered as random variables following normal probability distribution functions of the form N(300,10) and N(250,10). Considering discrete equipment sizes from the set {300, 500, 1000, 2000, 3000} the stochastic model size is 1531 continuous variables 50 binary variables and 1822 constraints comparing to 245 continuous 50 binary variables and 238 constraints of the deterministic model.

The optimal plant, obtained in 10.5 CPU s using GAMS/CPLEX in a Sparc10, corresponds to the selection of equipments E_1 and E_5 with size 3000, and E_2, E_6, E_9, E_{10} with size 300. This plant has a capital cost of 4.5E+3 and can meet the whole range of uncertain demand $260 \leq$ demand of product A ≤ 340, $210 \leq$ demand of product B ≤ 290. Notice that as in the previous examples using this formulation an additional optimization problem is required for the derivation of the detailed schedule for the optimal plant.

Group	Size factors				Processing times			
	Product				Product			
	A	B	C	D	A	B	C	D
1	1.5	-	-	-	4.0	-	-	-
2	2.0	-	-	2.2	6.5	-	-	6.5
3	-	1.6	-	1.7	-	3.9	-	7.0
4	-	2.5	1.4	-	-	5.5	4.5	-
5	-	1.9	-	-	-	4.2	-	-
6	-	-	2.4	1.8	-	-	3.5	4.7

Table 3.10: Data for Example 5

$$
\begin{gathered}
\tau_1 + \tau_2 + \tau_3 \leq H \\
\tau_1 + \tau_{10} \leq H \\
\tau_2 + \tau_{11} \leq H \\
\tau_3 + \tau_{12} \leq H \\
\tau_4 + \tau_5 + \tau_6 + \tau_{10} + \tau_{11} + \tau_{12} \leq H \\
\tau_4 + \tau_7 + \tau_{10} + \tau_{11} + \tau_{12} \leq H \\
\tau_5 + \tau_8 + \tau_{10} + \tau_{11} + \tau_{12} \leq H \\
\tau_6 + \tau_9 + \tau_{10} + \tau_{11} + \tau_{12} \leq H \\
\tau_7 + \tau_8 + \tau_9 + \tau_{10} + \tau_{11} + \tau_{12} \leq H
\end{gathered}
$$

Table 3.11: Horizon Constraints for Example 5

Example 6

The formulation proposed by Shah and Pantelides 1991 (Table 3.3), to describe the long-term campaign planning of multipurpose batch plants is used in a modified version of the example presented by Shah and Pantelides 1992, where two products are produced in three stages using any of the 8 available equipments (4 reactors, 2 crystallizers and 2 driers). The data of the problem are shown in Tables 3.12 3.13. The demand of product 1 is considered uncertain following normal probability distribution function of the form N(20,5). The stochastic design model involves 548 constraints and 276 variables (128 0-1 variables) comparing to 112 constraints with 64 variables (32 binary variables) of the deterministic model. Notice here that the stochastic formulation results to an increased number of binary variables since binary variables correspond to the selection of the units as well as schedule alternatives.

Product	Stage	Prerequisite stage	Task	Processing time	Material balance factor	Task type
1	1		reaction 1	9	0.0365	4
	2	1	reaction 1	10	0.124	6
			crystallization 1	11	0.098	7
	3	2	reaction 1	9	0.0781	4
			crystallization 1	11	0.0675	7
2	1		reaction 1	10	0.0435	2
	2	1	reaction 1	10	0.198	1
			crystallization 1	9	0.127	7
			drying	9	0.93	8
	3	2	reaction 1	11	0.0923	2
			crystallization 1	10	0.0763	7

Table 3.12: Recipe Data for Example 6

The optimal plant is obtained within 1.8 CPU s in Sparc10 using GAMS/CPLEX and corresponds to the selection of the reactors 1a and 2, the crystallizer 1 and the drier 2. This plant has a capital cost of 5.55 and can accommodate demand of product 1 in the range of [0,40]. The assumption of considering equipments with known capacity was then relaxed based on the consideration of discrete set of choices for equipment sizes which leads to the selection of the same units but with different capacities. In particular, reactor 2 of 2 m^3 and drier 2 of 2.5 m^3 were selected. Consequently, the optimal plant has smaller capital cost 5.3 but can still accommodate the same range of demand requirements.

Equipment	volume	Fixed Cost	Task Type
reactor 1	1	0.5	1,5,4
reactor 1a	5	1.0	1,5,4
reactor 2	2	1.25	2,3,6
reactor 2a	10	1.5	2,3,6
crystallizer 1	5	1.25	7
crystallizer 2	8	1.5	7
drier 1	10	1.0	8
drier 2	5	0.75	8

Table 3.13: Equipment Data for Example 6

Comparing to previous presented formulations the solution of the proposed stochastic design formulation results in the determination of the detailed production schedule. It should be pointed out here that proper consideration of uncertain demand is achieved through the incorporation of changing schedule with respect to demand realization as shown in Figure 3.10 for two different demand values.

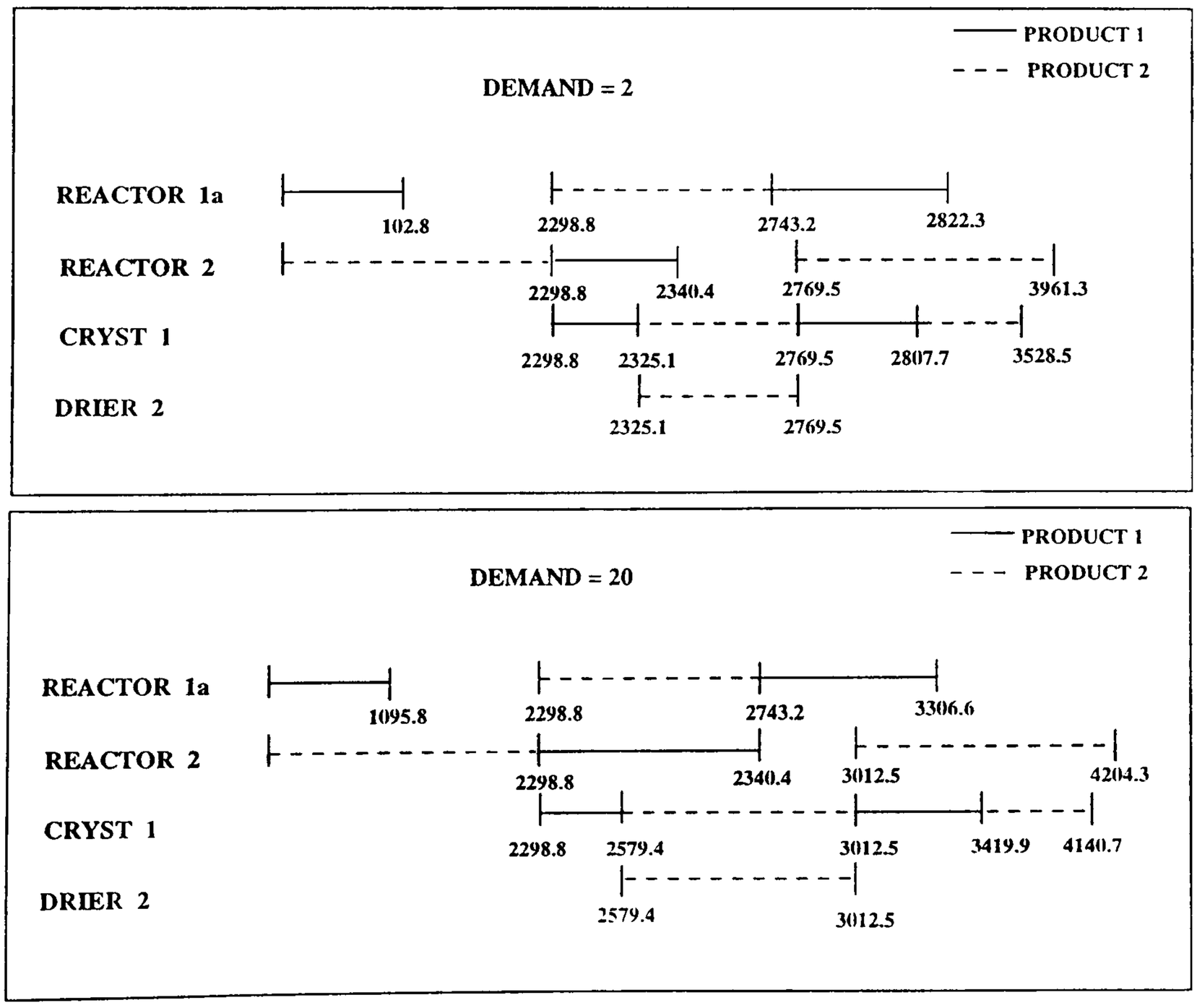


Figure 3.10: Gantt charts for different demand values - Example 6

Example 7

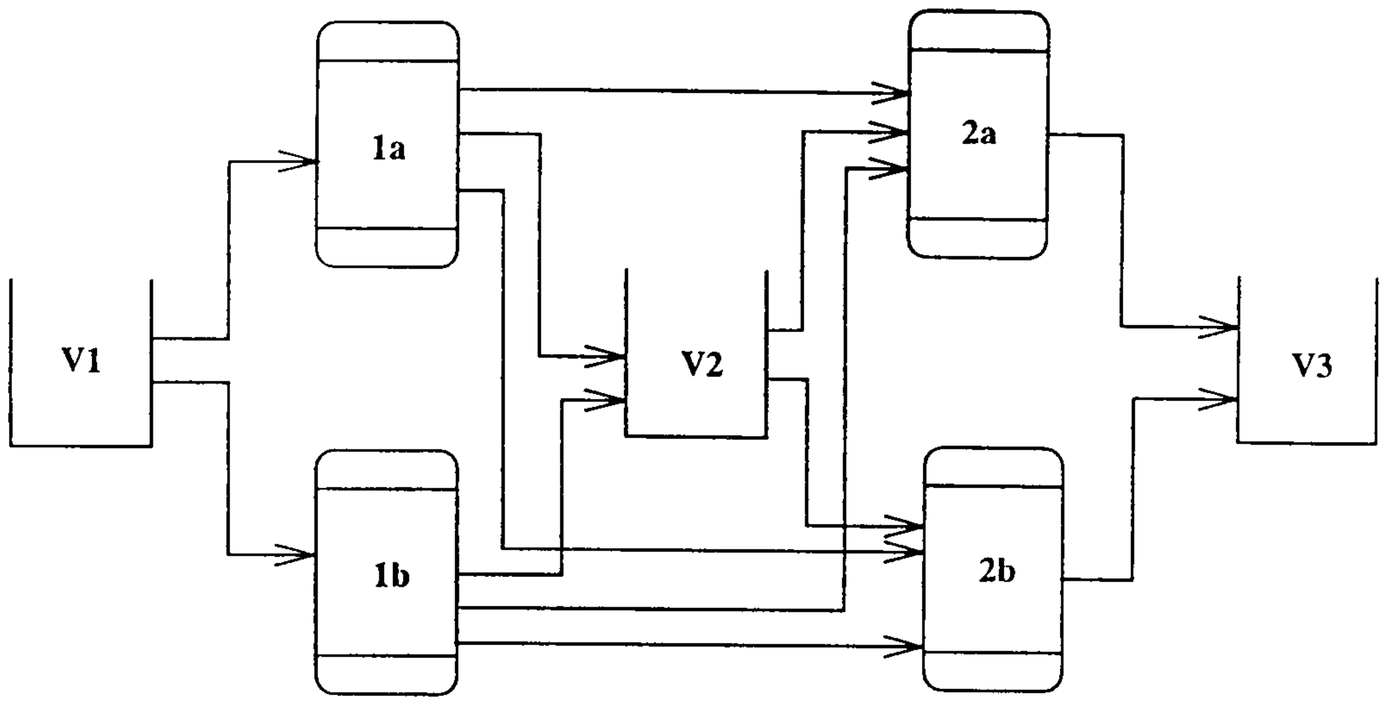


Figure 3.11: Plant superstructure of Example 7

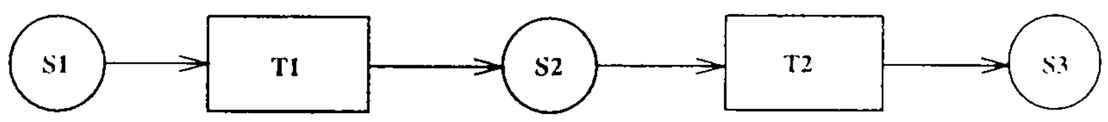


Figure 3.12: State task network of Example 7

Finally, in the last example the more detailed scheduling model proposed by Shah et al. 1993 (see Table 3.3), based on time discretization is employed at the design stage (Barbosa-Póvoa and Macchietto, 1994). The example examined here is the one presented by Barbosa-Póvoa and Macchietto, 1994 where in addition the demand of product is considered as uncertain following normal probability distribution function N(150,20). The example data concerning unit characteristics are given in Table 3.14 whereas the plant superstructure and the state task network representation are shown in Figures 3.11, 3.12. The stochastic model involves 262 variables (125 0-1 variables) and 509 constraints; it requires 18 CPU s solution time using GAMS/CPLEX on Sparc10.

The optimal plant corresponds to the selection of Unit 1b of 54 m^3 for task 1 and Unit 2b of 64 m^3 for task 2 as well as a storage vessel for state 2 of 10 m^3 and has an expected profit of \$21600. Comparing to the deterministic solution (Unit 1b of 45 m^3, Unit 2b of 51 m^3 and a storage vessel of 10 m^3) this plant involves larger equipments but has the capability to meet demand of product within the range of [90,200]. The detailed production schedules obtained from the solution for different demand values are shown in Figure 3.13. If the schedule remains unchanged with respect to demand the optimal plant corresponds to larger equipments of 81 m^3 for unit 1b and of 91 m^3 for unit 2b. an optimal schedule as shown in Figure 3.14 and an expected profit of \$21400. Notice

that considering production schedule to follow the demand realization which means better utilization of batch equipments leads to smaller yet more profitable plants.

Equipment	Task	Max capacity	Min capacity	Fixed cost	Variable cost
Unit 1a	Task T1	10	1750	20	0.5
Unit 1b	Task T1	10	250	10	0.1
Unit 2a	Task T2	10	2000	20	0.2
Unit 2a	Task T2	10	250	10	0.1
Vessel 1	State S1	-	Unl	-	-
Vessel 2	State S2	5	10	10	0.5
Vessel 3	State S3	-	Unl	-	-

Table 3.14: Equipment Data for Example 7

3.6. Concluding Remarks

A unified framework has been presented in this paper to address the problem of batch plant design and operations under uncertainty. A two-stage stochastic programming formulation was proposed which properly balances economic optimality with feasibility objectives. The formulation features (i) an expected profit objective comprising investment cost for equipment sizing, revenues from product sales and an explicit penalty term accounting for potential revenue losses due to unfilled orders and (ii) a relaxation of the feasibility requirement constraint. It was shown that basic properties can be established enabling the efficient solution of the proposed formulation for both cases of continuous and discrete equipment sizes. A particularly important result was that the integration of the expected profit evaluation can be performed within the bounds of uncertain parameter range, effectively avoiding the bilevel nature of the problem. An unexpected implication of this property was that despite the presence of uncertainty described by general probability distributional form, no extra complexity was introduced in the model, fully preserving the structure of the corresponding deterministic models!

Different policies regarding demand satisfaction, reflecting the attitude of decision maker can be effectively captured within the proposed unified formulation. The approach is general to most batch plant design/scheduling formulations appeared in the open literature involving aggregate scheduling constraints (as for example in Tables 3.1, 3.2) or detailed scheduling models (as in Table 3.3). A key issue that was exploited in this

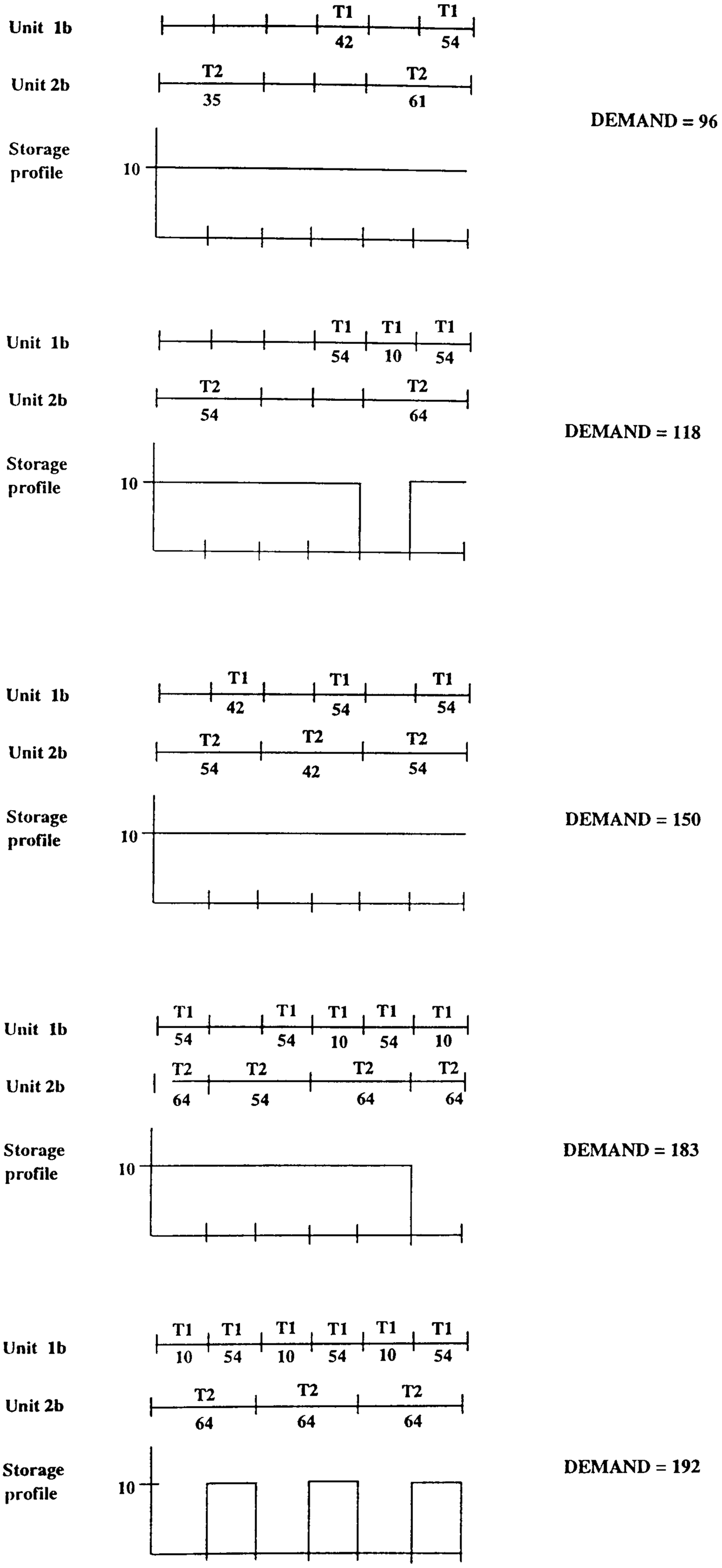


Figure 3.13: Gantt charts for different demand values (Example 7)

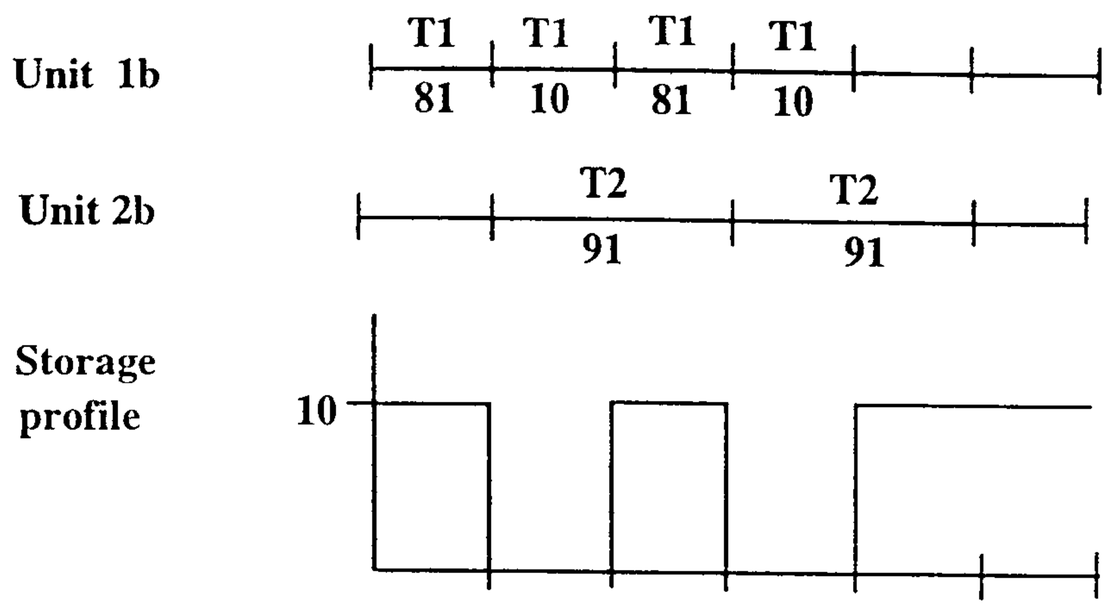


Figure 3.14: One schedule for different demand values (Example 7)

work was the option of changing the schedule pattern to follow demand variations which was proven to be advantageous from a design point of view, if especially the penalty for changeover is not significant.

From a computational point, the proposed modified global optimization approach for the case of continuous equipment sizes is promising, since only the solution of a fraction of optimization subproblems is required compared to the original GOP development; clearly there is a scope for further investigation in this area. Finally, it is interesting to note that many optimization tasks in the proposed approach, for batch continuous and discrete equipment sizes can in principle be performed independently; here parallel implementation developments look very promising (see for example, Pekny and coworkers, 1994, Floudas and coworkers, 1994).

Chapter 4

Production and Capacity Planning Under Uncertainty

Production planning with time horizon of few weeks or months as well as long-range planning including capacity expansion options is considered in this chapter where demands, prices and availabilities are assumed to be random variables. A decomposition based optimization approach is proposed, where planning decisions are taken by coupling economic optimality and plan feasibility. Example problems are presented to illustrate the steps of the proposed planning under uncertainty optimization algorithm.

4.1. Introduction

In any production system, many key parameters such as product demands, prices and availabilitites are only partially known; typically there is significant uncertainty regarding their future values. Consequently, in making planning decisions a company must not only consider a "short-term" economic criterion but also identify and assess the impact on its business of important uncertainties so as to develop strategies for dealing with them by providing contingency plans to be put into effect as the uncertainties are revealed. However, the proper treatment of uncertainty in planning decision making transforms the representation of the problem from a pure deterministic model that can be in principle solved by available software, to stochastic programming model whose solution typically requires the application of specialized decomposition techniques and advanced computer technologies (for example, parallel processors).

Solution approaches dealing with uncertainties in planning models have broadly proceeded along two directions: deterministic methods and probabilistic programming techniques. The former includes:

a. The scenario analysis approach, where a few realizations of the stochastic parameters are taken to be representative of the space of possible parameter outcomes and decisions are taken to maintain feasibility under each scenario. As presented by Brauers and Weber (1988), methods for scenario analysis differ mainly in the way they generate the scenarios to be examined. After the determination of future possible states and their corresponding probabilities these scenarios can be included in different phases of the planning process. In the simplest case, a specific plan gives higher objective function value when compared to alternative plans for all the different scenarios that are examined and therefore this will be chosen. More advanced techniques have also been presented for the aggregation of scenario solutions in an overall solution that will converge to the solution of the original stochastic optimization problem (Wets, 1988).

b. The multiperiod models which are characterized by discretization over time horizon. This model is used to account for predicted changes over a given time horizon. The consideration of uncertainty in forecasts can be made only by the examination of different scenarios. Grossmann et al. (1983) and Sahinidis and Grossmann (1991a), presented a multiperiod MILP model for the optimal selection of the production profiles and also of the capacity expansion policies given time varying demand and prices of chemicals. They also exploited the use of several solution approaches and concluded that the combination of strong cutting plane generation and B&B is the most promising strategy for the solution of these problems to optimality. Later, Sahinidis and Grossmann (1991b,1992) propose reformulation strategies for the above models that lead to great computational savings so as to render possible the examination of different scenarios. Picaseno-Gamiz and Sullivan (1988) presented also a multiperiod formulation for the optimization of the production schedule of continuous processing systems accounting for uncertainty by incorporating penalties in the objective function for not meeting production targets which also introduce nonlinear terms. Also Lustig et al. (1991), incorporate uncertainties into multiperiod model for long-range planning through the consideration of different scenarios. As the size of the resulting optimization model grows linearly with respect to the number of scenarios they reformulate the model to become suitable for interior point solutions methods which are able for solving large, sparse linear programs.

The probabilistic programming analysis takes into account the detailed statistical properties of the parameter variations and has evolved around two types of models:

the two-stage stochastic programming models with recourse and the chance constrained programming although most of the work presented in the literature follow the first of those approaches. Applications of stochastic programming with recourse models to long-range planning include the work Bloom (1983) and Bienstock and Shapiro (1988) who used stochastic programming with recourse model to describe the resource acquisition problems faced by an electric utility company; a Benders decomposition method was applied to solve the proposed two-stage programming with recourse model. Related electric utility planning problems have also been formulated as stochastic programming problems with recourse in the works of Borison et al. (1984) who presented a stochastic dynamic programming model for the determination of optimal purchase policies of generating technologies in the face of uncertainty and Modiano (1987) who developed a stochastic programming with recourse model to analyze the impact of demand uncertainties on electric utility capacity planning. Fathi-Afshar (1987) selected the parameters that have significant influence into decisions by some Monte Carlo technique and fed them into the optimization model. The solution gives the optimal decisions together with the value of the objective function and the same procedure is repeated until convergence is reached. Dantzig (1989) proposed a Benders decomposition algorithm to solve the two-stage stochastic programming formulation of the resource planning problem for large-scale electric power systems under uncertainty.

Friedman and Reklaitis (1975) and Shimizu (1989) suggested an approach for incorporating flexibility in a system where, by allowing for possible future additive corrections on the current decisions, the system can be optimized by applying an appropriate cost-for-correction in the objective function. For short/medium term linear planning models where capacity expansion policies are not taken into account, Ierapetritou et al. (1994) proposed an algorithm for two-stage stochastic linear planning models based on the solution of multiparametric linear programs; this however may become a non-trivial task especially as the number of first-stage decisions and uncertain parameters increase.

The problem of capacity expansions in planning models has also received a lot of attention in the literature. Himmeblau and Bickel (1980), solved the problem of when and how a chemical plant should be expanded in order to satisfy production requirements and maximize the present value of the net profit. They considered deterministic sale and demand forecasts over a given time horizon and only a finite set of possible plant expansions. They incorporated into their multiperiod model all possible alternatives and developed a

solution procedure based on branch and bound and nonlinear programming algorithms. However, the major limitations of their approach is the great computation effort needed and the large increase on model size with the number of alternatives considered mainly as the complexity of the plant increases. Shimizu and Takamatsu (1985), formulated a multiobjective MILP multiperiod planning model where they considered integer variables to represent expansions of specific units. They used an interactive goal programming algorithm for the solution of their model. However, they did not take into account variations in forecasts. Jimenez and Rudd (1987), presented a recursive MIP model for the petrochemical industry. They also corresponded the decisions of capacity expansions to binary variables but they did not consider the effect of uncertainty in future parameter values. Sahinidis et al. (1989) presented a multiperiod planning model for the optimal selection of the capacity expansion and/or shut down policies, selection of new processes, production profiles and the sales and purchases of chemicals over a given long time horizon for continuous plants where forecasts for prices and demands of chemicals are taken into account through the examination of different scenarios. A different approach has been followed by Davis et al., (1986). They first formulated the mathematical model of the capacity expansion problem considering the demand as a random point process and assumming non-zero lead times and then studied the optimization of capacity expansion by means of stochastic control theory. They pointed out that the resulting mathematical model falls into the class of stochastic processes known as piecewise-deterministic Markov processes and presented algorithms for computing the optimal policy in certain cases.

In this chapter a new planning methodology is proposed based on the approach presented in chapter 2 which results in the simultaneous optimization of expected profit and future plant feasibility. In the next sections, the two-stage programming planning model is first introduced; the key building blocks of the proposed approach are then discussed in detail and finally, three example problems are presented to illustrate the basic steps of the proposed approach and to provide more insight on the main features of the algorithm.

4.2. Two-stage Stochastic Formulation

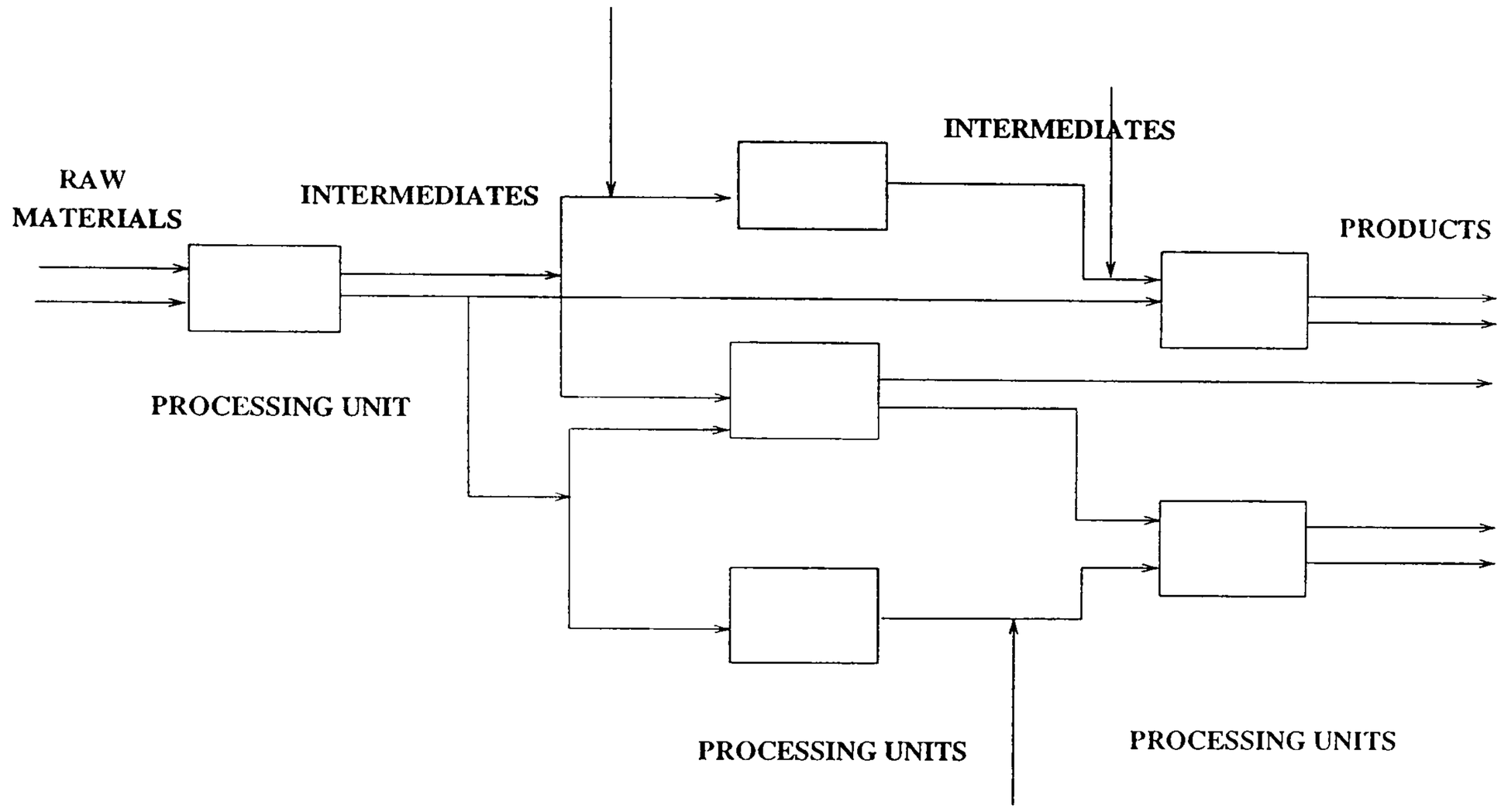


Figure 4.1: Production Network

The planning problem which is considered here can be stated as follows: A network of M continuous processes and N chemicals is given (see Figure 4.1). Also given are the prices, demands and availabilities of chemicals as well as investment and operating cost data over a time period (first-stage), whereas their exact values are not known for the future (second-stage); instead they are considered uncertain, described by continuous distribution functions. The problem then consists of determining (i) production profiles, (ii) sales and purchases of chemicals, and/or (iii) capacity expansions for the existing processes over each stage which will maximize an expected profit over the two stages by also ensuring future feasibility. A typical aggregate linear planning model consists of the following set of constraints:

(i) Production capacity constraints For example,

$$R_{tj} = R_{t-1j} + CE_{tj}, \quad j = 1,..,M$$

$$CE^L_{tj} y_{tj} \leq CE_{tj} \leq CE^U_{tj} y_{tj}, \quad t = 1,..,T$$

where R_{tj} denotes the production capacity of process j (j=1,..,M) during time period t; CE_{tj} represents the (potential) capacity expansion of process j in t; the occurrence or not of an expansion is denoted by a set of (0,1) variables y_{tj} ; CE^L_{tj}, CE^U_{tj} are constant lower and upper bounds of capacity expansion variables CE_{tj}.

(ii) Demand constraints

$$d_{ti}^{L} \leq S_{ti} \leq d_{ti}^{U}, \quad i = 1,..,N,\ t = 1,..T$$

where S_{ti} denotes the amount of chemical i (i=1,..,N) sold in time period t; d_{ti}^{L} and d_{ti}^{U} are the lower and upper bounds on the demands of chemical i during period t, respectively.

(iii) Availability constraints

$$a_{ti}^{L} \leq P_{ti} \leq a_{ti}^{U}, \quad i = 1,..,N,\ t = 1,..T$$

where P_{ti} denotes the amount of chemical i purchased in time period t; a_{ti}^{L}, a_{ti}^{U} are the lower and upper bounds on the availability of chemical i during period t, respectively.

(iv) Inventory requirements

$$I_{ti}^{fmin} \leq I_{ti}^{f} \leq I_{ti}^{fmax}, \quad i = 1,..,N$$

$$I_{ti}^{f} = I_{t+1i}^{in}, \quad t = 1,..,T$$

where I_{ti}^{in} and I_{ti}^{f} represent the initial and the final inventory of chemical i in t, respectively; $I_{ti}^{fmin}, I_{ti}^{fmax}$ are the minimum and maximum required amount of inventory for material i at the end of each time period (Dantzig, 1989).

(v) Material balances

$$P_{ti} + I_{ti}^{in} + \sum_{j=1}^{M} b_{ij} R_{tj} - S_{ti} - I_{ti}^{f} = 0, \quad i = 1,..,N,\ t = 1,..T$$

where b_{ij} is the stoichiometric coefficient for material i in process j.

(vi) Objective function

A profit function over the time horizon is considered as the difference between the revenue due to product sales and the overall cost (cost of raw materials, operating cost, investment cost and inventory cost).

$$Profit = \sum_{t=1}^{T}[\sum_{i=1}^{N}\gamma_{ti}S_{ti} + \sum_{i=1}^{N}\tilde{\gamma}_{ti}I_{ti}^{f} - \sum_{i=1}^{N}\lambda_{ti}P_{ti} - \sum_{i=1}^{N}\tilde{\lambda}_{ti}I_{ti}^{in} - \sum_{j=1}^{M}C_{tj}R_{tj} - \sum_{j=1}^{M}(\alpha_{tj}CE_{tj} + \beta_{tj}y_{tj})]$$

where : γ_{ti} are the sales price of material i in time period t; λ_{ti} the purchase price of material i in time period t; $\tilde{\gamma}_{ti}$ the value of final inventory of material i in time

period t; $\tilde{\lambda}_{ti}$ the value of starting inventory of material i in time period t (may be taken as the material purchase price); C_{tj} the operating cost of process j in time period t; α_{tj} the variable-size cost coefficients for the investment cost of capacity expansion of process j at time period t; β_{tj} the fixed-cost charges for the investment cost of capacity expansion of process j at time period t.

We consider here a two-stage stochastic planning problem in which the model parameters $(a_{ti}^L, a_{ti}^U, d_{ti}^L, d_{ti}^U, I_{ti}^{fmin}, I_{ti}^{fmax}, b_{ij}, \gamma_{ti}, \tilde{\gamma}_{ti}, \lambda_{ti}, \tilde{\lambda}_{ti}, C_{tj}, \alpha_{tj}, \beta_{tj})$ are known in the first stage, while for the second stage they can take a continuum of values following a several continuous or discrete distribution function J(θ). Then the previous planning model can be mathematically represented in the following compact format (Dantzig, 1989, Gassmann, 1990):

Problem (4.1)

$$\max_{x_1,y_1,y_1,CE_1,CE_2} \{c_1x_1 + a_1CE_1 + \beta_1y_1 + a_2CE_2 + \beta_2y_2 + \mathbf{E}_\theta \{\max_{x_2}\{c_2(\theta)x_2\}\}\} \tag{4.1}$$

subject to:

$$A_1x_1 + A_2CE_1 \leq b_1 \tag{4.2}$$

$$y_1CE_1^{min} \leq CE_1 \leq CE_1^{max}y_1 \tag{4.3}$$

$$A_3(x_1 + CE_1) + B_1(\theta)x_2 + B_2CE_2 \ \leq b_2(\theta) \tag{4.4}$$

$$y_2CE_2^{min} \leq CE_2 \leq CE_2^{max}y_2 \tag{4.5}$$

$$\theta \in \mathbf{R} \tag{4.6}$$

$$x_1, x_2 \geq 0, \ \ y_1, y_2 = 0, 1$$

where:

x_1, x_2 — vectors of first and second-stage operational decision variables (product sales, raw material purchases and production profiles)

CE_1, CE_2 — first and second-stage capacity expansion variables

y_1, y_2 — vectors of binary variables denoting capacity expansion alternatives, with elements

$$y_{1(2)j} = \begin{cases} 1 & \text{if process j is expanded during stage } 1(2) \\ 0 & \text{otherwise} \end{cases}$$

θ — vector of uncertain parameters with associated

	distribution function $J(\theta)$
$\mathbf{E}_\theta\{.\}$	expectation operator of $\{.\}$ over θ
c_1, $c_2(\theta)$	current and future costs of sales and purchases
a_1, a_2	current and future variable-size cost coefficients for the investment cost of capacity expansions
β_1, β_2	current and future fixed-cost charges for the investment cost of capacity expansions
b_1	current demands, availabilities and capacity bounds
$b_3(\theta)$	future demands, availabilities and capacity bounds
A_1, A_2, A_3, B_2	constant matrices
$B_1(\theta)$	matrix that may also involve uncertainty
$\mathbf{R}$	feasible region of x_1, $\mathrm{R}(x_1)= \{\theta \mid \forall\theta \in R(x_1)\ \exists x_2 :$ second stage constraints are satisfied$\}$

In the above formulation, the set of constraints 4.2 and 4.3 represent the first-stage operating requirements allowing for potential capacity expansions. Similarly, sets 4.4 and 4.5 refer to second-stage operating options, where θ is involved. For short-term planning $CE_1 = CE_2 = 0,\ y_1 = y_2 = 0$ and consequently problem (4.1) can be simplified in the following way:

Problem (4.2)

$$\begin{aligned} \max_{x_1}\ & c_1x_1 + \mathbf{E}_\theta\ \{\max_{x_2}\{c_2(\theta)x_2\}\} \\ s.t.\ & A_1x_1 \ \leq b_1 \\ & A_3x_1 + B_1(\theta)x_2 \ \leq b_2(\theta) \\ & x_1, x_2 \geq 0,\ \theta \in \mathbf{R} \end{aligned}$$

Problems (4.1) and (4.2) mathematically describe the following two-stage planning strategy. At the first stage the operating decision variables x_1 and/or the capacity expansion variables y_1, y_2, CE_1, CE_2 should be selected to maximize the average profit and also to ensure future feasibility, i.e. that a vector of future operating variables x_2 can be found to satisfy constraints 4.4. At the second stage, after a first-stage plan is implemented the solution of the inner optimization problem results in the selection of a feasible second-stage plan x_2 that optimize plant operation. Note that problem (4.1) involves linear planning models; however, convex nonlinear planning models can also be accommodated by the proposed planning framework as will become apparent in the next section.

The formulation in problem (4.1) is shown here for two stages; its extension to the multi-stage case using similar modelling arguments is indeed possible (although computationally much more intensive). Note also that a stage may be further divided in time periods to account, if needed, for more refined modelling requirements. These issues are not explicitly considered in this thesis.

A key feature of the model (4.1) is the explicit requirement for feasibility; i.e. the inclusion of constraint 4.6. This enables the evaluation of the expected profit inside the feasible region of the plan, where feasible second-stage decisions are ensured (see also chapter 2). In some situations, this evaluation might be conservative since it does not account for partial feasibility (for example, partial demand satisfaction with penalty term for the production-demand deviation; see Wellons and Reklaitis, 1989).

As far as the solution procedure is concerned, note that problem (4.1) corresponds to a special case of problem (4.3) presented in chapter 2. Consequently the proposed approach can be also used for the solution of planning problem (4.1) as it will be shown in more details in the following section.

4.3. Proposed Approach

Employing a Gaussian Quadrature formula for the evaluation of the expected profit problem (4.1) can be rewritten in the following way:

Problem (4.3)

$$\max_{x_1,y_1,y_2,CE_1,CE_2,x_2^{q_1q_2}} \{c_1x_1 + a_1CE_1 + \beta_1y_1 + a_2CE_2 + \beta_2y_2$$
$$+\frac{\theta_1^U - \theta_1^L}{2}\sum_{q_1=1}^{Q_1} w_1^{q_1}\frac{\theta_2^U(\theta_1^{q_1}) - \theta_2^L(\theta_1^{q_1})}{2}\sum_{q_2=1}^{Q_2} w_2^{q_2}\ (c_2(\theta_1^{q_1},\theta_2^{q_1q_2})x_2^{q_1q_2})\ J(\theta_1^{q_1},\theta_2^{q_1q_2})\}$$

subject to:

$$A_1x_1 + A_2CE_1 \leq b_1$$
$$y_1CE_1^{min} \leq CE_1 \leq CE_1^{max}y_1$$
$$A_3(x_1 + CE_1) + B_1(\theta_1^{q_1},\theta_2^{q_1q_2})x_2^{q_1q_2} + B_2CE_2\ \leq b_2(\theta_1^{q_1},\theta_2^{q_1q_2})$$
$$q_1 = 1,..,Q_1,\ q_2 = 1,..,Q_2$$

$$y_2 CE_2^{min} \leq CE_2 \leq CE_2^{max} y_2$$

$$(\theta_1^{q_1}, \theta_2^{q_1 q_2}) \in \mathbf{R}$$

$$x_1, x_2^{q_1 q_2} \geq 0, \;\; y_1, y_2 = 0, 1$$

The solution of problem (4.3) requires the determination of the feasible region $\mathbf{R}$, i.e. the bounds of the feasible space in each direction of the uncertain parameters. This can be achieved through a series of feasibility subproblems which have to be simultaneously considered. Recasting problem (4.3) in this manner leads to the following formulation:

Problem (4.4)

$$\max_{x_1, y_1, y_2, CE_1, CE_2, x_2^{q_1 q_2}} \{c_1 x_1 + a_1 CE_1 + \beta_1 y_1 + a_2 CE_2 + \beta_2 y_2$$

$$+ \frac{\theta_{\mathbf{1}}^{\mathbf{U}} - \theta_{\mathbf{1}}^{\mathbf{L}}}{2} \sum_{q_1=1}^{Q_1} w_1^{q_1} \frac{\theta_{\mathbf{2}}^{\mathbf{U q_1}} - \theta_{\mathbf{2}}^{\mathbf{L q_1}}}{2} \sum_{q_2=1}^{Q_2} w_2^{q_2} \; (c_2(\theta_1^{q_1}, \theta_2^{q_1 q_2}) x_2^{q_1 q_2}) J(\theta_1^{q_1}, \theta_2^{q_1 q_2})\}$$

subject to:

$$A_1 x_1 + A_2 CE_1 \leq b_1$$

$$y_1 CE_1^{min} \leq CE_1 \leq CE_1^{max} y_1$$

$$A_3(x_1 + CE_1) + B_1(\theta_1^{q_1}, \theta_2^{q_1 q_2}) x_2^{q_1 q_2} + B_2 CE_2 \; \leq b_2(\theta_1^{q_1}, \theta_2^{q_1 q_2})$$

$$q_1 = 1, .., Q_1, \; q_2 = 1, .., Q_2$$

$$y_2 CE_2^{min} \leq CE_2 \leq CE_2^{max} y_2$$

where:

$$\left.\begin{aligned} \theta_{\mathbf{1}}^{\mathbf{U}}, \theta_{\mathbf{1}}^{\mathbf{L}} &= \mathbf{arg} \max_{\theta_1^U, \theta_1^L} \{\theta_1^U - \theta_1^L\} \\ s.t. \;\; A_3(x_1 + CE_1) &+ B_1(\theta_1^U, \theta_2(.)) x_2(.) + B_2 CE_2 \; \leq b_2(\theta_1^U, \theta_2(.)) \\ A_3(x_1 + CE_1) &+ B_1(\theta_1^L, \theta_2(.)) x_2(.) + B_2 CE_2 \; \leq b_2(\theta_1^L, \theta_2(.)) \end{aligned}\right\} \quad \text{(B1)}$$

$$\left.\begin{aligned} \theta_{\mathbf{2}}^{\mathbf{U q_1}}, \theta_{\mathbf{1}}^{\mathbf{L q_1}} &= \mathbf{arg} \max_{\theta_2^{U q_1}, \theta_2^{L q_1}} \{\theta_2^{U q_1} - \theta_2^{L q_1}\} \\ s.t. \;\; A_3(x_1 + CE_1) &+ B_1(\theta_1^{q_1}, \theta_2^{U q_1}) x_2(.) + B_2 CE_2 \; \leq b_2(\theta_1^{q_1}, \theta_2^{U q_1}) \\ A_3(x_1 + CE_1) &+ B_1(\theta_1^{q_1}, \theta_2^{L q_1}) x_2(.) + B_2 CE_2 \; \leq b_2(\theta_1^{q_1}, \theta_2^{L q_1}) \end{aligned}\right\} \begin{array}{l} (B2^{q_1}), \\ q_1 = 1, .., Q_1 \end{array}$$

$$\theta_1^{q_1} = 0.5[\theta_1^U (1 + v_1^{q_1}) + \theta_1^L (1 - v_1^{q_1})], \;\; q_1 = 1, .., Q_1 \tag{4.7}$$

$$\theta_2^{q_1 \, q_2} = 0.5[\theta_2^{U q_1} (1 + v_2^{q_2}) + \theta_2^{L q_1} (1 - v_2^{q_2})], \; q_1 = 1, .., Q_1, \; q_2 = 1, .., Q_2 \tag{4.8}$$

where z(.), $\theta_2(.)$ denotes variables that are associated with each set of constraints.

The proposed decomposition scheme can then be employed for the solution of problem (4.4), which properly exploits the special structure of the problem as follows. For a given production plan and capacity expansion policy $(x_1, y_1, y_2, CE_1, CE_2)$ the linear feasibility subproblems (B1) and $(B2^{q_1})$ can be solved independently resulting in the identification of the feasible region (see Figure 4.2) and evaluation of the quadrature points from equations 4.7, 4.8.

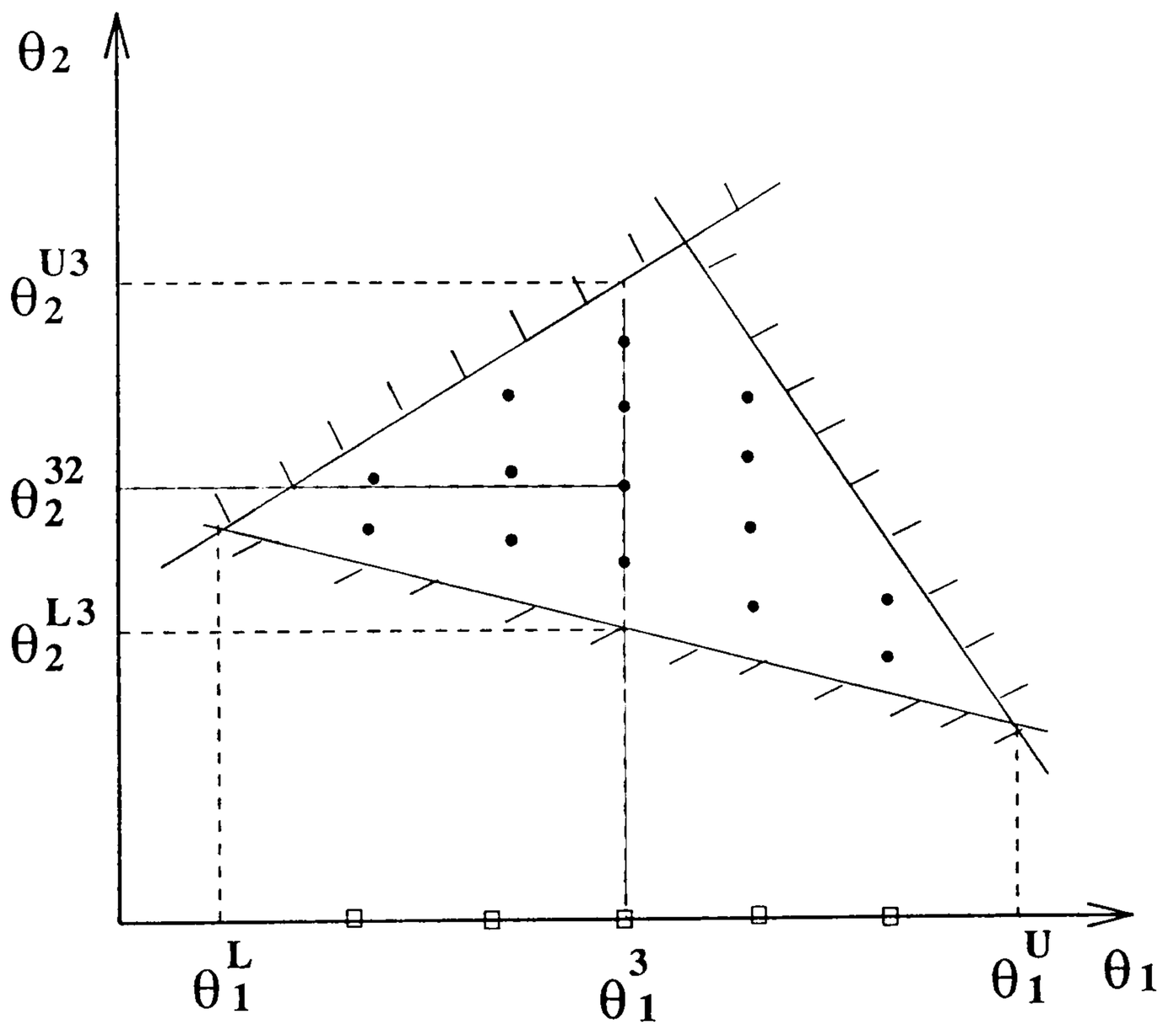


Figure 4.2: Quadrature Points inside Feasible Region

As soon as the quadrature points $(\theta_1^{q_1}, \theta_2^{q_1 q_2})$ are defined, problem (4.3) can be solved to evaluate the expected profit. Note that problem (4.3) can be further decomposed by first solving the following $Q_1 \times Q_2$ independent optimization subproblems (4.5):

Problem (4.5)

$$\max_{x_2^{q_1 q_2}} \{c_2(\theta_1^{q_1}, \theta_2^{q_1 q_2}) x_2^{q_1 q_2}\}$$

subject to

$$B_1(\theta_1^{q_1}, \theta_2^{q_1 q_2}) x_2^{q_1 q_2} \leq b_2(\theta_1^{q_1}, \theta_2^{q_1 q_2}) - A_3(x_1 + CE_1) - B_2 CE_2 \quad q_1 = 1, .., Q_1, \; q_2 = 1, .., Q_2$$

and then evaluate the expected profit through the Gaussian quadrature formula. Problems (4.5) correspond to linear programming (LP) formulations of much smaller size, which can effectively be solved within a parallel computing scheme with the subproblems distributed across processors. The solution of the feasibility subproblems (B1), ($B2^{q_1}$) as well as the profit maximization subproblems (4.5) provide also the required dual information for the construction of the following master problem (4.6) which identifies a new vector of decision variables and provides a valid upper bound to the solution of problem (4.4):

Problem (4.6)

$$EP_U^k = \max_{\mu_B, x_1, y_1, y_2, CE_1, CE_2} \mu_B$$

$$\begin{aligned} s.t.\ \mu_B \leq\ & c_1x_1 + a_1CE_1 + \beta_1y_1 + a_2CE_2 + \beta_2y_2 \\ & + \frac{\theta_1^U - \theta_1^L}{2} \sum_{q_1=1}^{Q_1} w_1^{q_1} \frac{\theta_2^{Uq_1} - \theta_2^{Lq_1}}{2} \sum_{q_2=1}^{Q_2} w_2^{q_2}\ c_2(\theta_1^{q_1}, \theta_2^{q_1q_2}) x_2^{q_1q_2} J(\theta_1^{q_1}, \theta_2^{q_1q_2}) \end{aligned}$$

$$\begin{aligned} & - \sum_{q_1=1}^{Q_1} \sum_{q_2=1}^{Q_2} \eta^{q_1q_2} [A_3(x_1 + CE_1) + B_1(\theta_1^{q_1}, \theta_2^{q_1q_2}) x_2^{q_1q_2} + B_2CE_2 - b_2(\theta_1^{q_1}, \theta_2^{q_1q_2}] \\ & - \lambda_1^U [A_3(x_1 + CE_1) + B_1(\theta_1^U, \theta_2(.)) x_2(.) + B_2CE_2 - b_2(\theta_1^U, \theta_2(.))] \\ & - \lambda_1^L [A_3(x_1 + CE_1) + B_1(\theta_1^L, \theta_2(.)) x_2(.) + B_2CE_2 - b_2(\theta_1^L, \theta_2(.))] \\ & - \sum_{q_1=1}^{Q_1} \lambda_2^{Uq_1} [A_3(x_1 + CE_1) + B_1(\theta_1^{q_1}, \theta_2^{Uq_1}) x_2(.) + B_2CE_2 - b_2(\theta_1^{q_1}, \theta_2^{Uq_1})] \\ & - \sum_{q_1=1}^{Q_1} \lambda_2^{Lq_1} [A_3(x_1 + CE_1) + B_1(\theta_1^{q_1}, \theta_2^{Uq_1}) x_2(.) + B_2CE_2 - b_2(\theta_1^{q_1}, \theta_2^{Uq_1})] \end{aligned}$$

$$A_1x_1 + A_2CE_1 \leq b_1$$

$$y_1CE_1^{min} \leq CE_1 \leq CE_1^{max}y_1$$

where:

μ_B	a scalar variable
EP_U^k	the predicted upper bound
$\eta^{q_1q_2}$	the corrected multipliers for the constraints of problems (4.5)
λ_1^U, λ_1^L	the corrected multipliers for the constraints of problem (B1)
$\lambda_2^{Uq_1}, \lambda_2^{Lq_1}$	the corrected multipliers for the constraints of problems ($B2^{q_1}$)

Therefore, an iterative procedure can be implemented, as shown in Figure 4.3, which involves the following steps:

Step 1: Select an initial plan $(x_1^1, y_1^1, y_2^1, CE_1^1, CE_2^1)$. Set the lower bound $EP_L = -\infty$, k=1 and select a tolerance ϵ.

Step 2: Solve the feasibility subproblems (B1), $(B2^{q_1})$ to obtain the boundary of the feasible region and the corresponding Lagrangian multipliers. For the case of infeasible subproblems solve the problem to minimize the infeasibilities.

Step 3: At each quadrature point $(\theta_1^{q_1}, \theta_2^{q_1 q_2})$ solve problem (4.5) to evaluate the optimal value of profit and obtain the corresponding Lagrangian multipliers.

Step 4: Calculate the expected profit (EP) using the Gaussian Quadrature formula (problem (4.3)); update the lower bound, $EP_L = \max\{EP, EP_L\}$.

Step 5a: Calculate the correction factors (see Chapter 2) and obtain the corrected multipliers $\eta^{q_1 q_2}$, $\lambda_1^U, \lambda_1^L, \lambda_2^{Uq_1}, \lambda_2^{Lq_1}$.

Step 5b: Solve the master problem (4.6) to obtain a new plan $(x_1^{k+1}, y_1^{k+1}, y_2^{k+1}, CE_1^{k+1}, CE_2^{k+1})$ and an upper bound EP_U^k.

Step 6: If $EP_U^k \leq EP_L + \epsilon$, stop; the solution is the plan $(x_1^k, y_1^k, y_2^k, CE_1^k, CE_2^k)$ with expected profit EP_L. Otherwise, set k=k+1 and return to Step 2.

The proposed iterative algorithmic procedure is guaranteed to converge to a global optimum in a finite number of iterations (Geoffrion, 1972); its solution results in the determination of an optimal plan and capacity expansion policy with a maximum expected profit over the two stages. In the next section, three example problems are presented to illustrate the features of the proposed planning under uncertainty algorithm.

4.4. Examples

Three planning problems are presented in this section. The first one corresponds to a small-scale chemical complex involving two uncertain parameters where capacity expansion options are not considered; it serves to illustrate in detail the analytical steps of the planning procedure. The second example involves three uncertain parameters with capacity expansion options; its solution shows the increase of required computations as a number of uncertain parameters increases, and motivates the need for parallel implementation. Finally, the third example, representing a refinery planning problem, demonstrates that the computational requirements for the implementation of the new algorithm do not critically depend on the model size.

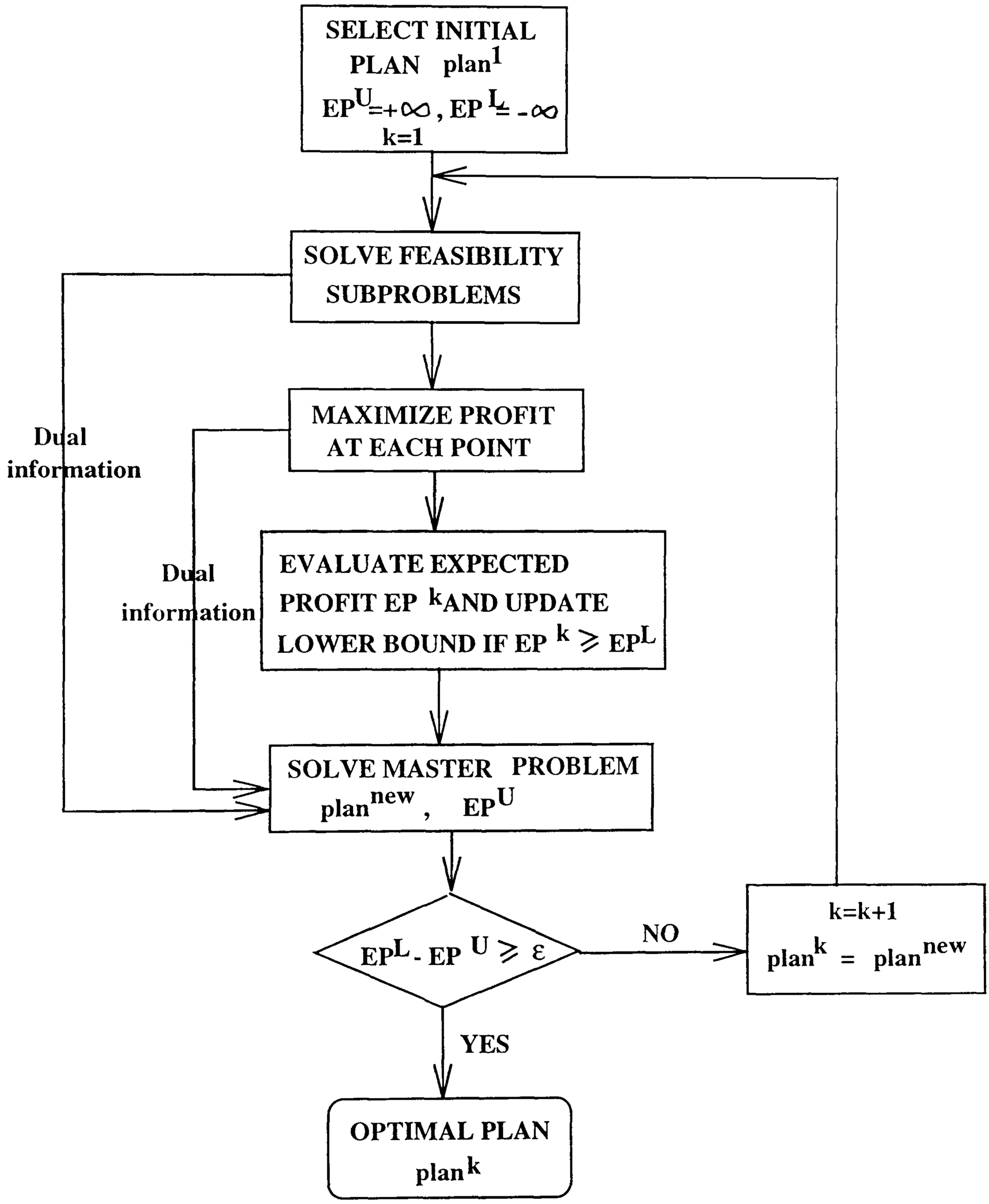


Figure 4.3: New planning under uncertainty Algorithm

Example 1

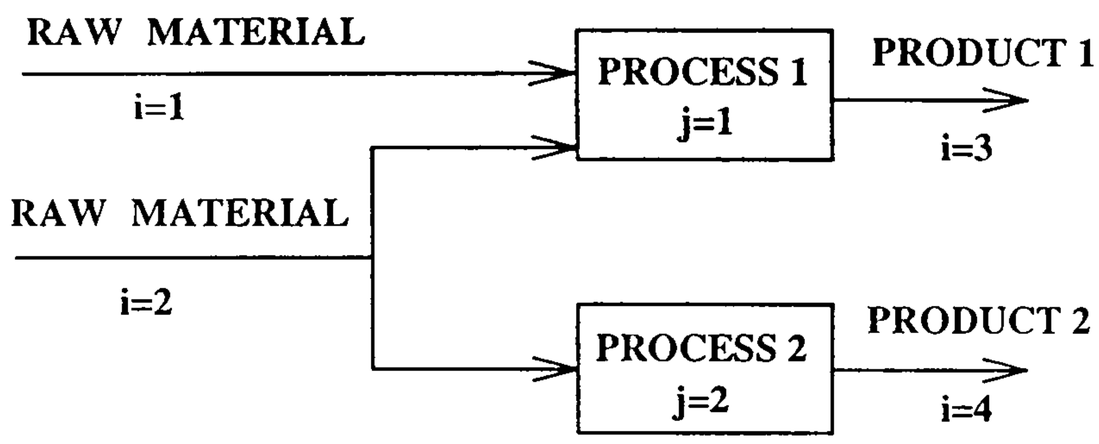


Figure 4.4: Chemical Complex - Example 1

Figure 4.4 depicts a small-scale chemical complex involving two processes with two products produced from two different raw materials. The following notation is used: s=1,2 represents the two stages, I= {i|i=1,2,3,4} is the set of materials and J= {j|j=1,2} is the set of processes. Then, the following set of constraints represents the two-stage production planning model:

(i) material balances over stage s

$$P_{s1} + I_{s1}^{in} - 0.4R_{s1} - I_{s1}^{f} = 0$$
$$P_{s2} + I_{s2}^{in} - 0.6R_{s1} - R_{s2} - I_{s2}^{f} = 0 I_{s3}^{in} + 0.5R_{s1} - I_{s3}^{f} - S_{s3} = 0$$
$$I_{s4}^{in} + 0.6R_{s2} - I_{s4}^{f} - S_{s4} = 0$$

where:
- R_{sj} the level at which process j is run at the stage s
- I_{si}^{in}, I_{si}^{f} the level of the inventory of material i at the beginning and at the end of stage s, respectively (with $I_{1i}^{in} = 0,\ I_{1i}^{f} = I_{2i}^{in}$)
- S_{si} the amount of material i sold during stage s
- P_{si} the amount of material i purchased during stage s

(ii) limitations on the utilization levels over the two stages

$$20 \leq R_{s1} \leq 100$$
$$30 \leq R_{s2} \leq 100$$

(iii) limitations on purchases due to the availability of raw material

$$20 \leq P_{11} \leq 100$$
$$30 \leq P_{12} \leq 200$$
$$20 \leq P_{21} \leq 100$$
$$10 \leq P_{22} \leq \theta_1$$

(iv) limitations on sales due to product demands

$$20 \leq S_{13} \leq 40$$
$$20 \leq S_{14} \leq 85$$
$$\theta_2 \leq S_{23} \leq 40$$
$$20 \leq S_{24} \leq 85$$

(v) maximum and minimum inventory requirements at the end of each stage

$$0 \leq I_{si}^{f} \leq 20$$

(vi) an objective to maximize the profit over the two stages:

$$\begin{aligned} \text{PROFIT} = {} & 100S_{13} + 80S_{14} + 10I_{11}^{f} + 15I_{12}^{f} + 20I_{13}^{f} + 25I_{14}^{f} - \\ & -10P_{11} - 15P_{12} - 30R_{11} - 35R_{12} + \\ & +90S_{23} + 80S_{24} + 10I_{21}^{f} + 15I_{22}^{f} + 25I_{23}^{f} + 20I_{24}^{f} - \\ & -30R_{21} - 35R_{22} - 10I_{21}^{s} - I_{22}^{s} - 30I_{23}^{s} - 30I_{24}^{s} \end{aligned}$$

Note that two uncertain parameters (θ_1, θ_2) are involved in the description of the model: (i) the availability of material i=2 at the second-stage which follows a normal distribution function N(50, 2.5) and (ii) the demand of material i=3 at the second-stage which is assumed to follow a normal distribution function N(20, 2.5).

Applying the steps of the proposed approach, the following results are obtained:

Step 1: An initial plan is selected for the first-stage variables: $(R_{11}, R_{12}, S_{13}, S_{14}, P_{11}, P_{12})$ = (90,36.67,40,20,56,110.67); $EP_L = -\infty$, k=1 and $\epsilon = 0.1$.

Step 2: The solution of the feasibility problem (B1) leads to the following bounds of θ_1: $40 \leq \theta_1 \leq 60$. Considering 5 quadrature points for θ_1 the results shown in Table 4.1 of the solution of $(B2^{q_1})$ subproblems are obtained.

q_1	1	2	3	4	5
$\theta_1^{q_1}$	40.938	44.615	50.000	55.385	59.062
$\theta_2^{Lq_1}$	10	10	10	10	10
$\theta_2^{Uq_1}$	30	30	30	30	30

Table 4.1: Bounds for θ_2 at $\theta_1^{q_1}$ for the initial plan

Step 3: Considering 5 quadrature points for θ_2 and solving problem (4.5) at each one of the 25 points the results shown in Table 4.2 are obtained.

q_1 q_2	1	2	3	4	5
1	488.1	488.1	488.1	488.1	488.1
2	500.4	500.4	500.4	500.4	500.4
3	518.3	518.3	518.3	518.3	518.3
4	525.0	525.0	525.0	525.0	525.0
5	525.0	525.0	525.0	525.0	525.0

Table 4.2: Optimal profit at the quadrature points (5x5 grid)

Step 4: The expected profit is evaluated through the Gaussian Quadrature formula yielding a value of 323.3 units; the lower bound is updated, EP_L = 323.3.

Step 5a,5b: After the evaluation of the corrected multipliers the master problem is formulated as follows:

$$
\begin{aligned}
EP_U^k = \max_{\mu_B, R_{11}, R_{12}, S_{13}, S_{14}, P_{11}, P_{12}} & \mu_B \\
s.t.\ \ & \mu_B \leq 13.5 + 12.4S_{13} - 2.3S_{14} + 17.5P_{12} - 9.7R_{11} - 18.1R_{12} \\
& 20 \leq R_{11} \leq 100 \\
& 30 \leq R_{12} \leq 100 \\
& 20 \leq P_{11} \leq 100 \\
& 30 \leq P_{12} \leq 200 \\
& 20 \leq S_{13} \leq 40 \\
& 20 \leq S_{14} \leq 85 \\
& 0 \leq P_{11} - 0.4R_{11} \leq 20 \\
& 0 \leq P_{12} - 0.6R_{11} - R_{12} \leq 20 \\
& 0 \leq S_{13} + 0.5R_{11} \leq 20 \\
& 0 \leq S_{14} + 0.6R_{12} \leq 20
\end{aligned}
$$

The solution of the master problem yields the following plan: $(R_{11}, R_{12}, S_{13}, S_{14}, P_{11}, P_{12}) = (100,33.3,40,20,40,113.3)$ and an upper bound of EP_U^1=778.7 units.

Step 6: Since the stopping criterion is not satisfied EP_U^1=778.7 > EP_L=323.3, set k=k+1 and return to Step 2.

The proposed approach requires 8 iterations to reach the optimal solution within a tolerance of 0.1 for the lower and upper bounds. The optimal solution is the plan that corresponds to the following values of the operating variables $(R_{11}, R_{12}, S_{13}, S_{14}, P_{11}, P_{12})$= (93.3,36.67,40,20,37.3,112.67). This plan has an expected profit of 504.2 units within a corresponding feasible region defined by the following bounds: for θ_1, $40 \leq \theta_1 \leq 60$, and for each quadrature point $\theta_1^{q_1}$ by bounds for θ_2 as shown in Table 4.3.

q_1	1	2	3	4	5
$\theta_1^{q_1}$	40.938	44.615	50.000	55.385	59.062
$\theta_2^{Lq_1}$	10	10	10	10	10
$\theta_2^{Uq_1}$	30	30	30	30	30

Table 4.3: Bounds for θ_2 at $\theta_1^{q_1}$ for the optimal plan

The progress of the convergence of the algorithm is shown in Figure 4.5. Using GAMS/MINOS for the solution of the linear subproblems and the master problem it requires a total of approximately 254 CPU s on SPARC 2 (32 CPU s for each iteration with approximately 30.5 CPU s spent at the solution of the subproblems and 1.5 CPU s at the solution of the master problem). However, one can easily envisage that if the independent optimization tasks were solved on parallel processors (with an almost perfect speed-up

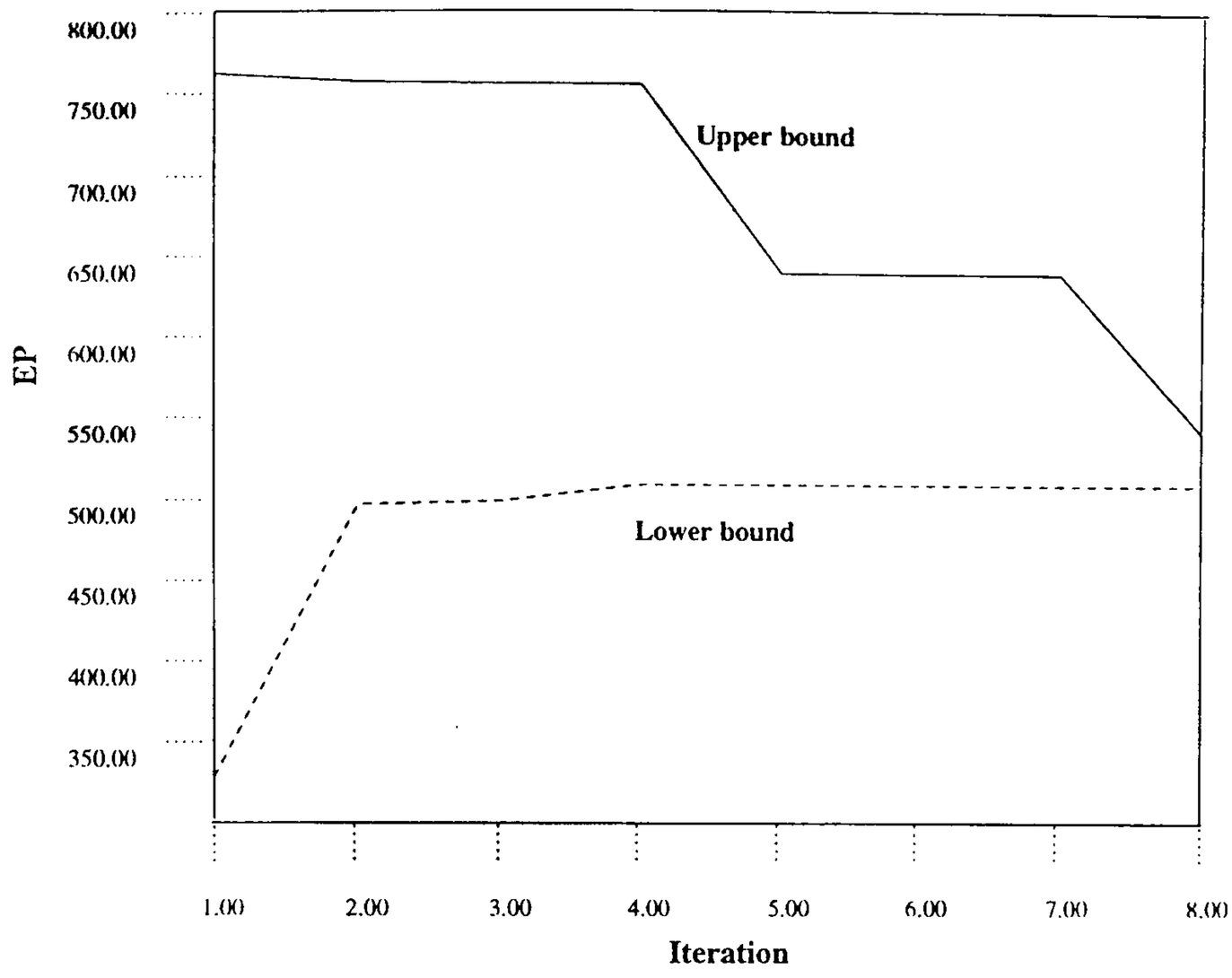


Figure 4.5: Progress of bounds - Example 1

factor) then the CPU time needed for each iteration could be reduced by 80%; this issue will become even more apparent in the next example.

Example 2

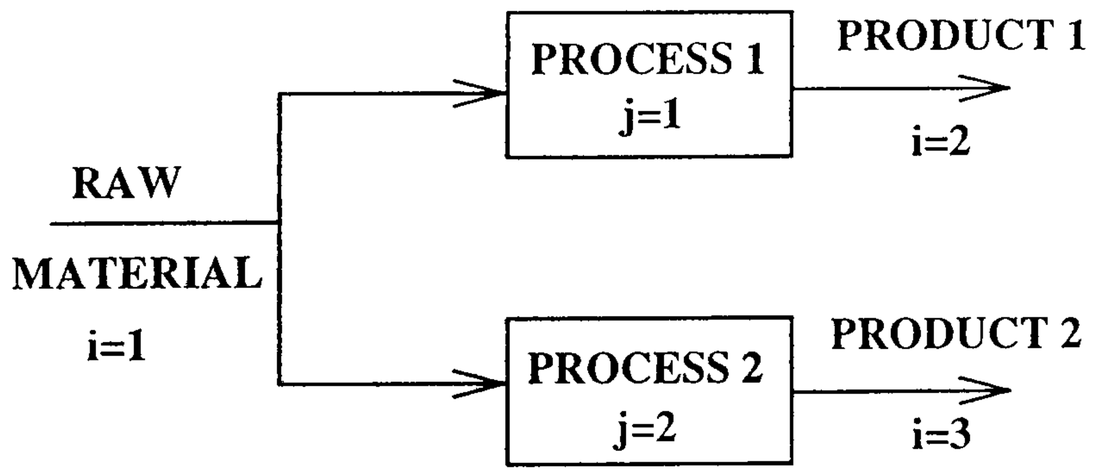


Figure 4.6: Chemical Complex - Example 2

Figure 4.6 shows a chemical complex involving two processes where a single material is transformed into two products. The notation used at example 1 is also followed here. The long-range two-stage planning model with capacity expansion options is represented by the following model:

(i) material balances over stage s

$$P_{s1} + I_{s1}^{in} - R_{s1} - R_{s2} - I_{s1}^{f} = 0$$
$$I_{s2}^{in} + 0.85R_{s1} - I_{s2}^{f} - S_{s2} = 0$$
$$I_{s3}^{in} + R_{s2} - I_{s3}^{f} - S_{s3} = 0$$

where: R_{sj} the level at which process j is run at the stage s
I_{si}^{in}, I_{si}^{f} the level of the inventory of material i at the beginning and at the end of stage s, respectively (with $I_{1i}^{in} = 0,\ I_{1i}^{f} = I_{2i}^{in}$)
S_{si} the amount of material i sold during stage s
P_{s1} the amount of material 1 purchased during stage s

(ii) limitations on the utilization levels over the two stages

$$
\begin{aligned}
0 &\leq R_{11} \leq 20 \\
0 &\leq R_{12} \leq 20 \\
0 &\leq R_{21} \leq 20 + CE_1 \\
0 &\leq R_{22} \leq 20 + CE_2 \\
0 &\leq CE_1 \leq 20y_1 \\
0 &\leq CE_2 \leq 20y_2
\end{aligned}
$$

where: CE_j the capacity expansion of unit j
y_j 0,1 variables to represent the decision of capacity expansion of unit j, 1 if capacity expansion of unit j takes place, 0 otherwise

(iii) limitations on sales due to product demands

$$
\begin{aligned}
15 &\leq S_{12} \leq 30 \\
15 &\leq S_{13} \leq 25 \\
\theta_1 &\leq S_{22} \leq 30 \\
\theta_2 &\leq S_{23} \leq 25
\end{aligned}
$$

(iv) limitations on purchases due to the availability of raw material

$$
\begin{aligned}
22 &\leq P_{11} \leq 40 \\
22 &\leq P_{21} \leq \theta_3
\end{aligned}
$$

(v) maximum and minimum inventory requirements at the end of each stage

$$
\begin{aligned}
0 &\leq I_{s1}^{f} \leq 2 \\
0 &\leq I_{s2}^{f} \leq 5 \\
0 &\leq I_{s3}^{f} \leq 5
\end{aligned}
$$

(vi) an objective function maximizing the profit over the two stages of the following form:

$$
\begin{aligned}
\text{PROFIT} = {} & 20S_{12} + 25S_{13} + 5P_{11} - 7.1R_{11} - 10R_{12} + \\
& + 25S_{22} + 30S_{23} - 12R_{22} - 7.1R_{21} - \\
& - 18CE_1 - 80y_1 - 7.5CE_2 - 80y_2
\end{aligned}
$$

Three uncertain parameters are considered: the demand of material i=2 at the second-stage (θ_1), the demand of material i=3 at the second-stage (θ_2) and the availability of raw material at the second-stage (θ_3). Their corresponding distribution functions are

Uncertain parameter	Distribution function	Mean value	Positive deviation	Negative deviation
θ_1	N(20, 2.5)	20	10	10
θ_2	N(15, 2.5)	15	10	10
θ_3	N(40, 2.5)	40	10	10

Table 4.4: Data for uncertain parameters for Example 2

shown in Table 4.4 (along with mean values and expected deviations for a confidence level 99.9%).

The application of the proposed algorithm leads to the following results. An initial plan is selected for the first-stage variables: $(R_{11}, R_{12}, S_{12}, S_{13}, P_{11},) = (20,20,15,20,40)$ and for the capacity expansion policy: $(y_1, y_2) = (1,0)$, $(CE_1, CE_2) = (10,0)$. The solution of the feasibility problems results in the identification of the bounds of the feasible region of the plan and the placement of the quadrature points within it (125 nodes if 5 quadrature points are considered for each uncertain parameter). Problem (4.5) is then solved to obtain the optimal profit at each one of these nodes; and the expected profit is evaluated through the Gaussian Quadrature formula yielding a value of 998.06 units; the lower bound is updated, $EP_L = 998.06$. After the evaluation of the corrected multipliers the master problem is formulated and solved. The following plan is then obtained $(R_{11}, R_{12}, S_{12}, S_{13}, P_{11},)$=(20,20,15,15,40), $(y_1, y_2) = (1,1), (CE_1, CE_2) = (20,20)$ and an upper bound of EP_U^1=1276.62 units. Since the stopping criterion is not satisfied EP_U^1=1276.62 $>$ EP_L=998.06, the iterative procedure proceeds. Convergence within a tolerance of 0.1 for the lower and upper bounds is achieved after 5 iterations. The optimal solution is the plan that corresponds to the following values of the operating variables $(R_{11}, R_{12}, S_{12}, S_{13}, P_{11},)$= (20,20,15,15,40) and a capacity expansion of process 1 by 6.6 units. This plan has an expected profit of 1189.5 units.

The progress of the convergence of the algorithm is shown in Figure 4.7. Using GAMS/MINOS for the solution of the linear subproblems and SCICONIC for the solution of the MILP master problem it requires a total of 205 CPU s on SPARC 2 per iteration with approximately 199 CPU s spent at the solution of the subproblems and 3 CPU s at the solution of the master problem. The increase in the required computation time compared to example 1 is mainly due to the large number of subproblems that have to be solved per iteration, namely 156 optimization subproblems for the case of 5 quadrature points (as compared to 31 for the case of 2 uncertain parameters). It is interesting

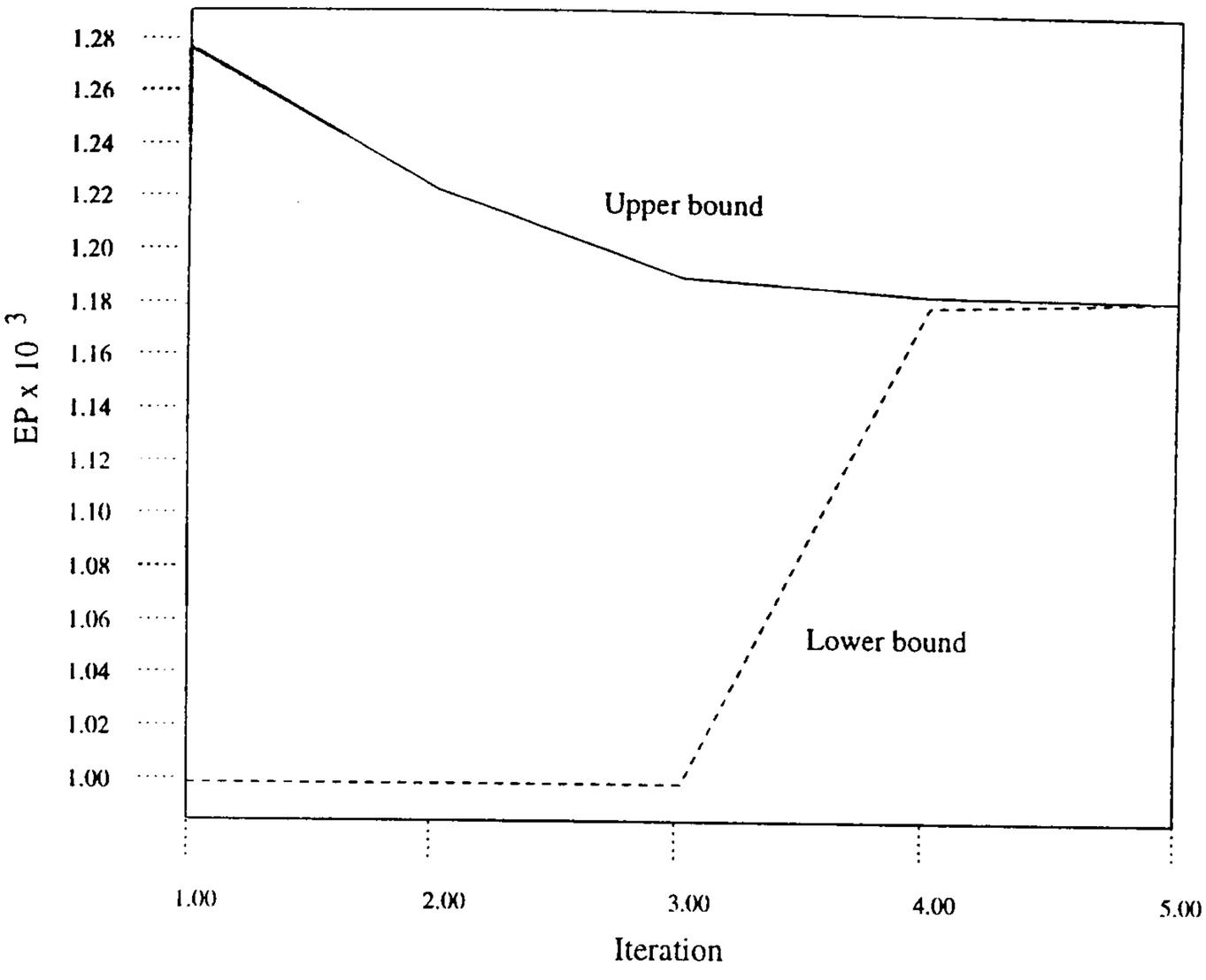


Figure 4.7: Progress of bounds - Example 2

to note that if only two uncertain parameters were considered, the time spent per iteration is reduced to 20 CPU s. Again however, most of the optimization subproblems are independent and can be solved in parallel to enhance computational performance. For example, after the bounds of θ_1 (θ_1^L, θ_1^U) are evaluated and the quadrature points $\theta_1^{q_1}$ are placed within $[\theta_1^L, \theta_1^U]$, the 5 subproblems for the determination of the bounds of θ_2 can be solved simultaneously. The effect of the consideration of different starting points on the performance of the algorithm is shown in Table 4.5; note that for this example, the number of iterations required from different starting points does not change significantly.

Initial Plan		Computation time	Number
Operational plan $(R_{11}, R_{12}, S_{12}, S_{13}, P_{11})$	Capacity Expansions (y_1, y_2, CE_1, CE_2)	CPU s per iteration	of iterations
(20,20,15,20,40)	(1,0,10,0)	205	5
(20,20,15,15,40)	(1,1,10,10)	205	6
(20,20,15,20,40)	(0,1,0,10)	205	5
(20,20,15,15,40)	(0,0,0,0)	205	5

Table 4.5: Convergence of the algorithm for different starting points - example 2

Example 3

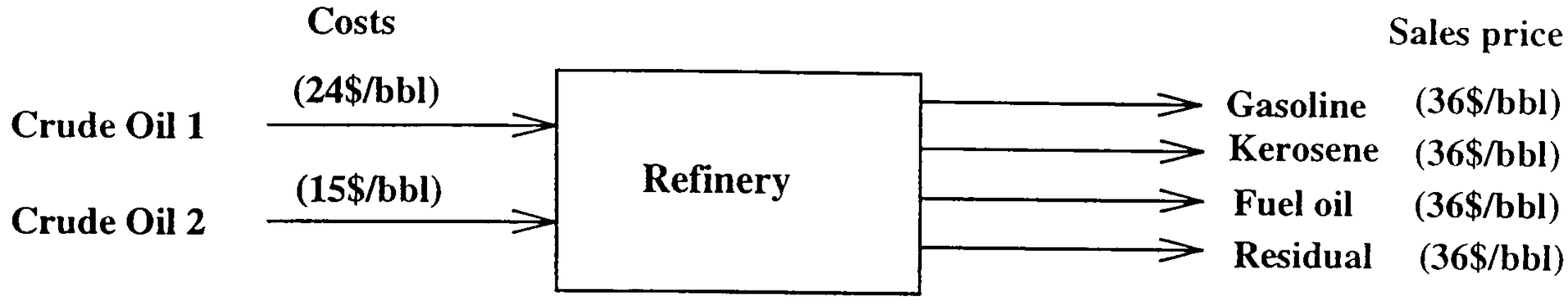


Figure 4.8: Refinery input and output schematic - Example 3

This example is a variation of the refinery planning problem considered in Edgar and Himmelblau (1988). Figure 4.8 is a simplified schematic of feedstocks and products for the refinery (where costs and prices are also given). Two crude oils are available for purchase subject to supply limitations. Four products are produced according to a yield matrix with limits on the production capacities (see Table 4.6). Both crudes and products can be stored subject to tank inventory limits. Products are available for sales according to market demands which are considered uncertain for gasoline and fuel oil during the second stage following normal distribution functions N(15, 1.25) and N(5,1), respectively. The objective is the maximization of the expected value of profit function, defined as the difference between income (from product sales) and cost (operating cost and cost of purchasing), over the two stages. The two-stage planning model consists of 28 inequalities and 36 equalities involving 40 variables.

	Yield		Maximum
	Crude oil 1	Crude oil 2	Capacity
Gasoline	0.8	0.44	24
Kerosene	0.5	0.4	15
Fuel oil	0.2	0.36	1
Residual	0.05	0.1	
Processing cost (per thousand bbl)	0.5	1	

Table 4.6: Data for the refinery crudes and products

The application of the proposed approach leads to the following results.

Step 1: An initial plan is selected to purchase 20 and 15 thousand bbl/day of crude oil 1 and 2, respectively, and to utilize 18 and 15 thousand bbl/day of crude oil 1 and 2, respectively, for the first-stage; $EP_L = -\infty$, k=1 and $\epsilon = 0.1$.

Step 2: The solution of the feasibility problem (B1) leads to the following bounds of θ_1: $13 \leq \theta_1 \leq 19.7$. Considering 5 quadrature points for θ_1 and solving $(B2^{q_1})$ at each of these points the results shown in Table 4.7 are obtained.

q_1	1	2	3	4	5
$\theta_1^{q_1}$	13.31	14.55	16.35	18.15	19.39
$\theta_2^{Lq_1}$	4.69	3.45	3.00	3.29	4.04
$\theta_2^{Uq_1}$	7.01	7.05	7.12	7.13	6.61

Table 4.7: Bounds for θ_2 at $\theta_1^{q_1}$ for the initial plan

Step 3: Considering 5 quadrature points for θ_2 and solving problem (4.5) at each of these points the results shown in Table 4.8 are obtained.

q_2 / q_1	1	2	3	4	5
1	420.31	432.98	446.13	459.27	468.25
2	418.95	444.76	477.99	498.34	512.23
3	467.13	491.24	514.51	532.57	540.82
4	499.05	513.89	535.63	547.70	555.40
5	515.75	525.68	540.21	554.75	560.13

Table 4.8: Optimal profit at the quadrature points

Step 4: The expected profit is evaluated through a Gaussian Quadrature formula yielding a value of 939.98 K$/day; the lower bound is updated, $EP_L = 939.98$.

Step 5a,5b: After the evaluation of the corrected multipliers the master problem is formulated and solved. A plan is then obtained that corresponds to purchasing and utilizing 20 and 12.5 thousand bbl/day of crude 1 and 2 respectively; an upper bound is found of EP_U^1=950.93 K$/day.

Step 6: Since the stopping criterion is not satisfied EP_U^1=950.93 > EP_L=939.98, set k=k+1 and return to Step 2.

The proposed approach requires only 2 iterations to reach the optimal solution within a tolerance of 0.1 for the lower and upper bounds. The optimal solution is the plan that corresponds to purchasing and utilizing 20 and 12.5 thousand bbl/day of crude 1 and 2 respectively. This plan has an expected profit of 948.5 K$/day within a corresponding feasible region defined by the following bounds: for θ_1, $13 \leq \theta_1 \leq 19.7$, and for each quadrature point $\theta_1^{q_1}$ by bounds for θ_2 as shown in Table 4.9.

The progress of the convergence of the algorithm is shown in Figure 4.9. Using GAMS/MINOS for the solution of the linear subproblems and for the linear master problem it requires a total of approximately 33 CPU s on SPARC 2 (16.5 CPU s for each

q_1	1	2	3	4	5
$\theta_1^{q_1}$	13.31	14.55	16.35	18.15	19.39
$\theta_2^{Lq_1}$	4.69	3.45	2.50	3.04	4.04
$\theta_2^{Uq_1}$	7.01	7.05	7.12	7.13	6.61

Table 4.9: Bounds for θ_2 at $\theta_1^{q_1}$ for theoptimalplan

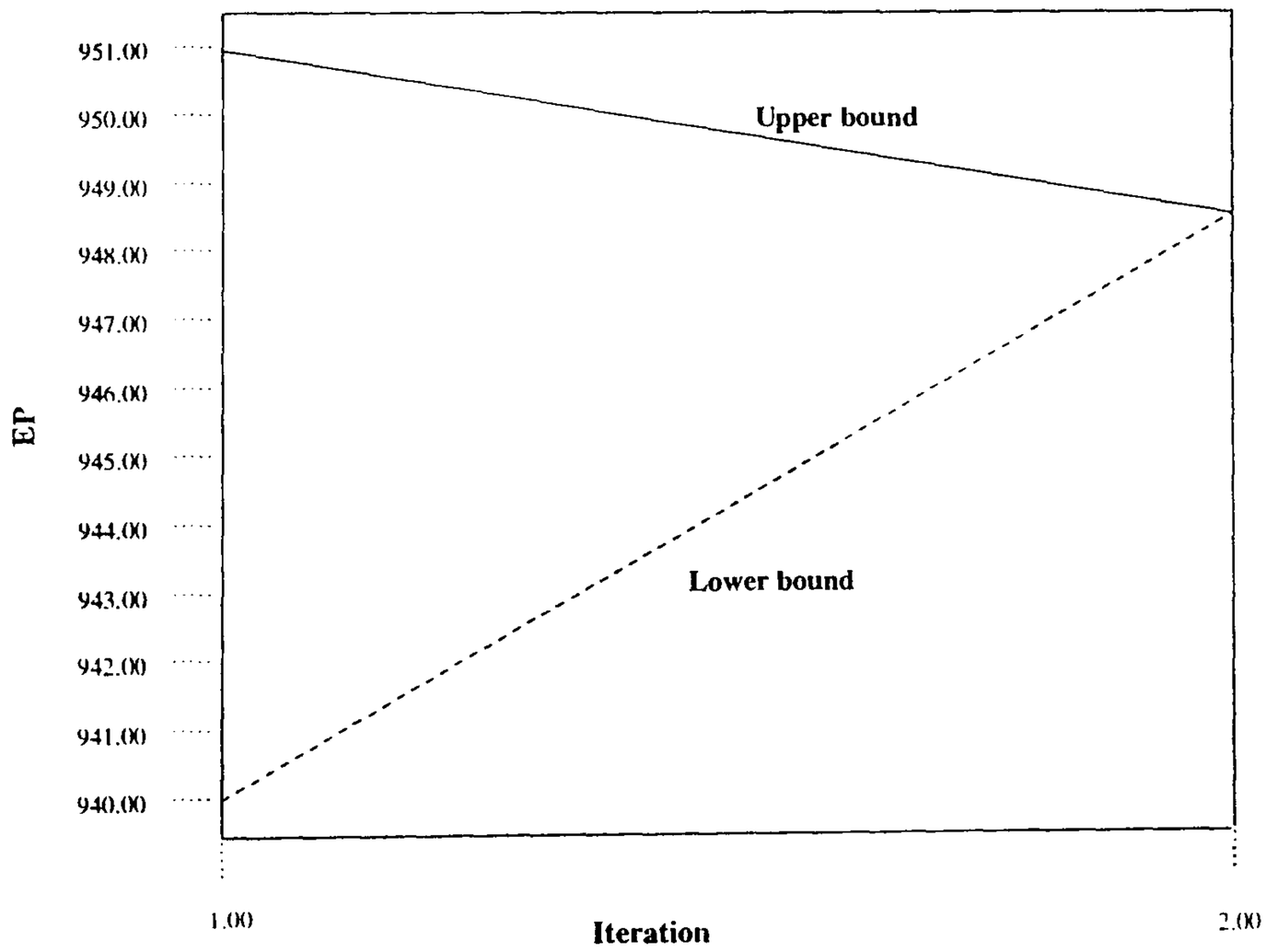


Figure 4.9: Progress of bounds - Example 3

iteration with approximately 15.5 CPU s spent at the solution of the subproblems and 1 CPU s at the solution of the master problem). Note, that the overall computational time remains small despite the relative increase of the model size.

4.5. Summary

The problem of selecting an optimal plan by also identifying opportunities for optimal capacity expansion policies of stochastic planning models has been addressed. A two-stage stochastic optimization formulation has been presented with the objective to maximize an expected profit while simultaneously ensuring future plan feasibility. Uncertainty in second-stage demands, prices and availabilities is considered to be described by general distribution function. The decomposition-based algorithm presented in chapter 2 has been employed which results in the optimal production planning and capacity expansion policy having the maximum expected profit at the optimal level of flexibility. The proposed algorithm constitutes a theoretical advancement over previous published work, since it enables plan optimization and feasibility to be performed simultaneously. An obvious limitation of the current implementation of the algorithm is its high computational requirements especially when the number of uncertain parameters is large; however, its highly distributed solution structure offers enough hope for future exploitation (see Acevedo et al. 1995).

Chapter 5

Value of Perfect Information and Decision Flexibility

In this chapter, the effect of uncertainty on future plant operation is investigated via the incorporation of Value of Perfect Information (VPI) within the approach presented in chapter 2. It offers a tool for analyzing the decision maker's attitude towards risk and accessing the importance of considering uncertainty at the decision stage. A number of example problems are used to illustrate the importance of obtaining this information especially when a decision must be made in the face of uncertainty whether to expand capacities and/or to introduce new technologies.

5.1. Introduction

The problem of measuring the ability of the system to cope with future variations of operating conditions, has been extensively addressed in the literature. For the design problems the proposed metrics are either deterministic considering the uncertain parameters θ to vary inside a specific range of tolerance, or stochastic which means that θ is discribed by a specific probability distribution function. Saboo et al. (1983), proposed a deterministic measure (Resilience Index, RI) to quantify the ability of a heat exchanger network to cope with inlet and target temperature changes. Geometrically, it corresponds to inscribing the largest polytope P inside the feasible region (Figure 5.1). Swaney and Grossmann, (1985a) proposed another deterministic flexibility index which provides a measure of the region of feasible operation in the space of uncertain parameters. The geometric interpretation of that metric is that it determines the maximum hyperrectangle T (Figure 5.2) that can be expanded around the nominal point with sides proportional to the expected deviations $\Delta\theta_j^+, \Delta\theta_j^-$. This hyperrectangle then defines the actual lower and upper bounds over which feasible operation can be guaranteed for the set of uncertain parameters. Comparing with

the metric proposed by Saboo et al. this metric expresses the disturbance load allowed in each stream independently of the others, whereas the RI defines the largest total disturbance load independent of the direction of disturbance that a network can withstand without becoming infeasible. It should be pointed out here that contrary to the RI the metric proposed by Swaney and Grossmann is applicable to any chemical process that operatesin steady state.

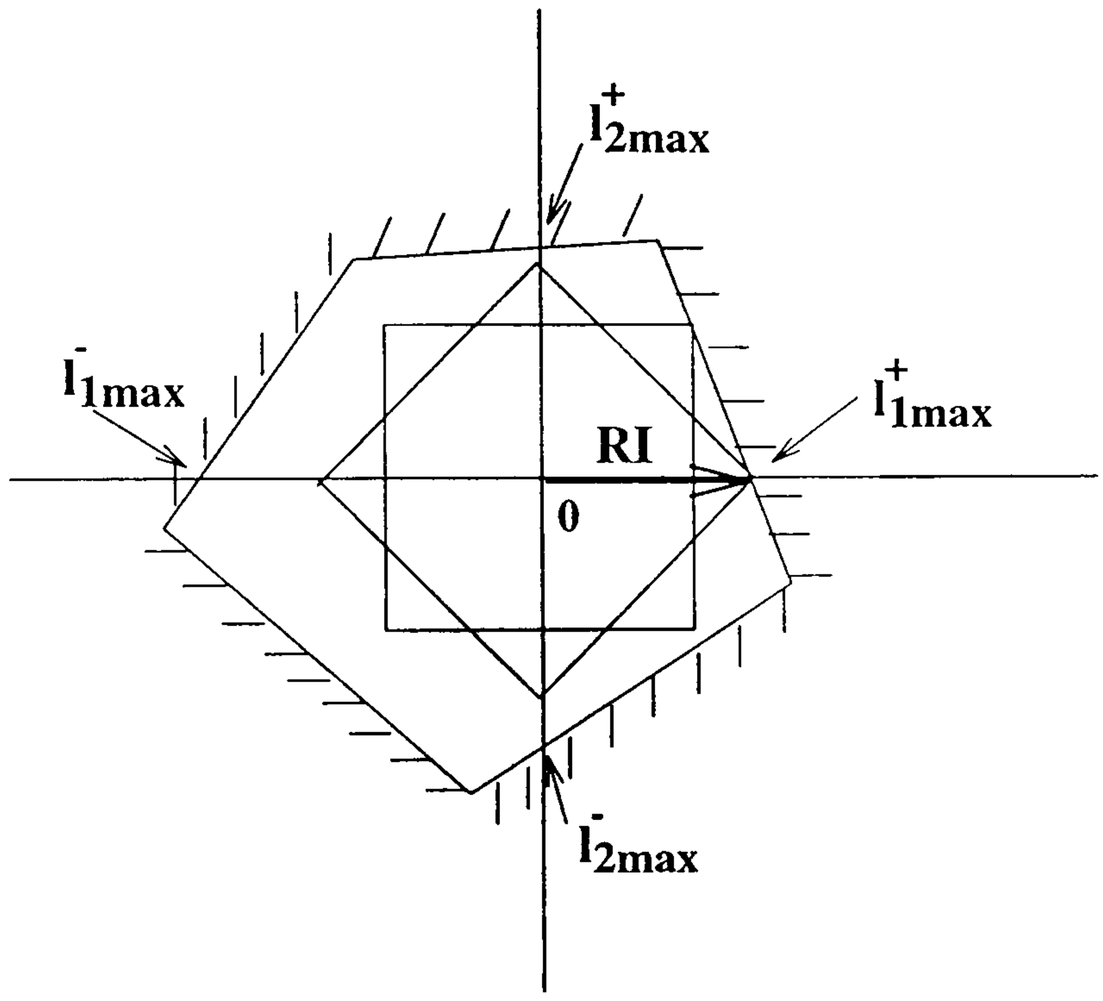


Figure 5.1: Flexibility index proposed by Saboo et al.

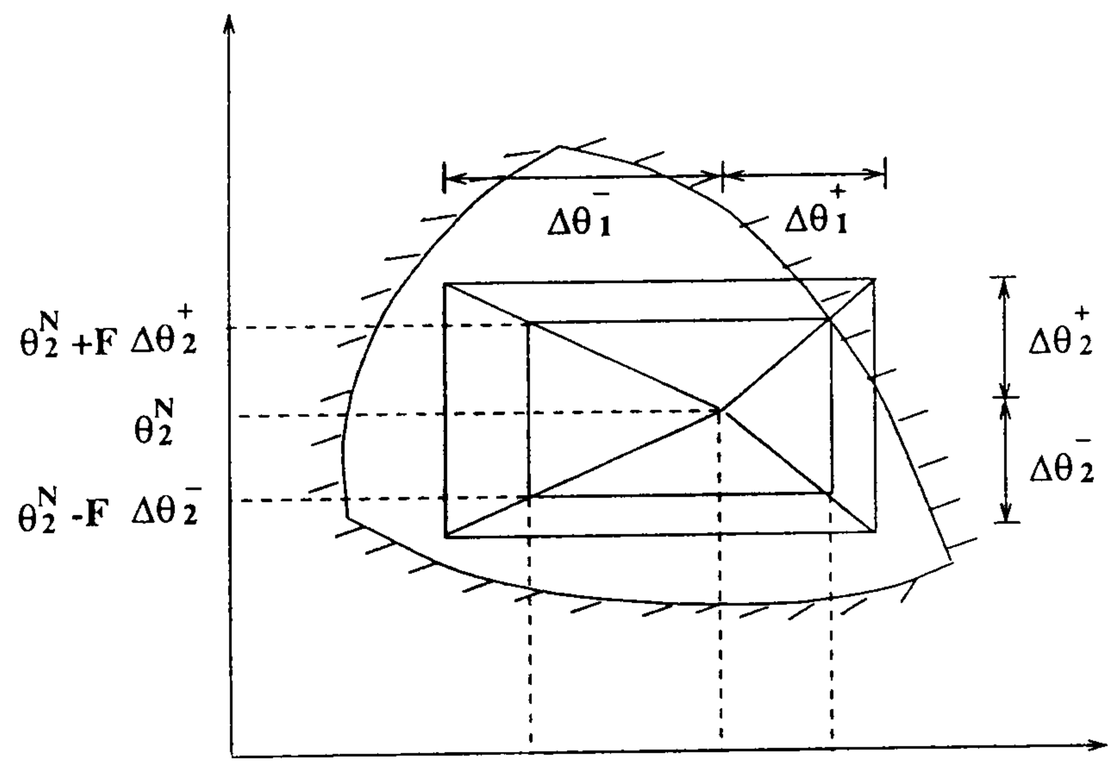


Figure 5.2: Flexibility index proposed by Swaney and Grossmann

Using the concepts of probability and fuzzy theory Kubic and Stein (1988), provide definitions and approximation techniques to measure "design reliability" i. e. the likelihood that a design will operate, but do not explicitly consider the operating de-

grees of freedom in a process. Pistikopoulos and Mazzuchi (1990), considering fixed design, proposed the stochastic flexibility metric (SF) to determine the probability of feasible operation assuming linear model and normal probability distribution function for the vector θ of the uncertain parameters. The estimation of this metric involves the evaluation of the integral:

$$SF(d) = \int_{\theta \epsilon \ feasible \ \ region} j(\theta) d\theta$$

where j(θ) is the joint distribution function of the uncertain parameters θ. Figure 5.3 illustrates the conservative nature of the deterministic metric proposed by Swaney and Grossmann, F, compared to the stochastic flexibility index of Pistikopoulos and Mazzuchi.

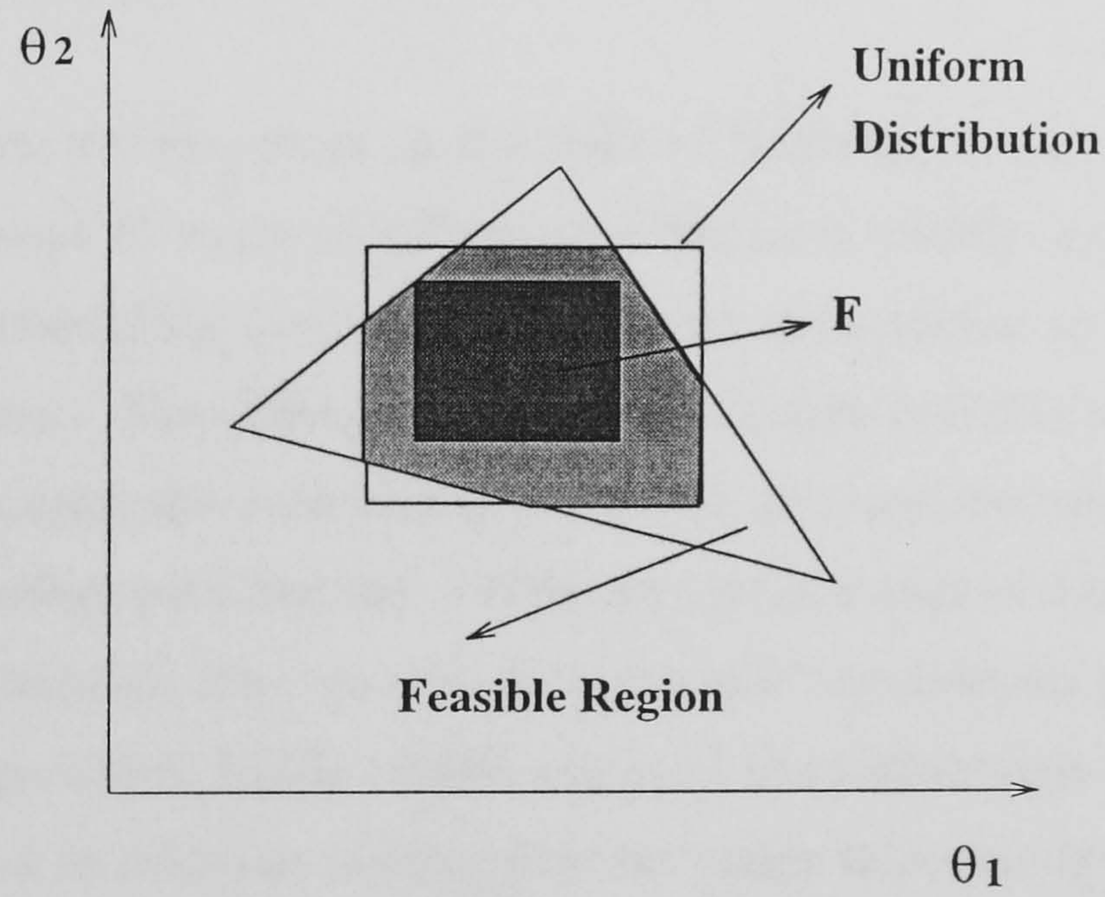


Figure 5.3: Stochastic Flexibility Index

For the case where uncertainties are also involved in the availability of each piece of equipment (discrete uncertainties), Straub and Grossmann (1990), proposed an expected stochastic flexibility (E(SF)) as a measure of the probability of feasible operation over both the discrete and continuous uncertainties (see also Pistikopoulos et al., 1990). This metric is given by:

$$E(SF) = \sum_{s=1}^{s=2^L} SF(s)P(s)$$

where: s state which is defined to represent different choices of design variables

P(s) probability of state s

L number of equipments

For planning problems, Lasserre and Roubellat, (1985) proposed the volume of the choice set associated with the first-period decision as a measure of the first-period decision flexibility. The choi e set is the set of all feasible plans starting at the beginning of the second period after the first-period plan has been implemented. An alternative measure has also been proposed by the same authors because of the size limitations of the previous one. This metric corresponds to the radius of the biggest hypersphere included in the choise set. They also use a multicriteria analysis method to generate the pareto set of solutions taking into account the plan flexibility and some economic criterion based on sensitivity analysis information.

In a separate development in the field of behavioral analysis of actions under uncertainty, the concept of value of information has been widely used mainly to analyze the importance of accounting (over time) for future information as the sequence of optimal decisions evolves. The difference of two alternative behavioral models of decision making under uncertainty, the *here-and-now* and the *wait-and-see* models is used to quantify the "value of perfect information" (VPI). In systems control theory, VPI is used to transform stochastic models into "pseudo-deterministic" equivalents (see Dempster, 1981; Davis, 1989). Among others, Raiffa (1968) analyzed the importance of the *expected value of perfect information* in decision making process under uncertainty; Manne (1974) used the *expected value of perfect information* to estimate the sensitivity of optimal initial decisions to the uncertainty on the date of availability of a breeder fission as an alternative energy resource. Modiano (1987) used this information to analyze the impact of demand uncertainties on capacity expansion policies. More recently Schmutzler (1991), used the value of information to analyze the influence of irreversibility/flexibility on the optimal decisions in a two-period model with uncertainty.

Despite the important developments in both areas of design/planning under uncertainty as well as in the decision making analysis, there is still no integrated and consistent way to link the latter attempts where the aim is to analyze the decision maker's attitude towards risk, to the former research efforts which focus on detailed planning decisions regarding for instance process capacity expansions in the face of uncertainty. In this chapter we attempt to formalize such a link for operational planning problems under uncertainty - considerations of future plan feasibility, different attitudes towards risk,

along with expected profit criteria are integrated in supporting the decision making of developing an optimal planning strategy. First, in the next section the concept of value of information is formally presented as the difference between the *wait-and-see* and *here-and-now* models. The explicit incorporation of the value of perfect information together with flexibility considerations leads to an overall strategy for planning under uncertainty. Combined metrics are also introduced to represent the relation between flexibility and the value of information. A number of example problems are discussed in detail in section 5.5 to illustrate some potential advantages of such an integrated approach to planning under uncertainty.

5.2. Value of Information

Before proceeding with the mathematical description of the metric used to evaluate the value of information, we will first attempt to analyze its concept in the context of operational planning situations, as described by problem (4.1) of chapter 4.

The value of "perfect" information can only be meaningful when the future is not entirely known. In such situations, the decision maker (DM) has to form expectations and beliefs about future outcomes - this will obviously shift the "optimal" actions that the DM would have taken otherwise. Moreover, the optimal desicion in the face of future uncertainty is greatly affected by DM attitude towards risk. Consequently, any further quantitative information would be an additional asset especially in addressing questions of the following form:

- what would be the benefit if it were possible to eliminate uncertainty before executing a plan?, or alternatively
- what is the loss of opportunity associated with a plan involving uncertainty?
- how much the DM is willing to pay to obtain perfect information - if the information regarding uncertainty realization were available at a cost?, or more generally,
- what is the price of having to deal with uncertainty?

Such questions indisputably seem rather qualitative and of relatively limited acceptability in all circumstances. Fortunately, for planning models such information provides useful extra feedback on the effect of uncertainty, as will be shown later in this chapter.

There is in fact a sound mathematical framework for formally assessing the value of information based on the difference between two alternative behavioral models of action under uncertainty, namely the here-and-now and wait-and-see models.

In the here-and-now model, we assume that some decisions (for example, installing extra capacity) have to be taken prior to resolution of uncertainty (here-and-now) - this is the first-stage. The second-stage then estimates decision rules contingent upon the first-stage decision. Clearly, while setting the first-stage decision variables, it is essential to assure feasibility of the second-stage variables and satisfy the model requirements for all possible realizations of the uncertainty.

In the wait-and-see model, the decision maker first waits for the realization of the uncertainty and then selects accordingly both the first and second-stage variables (for each possible realization). Such a situation arises naturally for example at the problem of buying primary resources of the production of end-use products when all the sector's primary supplies are bought in contingency markets or after the sector has observed end-use demands (Modiano, 1987). An optimal decision can then be obtained as a result of the deterministic optimization problem for each possible θ value.

For the stochastic planning model in (4.2), the wait-and-see and here-and-now problems, for a specific first-stage decision vector $\bar{x}_1$, can be mathematically represented by the following formulations:

$$\left.\begin{aligned} F1(\theta) &= \max_{x_1,x_2}\{c_1x_1 + c_2(\theta)x_2\} \\ s.t.\ A_1x_1 &\leq b_1 \\ B_1x_1 + B_2(\theta)x_2 &\leq b_2(\theta) \\ x_1, x_2 &\geq 0 \end{aligned}\right\} \textit{(wait-and-see)}$$

$$\left.\begin{aligned} F2(\bar{x}_1,\theta) &= \max_{x_2}\{c_1\bar{x}_1 + c_2(\theta)x_2\} \\ s.t.\ B_2(\theta)x_2 &\leq b_2(\theta) - B_1\bar{x}_1 \\ x_2 &\geq 0 \end{aligned}\right\} \textit{(here-and-now)}$$

The difference $F1(\theta) - F2(\bar{x}_1,\theta)$ represents the cost of uncertainty incurred by the decision maker when it follows a two-stage scheme:

$$VPI(\bar{x}_1,\theta) = F1(\theta) - F2(\bar{x}_1,\theta) \tag{5.9}$$

This function measures the Value of Perfect Information for θ realizations or the loss of opportunity the decision maker suffers by fixing a plan without having any information regarding uncertainty in the second stage. To assess the value of information considering the whole uncertain parameter space one needs to consider the expectancy of the difference of functions F1 and F2 over θ (defined in R). Thus the Expected Value of Information (conditional upon first-stage choice $\bar{x}_1$) is derived as:

$$EVPI(\bar{x}_1) = E_\theta\{F1(\theta) - F2(\bar{x}_1, \theta)\} \tag{5.10}$$

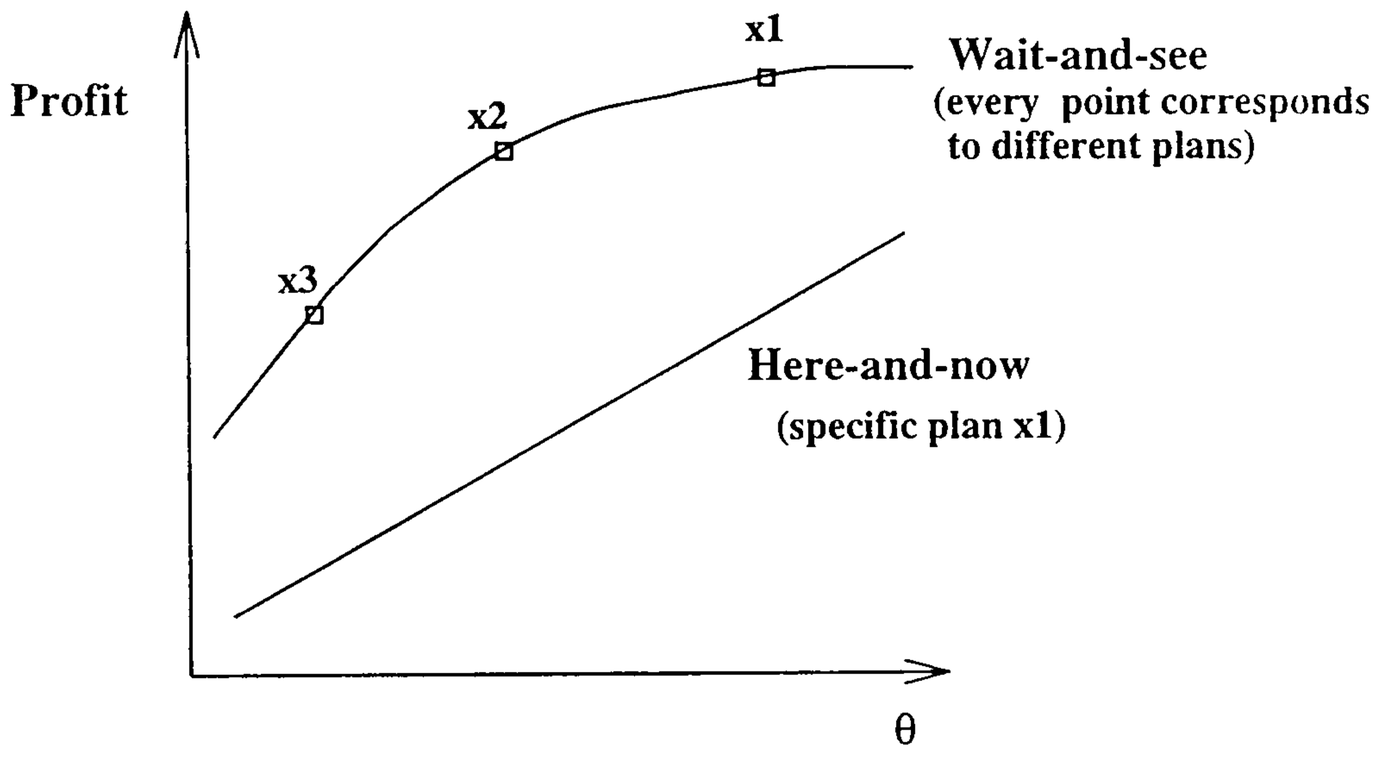


Figure 5.4: Wait-and-see and here-and-now models

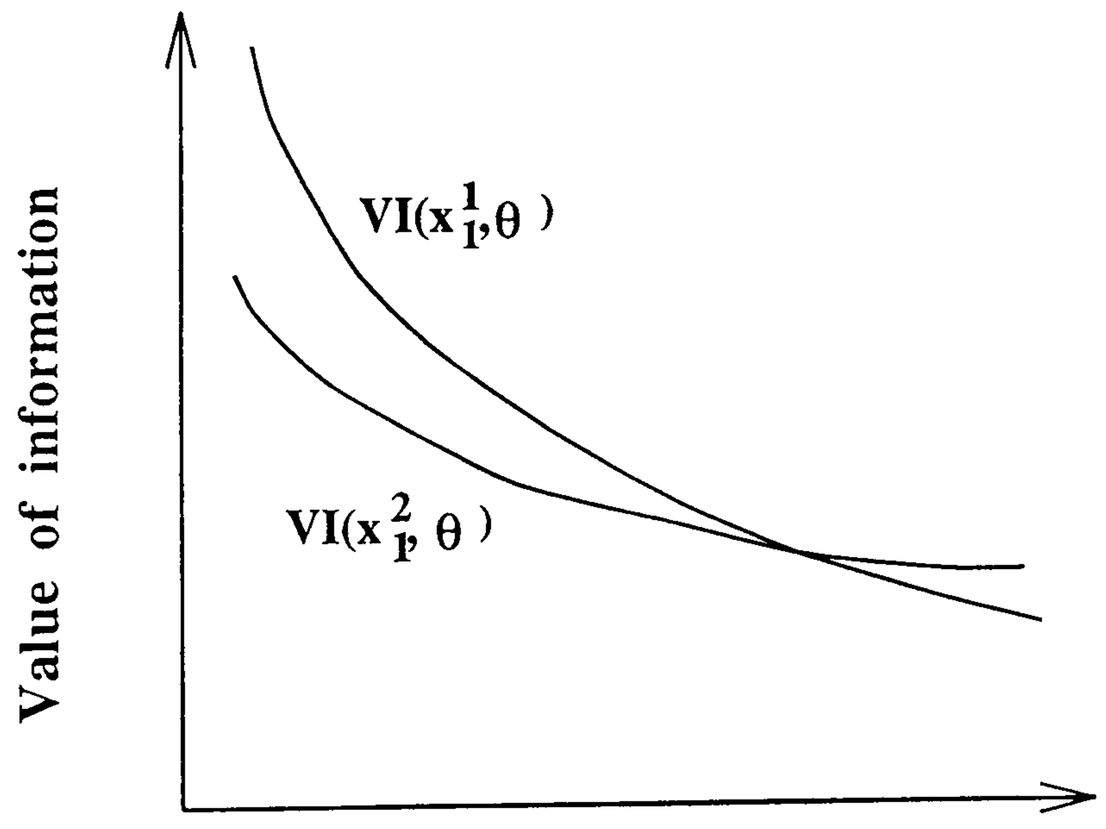


Figure 5.5: Value of information

Figure 5.4 shows typical results from the solution of the wait-and-see and here-and-now models for the problem of buying primary resources for the production of end-use products (Modiano, 1987). Figure 5.5 depicts the resulting functions of the value of information (as a function of the uncertainty θ) for two different plans x_1^1 and x_1^2 , whereas

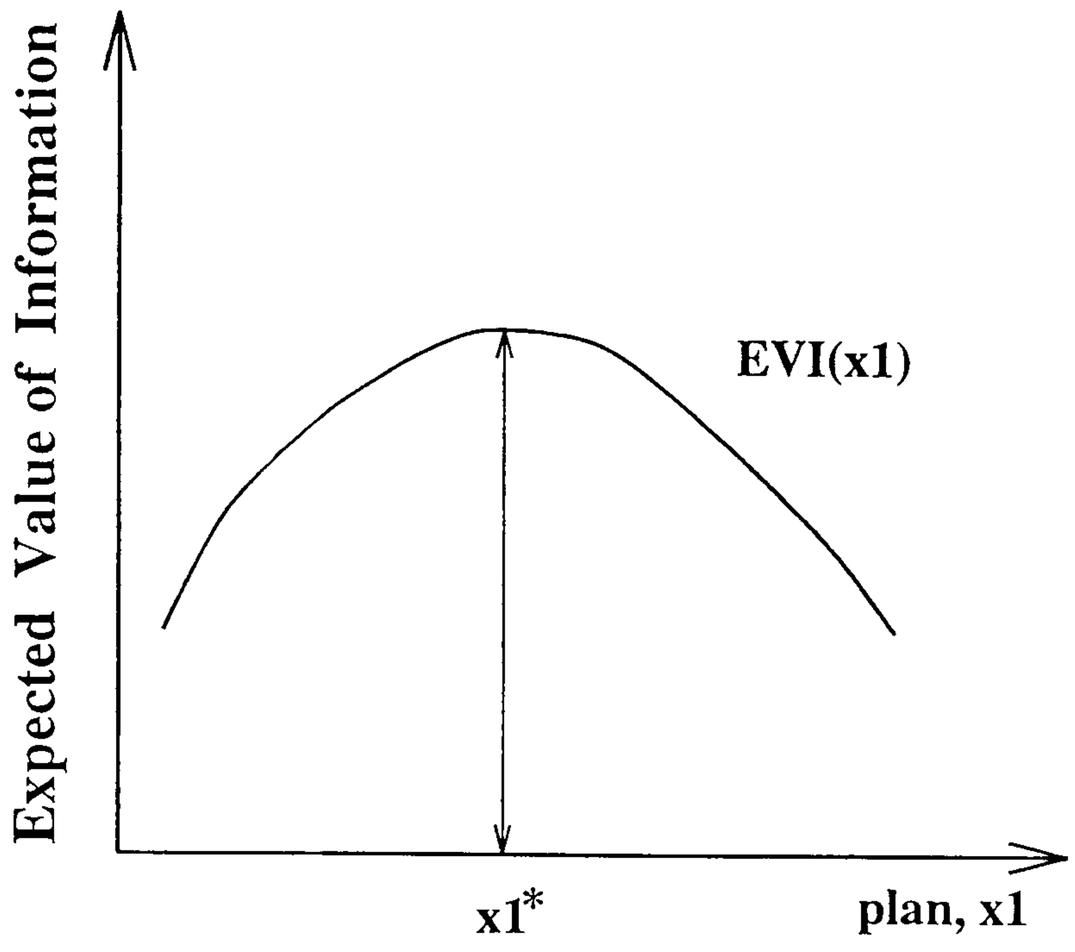


Figure 5.6: Expected value of information

the expected value of information (EVPI) as a function of first-stage planning decision x_1 corresponding to primary resources, is shown in Figure 5.6.

The trends that such an analysis reveals are quite interesting. Consider for instance Figure 5.6. In the first segment of the graph the EVPI curve rises: this is the situation where, since the resources are expensive to secure consumption of an additional unit, the sector is willing to pay more for perfect prediction of end-use product demand. However, as prices go down perfect information becomes less valuable (second segment of the graph, with x_1^* being a threshold value) since the expected opportunity cost of not having enough capacity to accommodate requirements becomes larger than the resource acquisition cost.

Although obtaining such information for VPI and EVPI could clearly add to the solution of planning models, the apparent computational implications pose a distinct obstacle. In the next section, however, we will show that by integrating the computations for the expected value of perfect information within the planning algorithm of chapter 4 the extra computational requirements are maintained to a minimum.

5.3. An Integrated Strategy for Operational planning under uncertainty

Based on the definitions in section 5.2 for the evaluation of the Value of Perfect Information and Expected Value of Perfect Information as in 5.9 and 5.10, the algorithm presented in chapter 4 can be extended to include the solution of the wait-and-see model at each quadrature point $(\theta_1^{q_1}, \theta_2^{q_1 q_2})$ as follows. Steps 1 and 2 are identical to the original algorithm.

Step 3 (expanded to include VPI and EVPI)

(a) At each quadrature point:

(i) Solve the profit maximization subproblem, which corresponds to the here-and-now model, i.e. problem (PQ).

(ii) Solve the following subproblem which corresponds to the wait-and-see model, i.e.

$$F1(\theta_1^{q_1}, \theta_2^{q_1 q_2}) = \max_{x_1^{q_1 q_2}, x_2^{q_1 q_2}} \{c_1 x_1^{q_1 q_2} + c_2(\theta_1^{q_1}, \theta_2^{q_1 q_2}) x_2^{q_1 q_2}\}$$

$$s.t.\ A_1 x_1^{q_1 q_2} \leq b_1$$

$$B_1 x_1^{q_1 q_2} + B_2(\theta_1^{q_1}, \theta_2^{q_1 q_2}) x_2^{q_1 q_2} \leq b_2(\theta_1^{q_1}, \theta_2^{q_1 q_2})$$

$$x_1^{q_1 q_2}, x_2^{q_1 q_2} \geq 0$$

(iii) Calculate the value of information $VPI(\theta_1^{q_1}, \theta_2^{q_1 q_2})$ through equation 5.9.

(b) Calculate the expected profit EP^L through the Gaussian quadrature formula and the expected value of perfect information as follows:

$$\text{EVPI} = \frac{\theta_1^U - \theta_1^L}{2} \sum_{q_1=1}^{Q_1} w_1^{q_1} \frac{\theta_2^{Uq_1} - \theta_2^{Lq_1}}{2} \sum_{q_2=1}^{Q_2} w_2^{q_2}\ VPI(\theta_1^{q_1}, \theta_2^{q_1 q_2}) J(\theta_1^{q_1}, \theta_2^{q_1 q_2}) \tag{5.11}$$

This integrated approach as shown schematically in Figure 5.7, offers a platform for investigating the impact of uncertainty on operational planning models. On the one hand, future feasibility is properly balanced on an expected profit basis. On the other hand, the evaluation of the Value of Information properly quantifies the importance of uncertainty in determining future operation.

For a specific plan, low values of VPI within some uncertainty space imply that no further control action is required there - this transforms the problem to a deterministic equivalent (as discussed in detail in examples 1 and 2). For different plans, EVPI

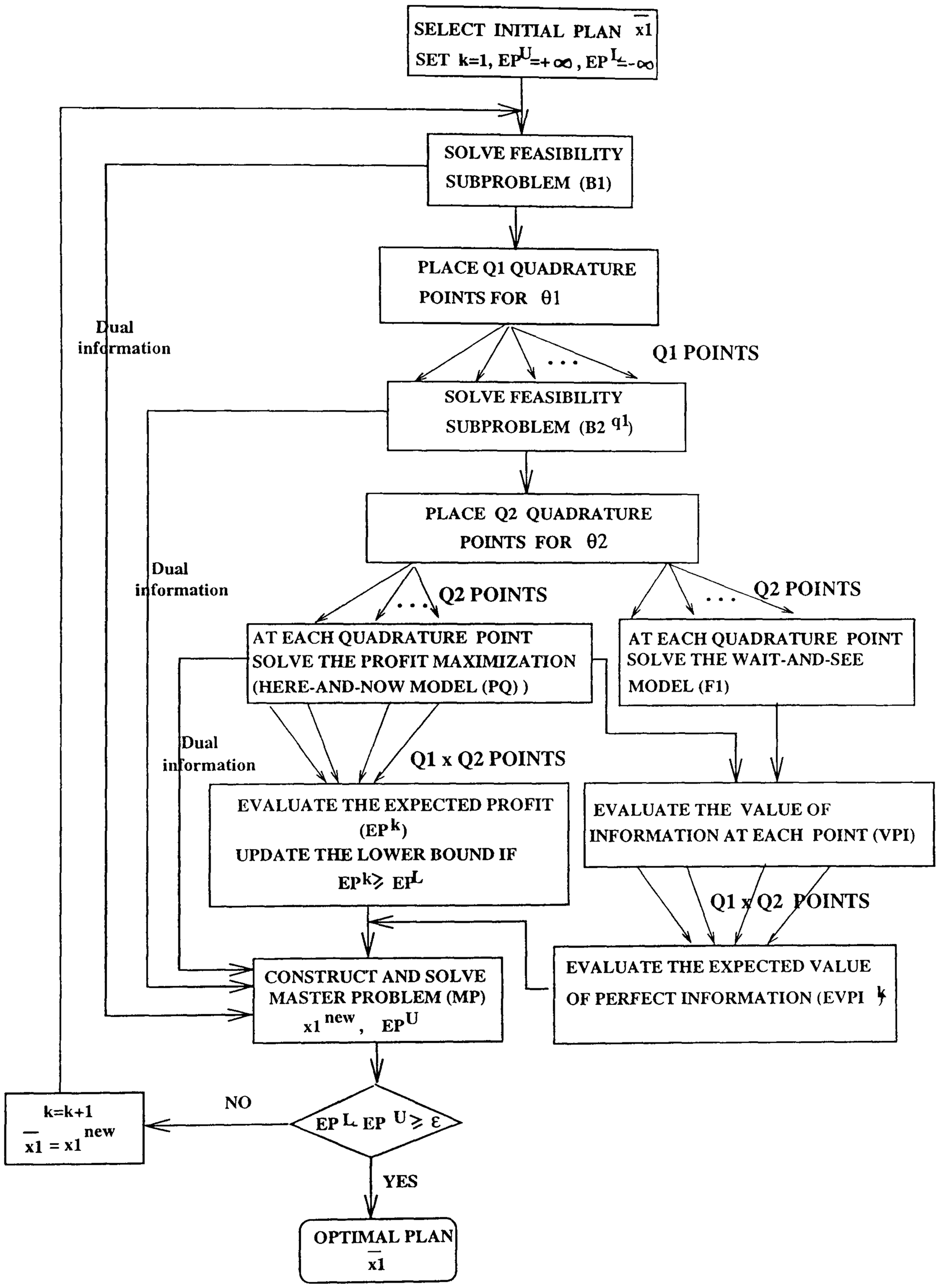


Figure 5.7: A strategy for Operational Planning under Uncertainty

provides a measure for establishing the decision maker's attitude towards risk: the higher the value of EVPI is,the more valuable acquiring future information becomes - this situation corresponds to high risk decisions involving large opportunity losses, certainly not a particularly acceptable choice of a risk aversion strategy. Furthermore, for capacity expansion projects (see examples 2 and 3 in section 4.5) involving long-term contracts and expensive economic decisions, EVPI can be used in conjunction with plan flexibility to identify the most profitable policy (with opportunity losses kept to an acceptable level).

Note that the evaluation of EVPI is only performed at a number of quadrature points, thus avoiding a conservative estimate of its value over the entire region of θ, $\theta \in \mathbf{R}$. Note also that the additional computations required correspond to the solution of the full wait-and-see model at each quadrature point, still quite a demanding job. If one considers, however, the potential benefits that could be achieved from computing these metrics for planning problems especially in terms of implementing future operational policies, then it is a penalty worth paying earlier (at the planning level), rather than later (during operation).

Finally, note that the integrated approach of Figure 5.7 allows plans to be excluded if EVPI and VPI metrics are considered to be prohibitively high (above specified by the decision maker target values EVPI^T and VPI^T, respectively). The exclusion can be either done through the direct incorporation of a cut in the master problem (MP) or alternatively by defining a combined flexibility - VPI index as shown next.

5.4. Combined flexibility-VPI metrics

5.4.1. Flexibility Index

In the following analysis, the flexibility index proposed by Swaney and Grossmann (1985a) will be used as a basis for the formulation. In the context of the two-period linear planning problem, this index defines the maximum parameter region inside which given a current plan (decisions about operational conditions in the first period) a consecutive plan (second period decisions) can be assured. In relation to the design problem, the first and second period decisions correspond here to the design and control variables, respectively. The flexibility index can then be defined to represent the largest rectangle that can be inscribed inside the plan's feasible region. Then, the mathematical formulation of the flexibility index of a plan for the two-period linear planning problem is as follows:

Problem (FP1)

$$F = \max \delta$$

$$s.t.\ \chi(x_1) = \max_{\theta \epsilon T} \min_{x_2} \max_{j \epsilon J} \{\beta_{1,j} x_1 + \beta_{2,j}(\theta) x_2 - b_{2,j}(\theta)\} \leq 0$$

$$T(\delta) = \{\theta | \theta^N - \delta \Delta\theta^- \leq \theta \leq \theta^N - \delta \Delta\theta^+\}$$

$$\delta \geq 0$$

where the vectors $\beta_{1,j}$, $\beta_{2,j}(\theta)$ correspond to the j row of B_1, $B_2(\theta)$, whereas $b_{2,j}(\theta)$ corresponds to the j element of $b_2(\theta)$. The max-min-max constraint in the above formulation (FP1) is considered to assure feasibility over the set T(δ); i.e. for every θ value inside T(δ) the second period decisions x_2 can be adjusted to meet the constraints $\beta_{1,j} x_1 + \beta_{2,j}(\theta) x_2 - b_{2,j}(\theta) \leq 0, j \epsilon J$.

Note that problem (FP1) includes as a constraint problem $\chi(x_1)$, which can be further decomposed as follows:

Problem (FP2)

$$\chi(x_1) = \max_{\theta \epsilon T} \ \psi(x_1, \theta)$$

$$s.t.\ \psi(x_1, \theta) \leq 0$$

$$\text{where:} \quad \psi(x_1, \theta) = \min_{x_2, u} u$$

$$s.t.\ \ \beta_{1,j} x_1 + \beta_{2,j}(\theta) x_2 - b_{2,j}(\theta) \leq u \ \ j \epsilon J$$

where the function $\psi(x_1, \theta) = 0$ defines the boundary of the feasible region in the space of the uncertain parameters θ.

Computationally, the evaluation of the flexibility index for the two-period linear planning model can be performed either through a vertex enumeration algorithm (implicit or explicit, Swaney and Grossmann, 1985b) or by applying the active set strategy (Grossmann and Floudas, 1986). Alternatively, the analytical expressions of Pistikopoulos and

Grossmann (1988a) for the feasibility function $\psi(x_1, \theta)$:

$$\psi^k(x_1, \theta) = \sum_{j \epsilon J_A^k} \lambda_j^k (\beta_{1,j} x_1 + \beta_{2,j}(\theta) x_2 - b_{2,j}(\theta)) \tag{5.12}$$

may be used where λ_j^k denotes the lagrange multiplier of constraint j in active set J_A^k of problem (FP2).

For the case that future uncertainty θ is described by joint[1] probability function $P_D(\theta)$, the stochastic flexibility index SF of Pistikopoulos and Mazzuchi, (1990) is used:

$$\mathrm{SF}(\bar{x}_1) = \int \quad ... \quad \int \; p_D(\theta)\, d\theta$$
$$\theta \in \mathbf{R}(\bar{x}_1)$$
$$\mathbf{R}(\bar{x}_1) = \{\theta \mid \forall \theta \in \mathbf{R} \exists x_2 : B_1 \bar{x}_1 + B_2(\theta) x_2 \; \leq b_2(\theta)\}$$

Qualitatively, in the context of operational planning such an index represents the fraction of the uncertain parameter space that can be accommodated by properly adjusting future decisions x_2, given a first-stage decision $\bar{x}_1$; i.e. it is a measure of the inherent future plan feasibility. Algorithms for the efficient evaluation of SF are described in Pistikopoulos and Mazzuchi (1990), and Straub and Grossmann (1992).

5.4.2. Flexibility-VPI metric

In the previous sections metrics have been presented to measure:

(i) the ability of a current plan to meet future requirements, and

(ii) the value of information involved in decision making.

Intuitively, one would expect that there is a relation between the flexibility of a plan and a value of information. To establish this relationship, we introduce the following combined flexibility-VPI index (for a specific plan, $\bar{x}_1$):

Problem (F-VPI)

$$\text{F-VPI}(\bar{x}_1) = \max \delta$$

---

[1]the case of independent probability distributions is straightforward, see Pistikopoulos and Mazzuchi (1990)

$$s.t.\ \chi(\bar{x}_1) = \max_{\theta \epsilon T} \min_{x_2} \max_{j \epsilon J} \{\beta_{1,j}\bar{x}_1 + \beta_{2,j}(\theta)x_2 - b_{2,j}(\theta)\} \leq 0$$

$$T(\delta) = \{\theta | \theta^N - \delta\Delta\theta^- \leq \theta \leq \theta^N + \delta\Delta\theta^+\}$$

$$\delta \geq 0$$

$$\mathrm{mVPI}(\bar{x}_1) \leq \mathrm{VPI}^T$$

where:

$$\left.\begin{array}{l} \mathrm{mVPI}(\bar{x}_1) = \max\limits_{\theta|\bar{x}_1} [F_1(\theta) - F_2(\theta, \bar{x}_1)] \\ \theta \epsilon T(\delta) = \{\theta | \theta^N - \delta\Delta\theta^- \leq \theta \leq \theta^N + \delta\Delta\theta^+\} \\ \delta \geq 0 \end{array}\right\} \textbf{Problem (VPIP)}$$

$$\left.\begin{array}{l} F_1(\theta) = \max\limits_{z_1, z_2|\theta} \{c_1 z_1 + c_2(\theta) z_2\} \\ s.t. A_1 z_1 \leq b_1 \\ B_1 z_1 + B_2(\theta) z_2 \leq b_2(\theta) \end{array}\right\} \textbf{Problem (F1)}$$

$$\left.\begin{array}{l} F_2(\theta, \bar{x}_1) = \max\limits_{x_2|\bar{x}_1, \theta} \{c_1\bar{x}_1 + c_2(\theta)x_2\} \\ s.t. B_2(\theta)x_2 \leq b_2(\theta) - B_1\bar{x}_1 \end{array}\right\} \textbf{Problem (F2)}$$

where mVPI reperesents the maximum value of VPI within the feasible region of the plan $\bar{x}_1$.

The interpretation of such an index is as follows: given a target VPI^T posed by the decision maker to represent his/her attitude towards risk, the metric depicts the part of the feasible uncertain parameter space, where future uncertain outcomes can be neglected and substituted by a mean value. This effectively transforms the stochastic program within the depicted range into a deterministic equivalent with uncertainty replaced by a corresponding mean value. Opportunity losses are guaranteed to be below the target value of VPI^T by implementing the resulting (from the solution of the deterministic problem) optimal future decision strategy x_2.

5.4.2.1. Evaluation Procedure

Note that the problem (VPIP) corresponds to a parametric multi-level optimization problem since it involves uncertain parameters and constraints that are optimization problems. A solution procedure can be derived for addressing problem (F-VPI) based on the following observations:

- the requirement of having, for a given plan, maximum VPI over the feasible region less than a specified target value is equivalent to the consideration of the value of perfect information being less than this target value for all values of θ inside the feasible region. In mathematical terms instead of considering the constraint $\text{mVPI}(x_1) \leq \text{VPI}^T$, the following constraint is included:

$$\text{VPI}(\theta) \leq \text{VPI}^T, \ \ \forall \theta \epsilon T(\delta)$$

where $\text{VPI}(\theta)$ is the VPI function for a specific plan; i.e. $\text{VPI}(\theta) = F_1(\theta) - F_2(\theta, \bar{x}_1)$.

- the requirement of having VPI less than a specified value limits the feasible region of the plan examined. Therefore, this constraint can be considered as an additional constraint in the flexibility analysis problem.

In mathematical terms the above two observations can be represented as follows:

$$\text{F-VPI}(\bar{x}_1) = \max \delta$$

$$s.t. \ \max_{\theta \epsilon T(\delta)} [\min_{x_2} \max_{j \epsilon J} \{\beta_{1,j} \bar{x}_1 + \beta_{2,j}(\theta) x_2 - b_{2,j}(\theta)\}] \leq 0, \ \ |J| = m$$

$$\max_{\theta | \bar{x}_1} [F_1(\theta) - F_2(\theta, \bar{x}_1)] - \text{VPI}^T \leq 0$$

$$\Downarrow$$

$$\max \delta$$

$$s.t. \ \max_{\theta \epsilon T(\delta)} \left\{ \begin{array}{l} \min_{x_2} \max_{j \epsilon J} \{\beta_{1,j} \bar{x}_1 + \beta_{2,j}(\theta) x_2 - b_{2,j}(\theta)\} \leq 0 \\ \\ F_1(\theta) - F_2(\theta, \bar{x}_1) - \text{VPI}^T \leq 0 \end{array} \right\}$$

$$\Downarrow$$

$$\max \delta$$

$$s.t. \ \max_{\theta \epsilon T(\delta)} \{\min_{x_2} \max_{j \epsilon J^*} \{f_j = \beta_{1,j} \bar{x}_1 + \beta_{2,j}(\theta) x_2 - b_{2,j}(\theta)\} \leq 0\}$$
$$|J^*| = m + 1$$

where the m+1 constraint corresponds to the constraint: $f_{m+1} = F_1(\theta) - F_2(\theta, \bar{x}_1) - \text{VPI}^T \leq 0$.

By applying the active set strategy, this problem can then be transformed to the following formulation:

Problem (F-VPI′)

$$\text{F-VPI}(\bar{x}_1) = \min \delta$$

$$\begin{aligned}
s.t.\ \ & r_j + f_j(x_1, x_2, \theta) = 0 \quad j = 1, ...m \\
& r_V + [\text{VPI} - \text{VPI}^T] = 0 \\
& \sum_{j=1}^{m} \lambda_j + \lambda_V = 1 \\
& \sum_{j=1}^{m} \lambda_j \frac{\partial f_j}{\partial x_2} = 0 \\
& \lambda_j - y_j \leq 0 \\
& r_j - U(1 - y_j) \leq 0 \\
& \lambda_V - y_V \leq 0 \\
& r_V - U(1 - y_V) \leq 0 \\
& \sum_{j=1}^{m} y_j + y_V \leq n_{x_2} + 1 \\
& \theta^N - \delta\Delta\theta^- \leq \theta \leq \theta^N + \delta\Delta\theta^+ \\
& \delta \geq 0, \ \ y_j, y_V = 0, 1, \ \ \lambda_j, \ \ \lambda_V, \ r_j, \ \ r_V \geq 0
\end{aligned}$$

where n_{x_2} is the number of the x_2 variables; r_j, r_V are slack variables, λ_j, λ_V are associated Lagrange multipliers; y_j, y_V are 0,1 variables (y_j=1 if constraint j is active; 0 otherwise).

It should be pointed out that the importance of the mixed-integer linear programming (MILP) formulation in (F-VPI′) is that it is a single optimization problem. Therefore, by properly analyzing the nature of the problem the direct solution of the multi-level problem in (F-VPI) has been avoided.

The algorithmic procedure for obtaining the combined flexibility-VPI metric can then be summarized in the following steps:

Step 0. Specify a plan $\bar{x}_1$.

Step 1. Solve the two parametric LP problems (F1) and (F2) for a specific plan x_1 by applying the algorithm presented in Appendix C.1.

Step 2. Generate the expressions of the VPI function VPI(θ) as a function of the uncertain parameters (see Appendix C.2).

Step 3. (i) Specify a target value VPI^T.

(ii) Determine the combined flexibility-VPI index by solving the corresponding MILP problem in (F-VPI′).

5.4.2.2. An illustrative example

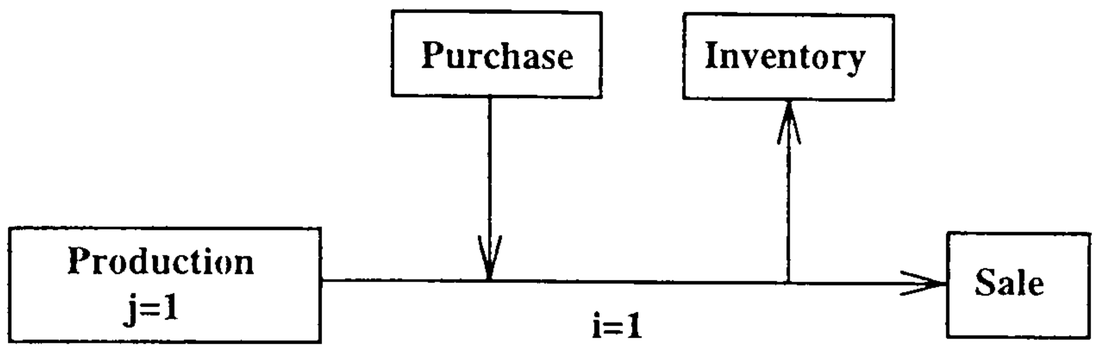


Figure 5.8: Material flow

Consider the following small-scale chemical complex, shown in Figure 5.8, involving only one material and one process. The material balance for each stage takes the following form:

$$P_{11} + I_{11}^{in} + b_{11}R_{11} - S_{11} - I_{11}^{f} = 0$$

$$P_{21} + I_{21}^{in} + b_{11}R_{21} - S_{21} - I_{21}^{f} = 0$$

where R_{11}, R_{21} are the process utilization level in the first and second stage, respectively; S_{11}, S_{21} are the amounts of material sold in the first and second stage, respectively; P_{11}, P_{21} are the amounts of material purchased in the first and second stage, respectively, that are set to zero; b_{11} is the stoichiometric coefficient that is assumed for this example to be equal to 1; I_{11}^{f}, I_{21}^{f} correspond to the material inventories at the end of the first and second stage, and I_{11}^{in}, I_{21}^{in} the initial inventory of the material at the first and second stage, respectively. It is further assumed that no inventory exists at the beginning of the first stage ($I_{11}^{in} = 0$) and at the end of the second stage ($I_{21}^{f} = 0$). It is also required that the inventory of the material at the end of the first stage be positive, in order to ensure the material availability ($I_{11}^{f} > 0$). In addition, the initial inventory in second stage is the same as the inventory at the end of the first stage ($I_{11}^{f} = I_{21}^{in}$).

Based on the above assumptions the material balances can be further simplified into the following equations:

$$R_{11} - S_{11} = I_{11}^{f} \tag{5.13}$$

$$I_{21}^{in} + R_{21} - S_{21} = 0 \tag{5.14}$$

and after the elimination of I_{11}^f:

$$R_{11} + R_{21} - S_{11} - S_{21} = 0 \tag{5.15}$$

Upper bounds are imposed on the levels of the amounts of material that can be produced due to the availability limitations at each stage. In order to achieve a certain level of efficiency the process has to meet a minimum utilization level at each stage:

$$0 \leq R_{11} \leq 5 \tag{5.16}$$

$$3 \leq R_{21} \leq 4 \tag{5.17}$$

Bounds are also imposed on the levels of the amounts of material that can be sold due to demand considerations imposed from market restrictions.

$$0 \leq S_{11} \leq 4 \tag{5.18}$$

$$0 \leq S_{12} \leq \theta \tag{5.19}$$

Note that uncertainty is considered on the value of the upper bound of the product demand during the second stage represented by the uncertain parameter θ. The expected value of the material demand during the second stage, corresponding to the nominal value of θ, is assumed to be equal to 5 ($\theta^N = 5$).

The objective is then to maximize a profit function, which is defined as follows:

$$\begin{aligned}\text{Expected Profit} \;=\; & \underbrace{\gamma_{11}S_{11} + \tilde{\gamma}_{11}I_{11}^f - C_{11}R_{11}}_{1st\ period} + \\ & E_\theta\{\underbrace{\gamma_{21}(\theta)S_{21} - \lambda_{21}(\theta)P_{21} - \tilde{\lambda}_{21}(\theta)I_{21}^{in} - C_{21}(\theta)R_{21}}_{2nd\ period}\}\end{aligned}$$

which, after the elimination of I_{11}^f and I_{21}^{in} from equations 5.13 and 5.14, takes the following form:

$$\begin{aligned}\text{Expected Profit} \;=\; & (\gamma_{11} - \tilde{\gamma}_{11})S_{11} + (\tilde{\gamma}_{11} - C_{11})R_{11} + \\ & E_\theta\{(\gamma_{21}(\theta) - \tilde{\lambda}_{21}(\theta))S_{21} + (\lambda_{21}(\theta) - C_{21}(\theta))R_{21}\}\end{aligned}$$

Here it is assumed that the sales and purchase price of the material, the value of starting and final inventory and also the operating cost of process at the second stage are known with values: $\gamma_{21} - \tilde{\lambda}_{21} = 6$ and $\lambda_{21} - C_{21} = -4$. Also for the first time period: $\gamma_{11} - \tilde{\gamma}_{11} = 3$ and $\tilde{\gamma}_{11} - C_{11} = -2$. The profit function can then be simplified as follows:

$$\text{Profit} = \underbrace{(3S_{11} - 2R_{11})}_{1st\ stage} + \underbrace{(6S_{21} - 4R_{21})}_{2nd\ stage}$$

where θ is assumed to follow a normal probability distribution with mean value equal to 5 and standard deviation equal to 2. The solution of the above problem at the nominal (mean) value of θ, $\theta^N = 5$, yields the plan $(x_{1,1}, S_{1,1})$=(5,3).

Flexibility Analysis for the plan (R_{11}, S_{11})=(5,4)

The constraints for this plan are as follows:

$$\left.\begin{array}{l} 3 \le R_{21} \le 4 \\ R_{21} = S_{21} - 1 \\ 0 \le S_{21} \le \theta \\ 3 \le \theta \le 7 \end{array}\right\} \left.\begin{array}{l} 4 \le S_{21} \le 5 \\ 0 \le S_{21} \le \theta \\ 3 \le \theta \le 7 \end{array}\right\} \begin{array}{l} f_1 = S_{21} - 5 \le 0 \\ f_2 = -S_{21} + 4 \le 0 \\ f_3 = S_{21} - \theta \le 0 \end{array}$$

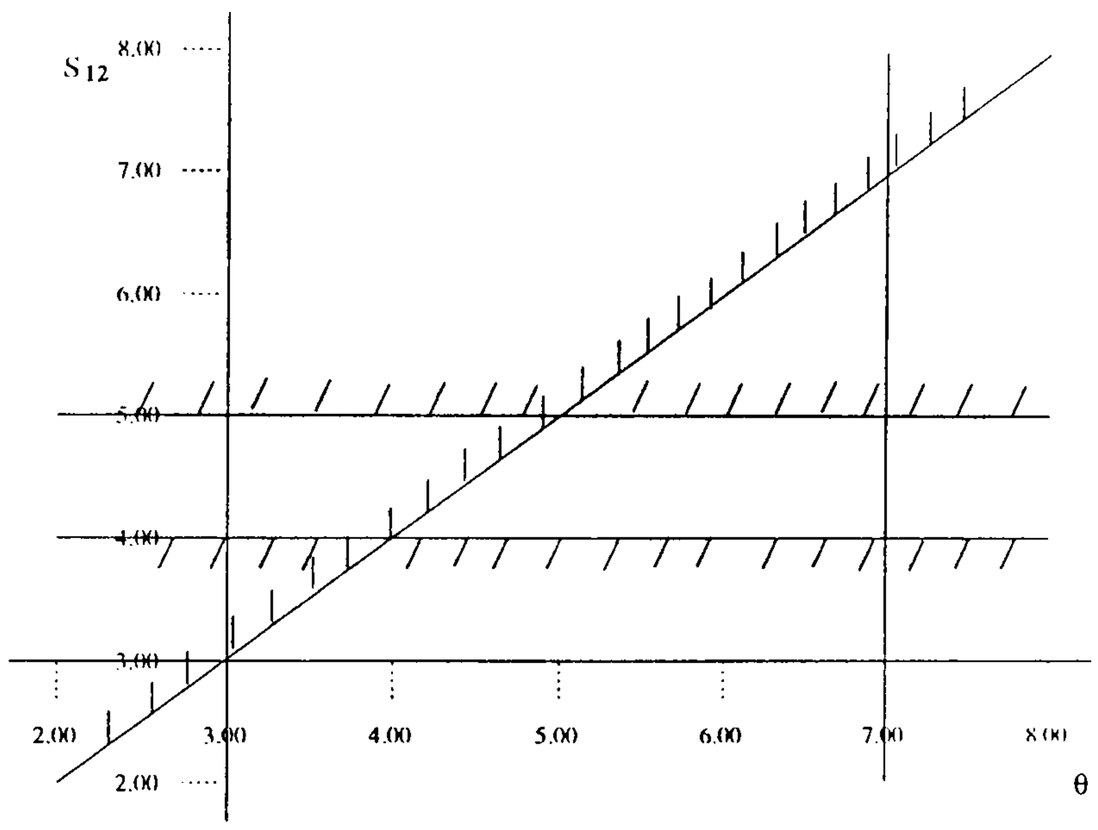


Figure 5.9: Feasible region of plan (5,4)

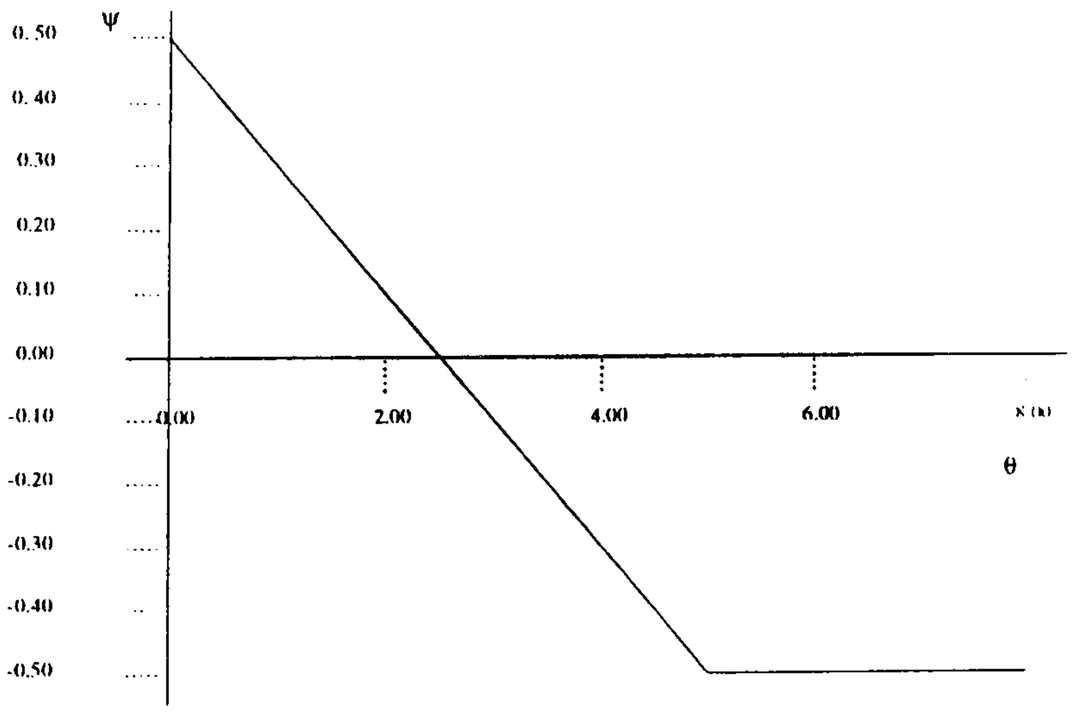


Figure 5.10: Feasibility function of plan (5,4)

The corresponding feasible region is depicted in Figure 5.9. Following the active set strategy two active sets can be identified. The first active set involves f_1 and f_2 leading

to the feasibility function ψ^1= -1/2 and the second one involves f_2 and f_3 yielding the feasibility function $\psi^2 = 1/2(4-\theta)$. As the feasibility function $\psi(R_{11}, S_{11}, \theta)$ corresponds to the larger of the above expressions, the following function is generated as shown in Figure 5.10.

$$\psi(R_{11}, S_{11}, \theta) = \begin{cases} 1/2(4-\theta) & \text{if } 3 \leq \theta \leq 5 \\ -1/2 & \text{if } 5 \leq \theta \leq 7 \end{cases}$$

It follows then from Figures 5.9 and 5.10, that the plan is feasible for the range $4 \leq \theta \leq 7$. The critical parameter value is 4 and the flexibility index evaluation yields a value of 0.5.

VPI for the plan (R_{11}, S_{11})=(5,4)

The wait-and-see model (F1) for this problem is as follows:

$$F_1(\theta) = \max_{S_{11}, S_{21}, R_{11}, R_{12}|\theta} \{3S_{11} - 2R_{11} + 6S_{21} - 4R_{21}\}$$

$$s.t.\ \ 0 \leq R_{11} \leq 5$$

$$0 \leq S_{11} \leq 4$$

$$3 \leq R_{12} \leq 4$$

$$0 \leq S_{12} \leq \theta$$

$$R_{11} - S_{11} + R_{12} - S_{12} = 0$$

Similarly, the here-and-now model (F2) is represented as follows:

$$F_2(\theta, S_{11}, R_{11}) = \max_{S_{21}, R_{21}|\theta, S_{11}, R_{11}} \{6S_{21} - 4R_{21} + 2\}$$

$$s.t.\ \ 3 \leq R_{21} \leq 4$$

$$5 - 4 + R_{21} - S_{21} = 0$$

$$0 \leq S_{21} \leq \theta$$

The solution of these two parametric LP subproblems results in the following expressions:

$$F_1(\theta) = \begin{cases} 4\theta - 2 & 3 \leq \theta \leq 4 \\ 3\theta + 2 & 4 \leq \theta \leq 7 \end{cases}$$

$$F_2(\theta, 4, 5) = \begin{cases} 2\theta + 6 & 4 \leq \theta \leq 5 \\ 16 & \theta \geq 5 \end{cases}$$

The VPI function is then defined as the difference between these two functions (see Figure 5.11):

$$\text{VPI}(\theta, 4, 5) = \begin{cases} \theta - 4 & 4 \leq \theta \leq 5 \\ 3\theta - 14 & \theta \geq 5 \end{cases}$$

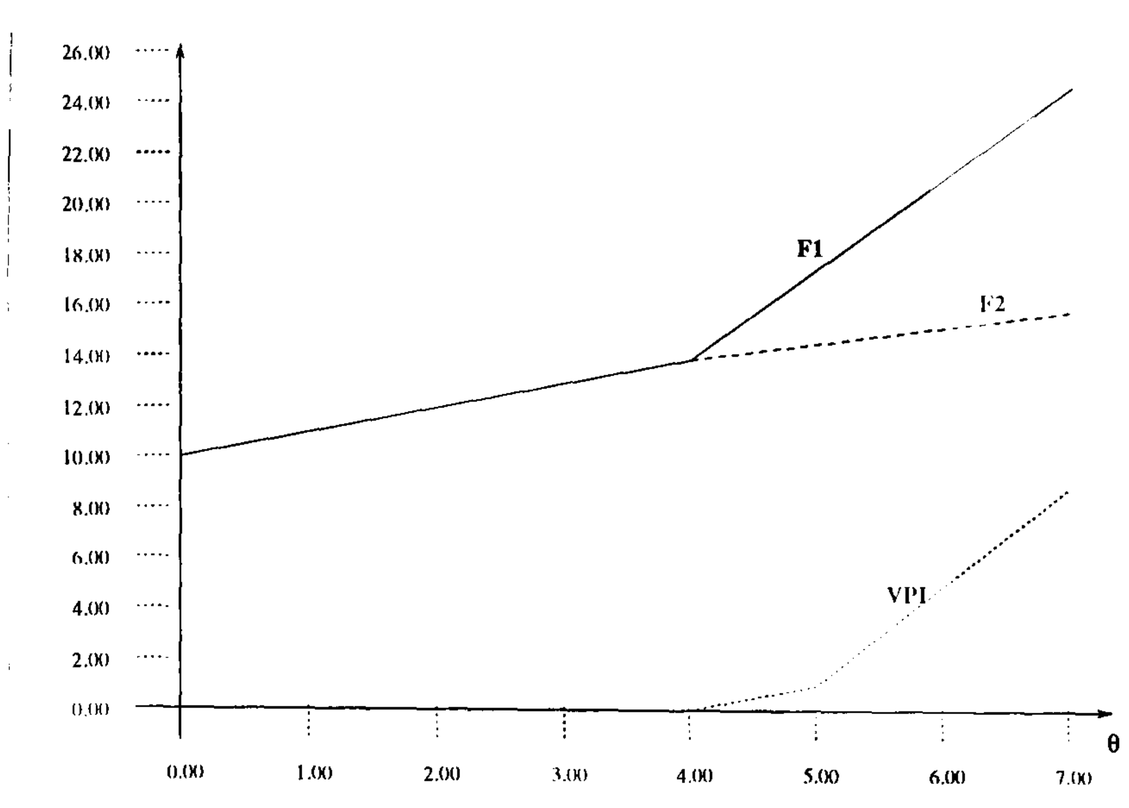


Figure 5.11: VPI function of plan (5,4)

Note that the VPI function is only defined for values of θ corresponding to feasible operation, $\theta \geq 4$.

Combined Flexibility-VPI Analysis for the plan (R_{11}, S_{11})=(5,4)

Problem (F-VPI′) can then be formulated as follows:

$$F(x_1, \theta) = \min \delta$$

$$\left.\begin{array}{l} s.t.\ \ r_1 + S_{12} - 5 = 0 \\ \qquad r_2 - S_{12} + 4 = 0 \\ \qquad r_3 + S_{12} - \theta = 0 \\ \qquad r_V + \text{VPI} - \text{VPI}^T = 0 \end{array}\right\} \textit{initial constraints}$$

$$\left.\begin{array}{l} \text{VPI} = (4\theta_1 - 2\delta_1 + 3\theta_2 + 2\delta_2) - (2\theta_3 + 6\delta_3 + 16\delta_4) \\ \delta_1 + \delta_2 = \delta_3 + \delta_4 \\ \theta_1 + \theta_2 = \theta_3 + \theta_4 = \theta \\ 3\delta_1 \leq \theta_1 \leq 4\delta_1 \\ 4\delta_2 \leq \theta_2 \leq U\delta_2 \\ 4\delta_3 \leq \theta_3 \leq 5\delta_3 \\ 5\delta_4 \leq \theta_4 \leq U\delta_4 \end{array}\right\} \text{VPI } \textit{expression}$$

$$\left.\begin{aligned}&\lambda_1+\lambda_2+\lambda_3+\lambda_R=1\\&\lambda_1-\lambda_2+\lambda_3=0\end{aligned}\right\}\ \textit{stationary conditions}$$

$$\left.\begin{aligned}&\lambda_i-y_j\le 0\ \ j=1,2,3\\&r_j-U(1-y_j)\le 0\ \ j=1,2,3\\&\lambda_V-y_V\le 0\\&r_V-U(1-y_V)\le 0\end{aligned}\right\}\ \textit{complementarity conditions}$$

$$\sum_{j=1}^{3} y_j+y_V\le 2$$

$$5-2\delta\le\theta\le 5+2\delta$$

$$\delta\ge 0,\ \ y_j,y_V=0,1,\ \ \lambda_j,\ \ \lambda_V\ge 0$$

$$r_j,\ \ r_V\ge 0\qquad \text{the slacks of the inequalities}$$

The above formulation is solved for different specified values of VPI^T and the results are summarized in Table 5.1. The same analysis is performed for plan (R_{11}, S_{11})=(4,4) with the results shown in Table 5.1. Note that the additional requirement $\text{VPI} \le \text{VPI}^T$ limits the feasible region of the plan in such a way that the smaller the value of VPI^T the smaller the flexibility of the plan. This observation motivates the idea that trade-offs exist between flexibility and VPI for a specific plan, which can be further explored through the construction of a trade-off curve. In the next section, an algorithm is presented for the systematic generation of such a trade-off curve.

VPI target	Combined Flexibility-VPI index for the plan (5,4)	Combined Flexibility-VPI index for the plan (4,4)
1	0.00	0.00
2	0.167	0.00
3	0.33	0.00
5	0.50	0.00
7	0.50	0.33
9	0.50	0.667
11	0.50	1.00

Table 5.1: Flexibility-VPI analysis results for plan (5,4)

5.4.3. Trade-off Curve of VPI vs Flexibility

If a target value of VPI (VPI^T) is specified for a fixed plan, a combined flexibility-VPI index F-VPI can be evaluated as discussed in the previous section. Here, it will be shown that an additional advantage of the proposed integrated analysis is that it can be easily

extended in order to explore the trade-offs that exist between VPI and the flexibility via the generation of a trade-off curve. When the objectives of F_1, F_2 subproblems are expressed linearly with respect to θ the trade-off curve will be a piecewise linear function where each segment is characterized either by different limiting active sets or by different VPI expressions (as a function of the uncertain parameters θ). This suggests that for generating such a trade-off curve, it suffices to identify its corresponding break points so as to avoid the parametric solution of problem (F-VPI′) for a large number of VPI^T values. A methodology for systematically constructing the trade-off curve of the combined flexibility-VPI index versus the VPI target follows.

For a given active set J_A^k, the combined flexibility-VPI index evaluation problem in (F-VPI′) takes the following form:

Problem (PT1)

$$\delta^k = \min \delta$$
$$s.t.\ \psi^k(x_1, \theta) = 0$$
$$T(\delta) = \{\theta | \theta^N - \delta\Delta\theta^- \leq \theta \leq \theta^N - \delta\Delta\theta^+\}$$
$$\delta \geq 0$$

where $\psi^k(x_1, \theta)$, the feasibility function for plan x_1, is given by:

$$\psi^k(x_1, \theta) = \min u$$

$$s.t. f_j(x_1, x_2, \theta) \leq u \quad j \epsilon J_A^k$$

$$\text{VPI}(\theta, x_1) - \text{VPI}^T \leq u$$

For the linear case, Pistikopoulos and Grossmann (1988a) showed that the feasibility function can be expressed through the following equation:

$$\psi^k(x_1, \theta) = \sum_{j \epsilon J_A^k} \lambda_j^k f_j(x_1, x_2, \theta) + \lambda_V(\text{VPI}(\theta, x_1) - \text{VPI}^T) \tag{5.20}$$

where λ_j^k, λ_V are the Lagrange multipliers for the corresponding active constraints. They also showed that the critical directions $\Delta\theta_i^{c,k}$ can be obtained in terms of the expected deviations as follows:

a. if $\dfrac{\partial\psi^k}{\partial\theta_i} \leq 0$ then $\Delta\theta_i^{c,k} = -\Delta\theta_i^-$

b. if $\dfrac{\partial\psi^k}{\partial\theta_i} \geq 0$ then $\Delta\theta_i^{c,k} = +\Delta\theta_i^+$

By considering the critical directions of θ_i and equation 5.20, problem (PT1) can be rewritten as follows:

Problem (PT1′)

$$\delta^k = \min \delta$$

$$s.t. \sum_{j \epsilon J_A^k} \frac{\lambda_j^k}{\lambda_V} f_j(x_1, x_2, \theta) + \text{VPI}(\theta, x_1) = \text{VPI}^T$$

$$\theta_i = \theta_i^N + \delta \Delta\theta_i^{c,k}$$

$$\delta \geq 0$$

where the feasibility constraint was divided by λ_V (assumming that the VPI constraint is active, $\lambda_V \neq 0$). The Lagrangian of problem (PT1′) is given by:

$$L^k = \delta + v^k \left[\sum_{j \epsilon J_A^k} \frac{\lambda_j^k}{\lambda_V} f_j(x_1, x_2, \theta) + \text{VPI}(\theta, x_1) - \text{VPI}^T \right] + \sum_i \mu_i (\theta_i - \theta_i^N - \delta \Delta\theta_i^{c,k})$$

with the following stationary conditions:

$$a. \quad \frac{\partial L^k}{\partial \delta} = 1 - \sum_i \mu_i \Delta\theta_i^{c,k} = 0$$

$$b. \quad \frac{\partial L^k}{\partial \theta_i} = v^k \left[\sum_{j \epsilon J_A^k} \frac{\lambda_j^k}{\lambda_V} \frac{\partial f_j}{\partial \theta_i} + \frac{\partial \text{VPI}}{\partial \theta_i} \right] + \mu_i = 0$$

Multiplying equation (b) by $\Delta\theta_i^{c,k}$, adding over i, and combining it with equation (a) the following equation obtained for the v^k multiplier:

$$v^k = -1 / \left[\sum_i \Delta\theta_i^{c,k} \sum_{j \epsilon J_A^k} \frac{\lambda_j^k}{\lambda_V} \frac{\partial f_j}{\partial \theta_i} + \sum_i \Delta\theta_i^{c,k} \frac{\partial \text{VPI}}{\partial \theta_i} \right] \tag{5.21}$$

Since, from (PT1′), the multiplier:

$$v^k = -\frac{\partial \delta^k}{\partial \text{VPI}^T}$$

and has a constant value, the flexibility index for an active set that involves the VPI constraint is then given by:

$$\delta^k = \delta_o^k - v^k \Delta\text{VPI}^T$$

where δ_o^k is the flexibility index for a VPI^T value slightly greater than the value at which the VPI requirement constraint becomes active.

The allowable increase of VPI^T with which the active set remains the same can be determined from the solution of the following problem:

$$\max \Delta\text{VPI}^T$$

$$s.t.\ \delta \leq \delta^k \quad k = 1, ..., n_{AS}$$

$$\delta \geq 0$$

where n_{AS} is the number of active sets of the combined flexibility-VPI problem (F-VPI′). The flexibility index for the active set that involves the constraint VPI - $\text{VPI}^T = 0$ is given by $\delta^k = \delta_o^k - v^k \Delta\text{VPI}^T$, while the flexibility indices for the other active sets take constant values (F′), which can be obtained by solving problem (F-VPI′) without including the VPI constraint. In the latter case, the above problem can then be reduced to the solution of the following single equation:

$$\delta_o^k - v^k \Delta\text{VPI}^T = F' \tag{5.22}$$

Based on the above analysis the algorithmic procedure to determine the break points in generating the trade-off curve of VPI versus flexibility is as follows:

Step 0: Select a plan x_1.

Step 1: Evaluate the value of VPI, $\text{VPI}(\theta^N)$, at the nominal value of the uncertain parameters θ^N. The combined flexibility-VPI is equal to zero for VPI between 0 and $\text{VPI}(\theta^N)$.

Step 2: Set VPI^T to a value slightly greater than $VPI(\theta^N)$; solve problem (F-VPI′) to determine the combined flexibility-VPI index. The current active set, from the solution of (F-VPI′), is J_A^k.

Step 3: (i) If the active set J_A^k does not include the VPI constraint, then the flexibility index remains constant for $\text{VPI} \leq \max \text{VPI}^T$ and the procedure terminates.

(ii) If the VPI constraint is included in the active set, J_A^k, the flexibility index of the plan is computed without considering the VPI constraint. Then, equation 5.22 is solved to determine what is the allowable increase, ΔVPI^T, of the VPI target so that the active set of constraints remains the same.

Step 4: Set the new break point $\text{VPI}_{new}^T = \text{VPI}_{old}^T + \Delta\text{VPI}^T + \epsilon$ where ϵ is a small positive number, set k=k+1 and go back to step 2.

The main advantage of the above algorithm is that it avoids the need for solving problem (F-VPI′) at an infinite, in theory, number of VPI^T values; instead, by systematically identifying the break points of the different segments, the flexibility vs. VPI trade-off curve is generated. The steps of the algorithmic procedure will be clarified by revisiting the example of section 5.4.2.2.

Iteration 1

Step 0: Select the plan (R_{11}, S_{11})=(5,4).

Step 1: The value of regret for the nominal value of θ ($\theta^N = 5$) is equal to 1; $\text{VPI}(\theta^N)$=1, thus the combined flexibility-VPI equals to 0 for VPI^T between 0 and 1.

Step 2: Setting VPI^T=1.2 the combined flexibility-VPI problem (F-VPI′) yields F-VPI=0.033 and λ_V=1 (the active set consists only of the VPI constraint).

Step 3: (ii) The flexibility index of the plan without considering VPI requirement has the value of F′=0.5. Since from 5.20 the feasibility function for this active set is $\psi^1 = \text{VPI} - \text{VPI}^T = 3\theta - 14 - \text{VPI}^T$, the critical direction corresponds to the positive deviation $\Delta\theta^{c,1} = +2$. The value of v^1, calculated from 5.21, is found to be $v^1 = 6$. With this value the solution of equation 5.22 yields the maximum allowable increase of VPI^T at a value of $\Delta\text{VPI}^T = 2.8$.

Step 4: Set VPI^T =1.2 + 2.8 + 0.1 = 4.1, k=2 and go back to Step 2.

Iteration 2

Step 2: The combined flexibility-VPI problem yields F-VPI=0.5; the resulting active set does not include the VPI constraint.

Step 3: The combined index remains constant at a value of 0.5 for $4.1 \leq \text{VPI}^T \leq$ max VPI where max VPI = $\text{VPI}(\theta{=}7) = 7$; stop.

Figure 5.12 depicts the resulting trade-off curve for plan (5,4). The dotted curves correspond to different plans. A careful examination of the trade-off curves further reveals the following important features:

(i) **The existence of trade-offs for different plans**; if the decision maker imposes a low "risk" value trying to choose a plan as close as possible to the wait-and-see model, then he has to select a plan with small flexibility. For example, if a VPI target of 0.8 is imposed, then plan (5,3) with flexibility-VPI index of 0 is selected. On the other hand, if the decision maker is willing to take a larger risk this results in gains with respect to plan flexibility. For example, if a VPI target of 4 is set, then plan (5,4) can be selected which features a combined flexibility-VPI index of 0.5.

(ii) **The existence of trade-offs for a specific plan**; the decision maker can balance the risk he is willing to take to the flexibility he wants to

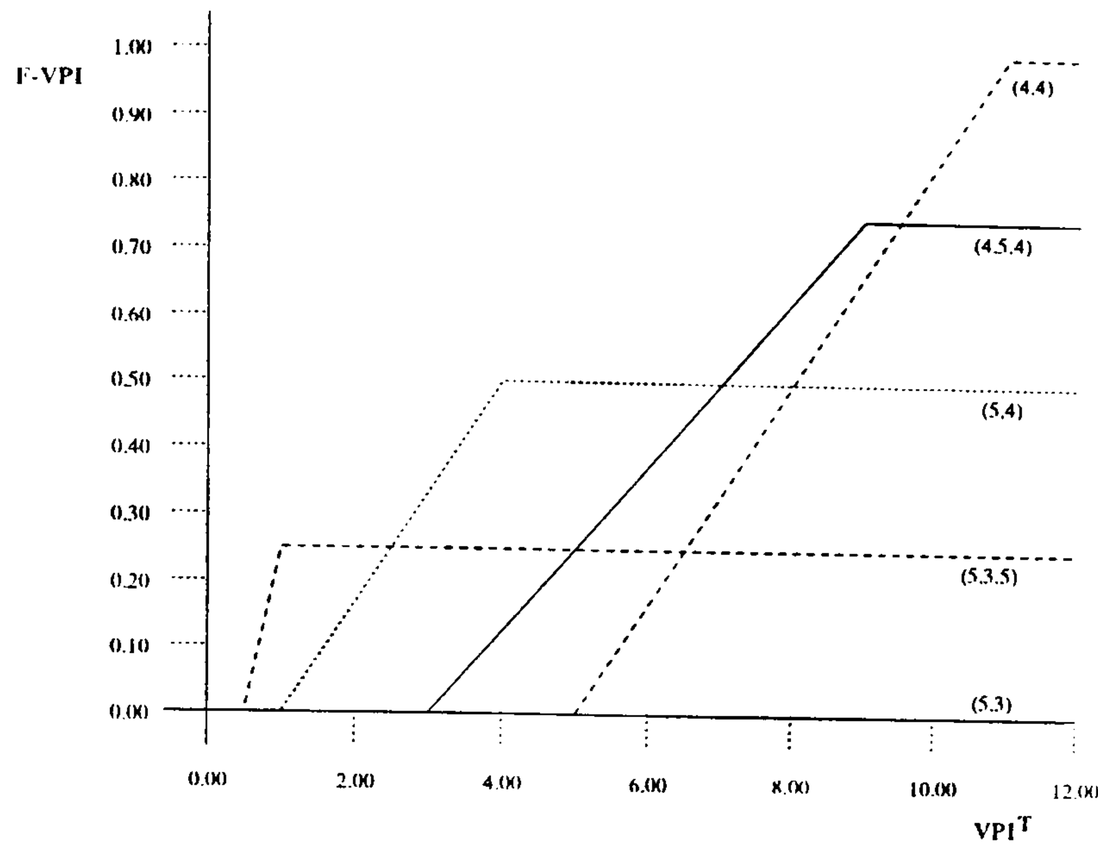


Figure 5.12: Combined Flexibility-VPI metric vs. VIP target

gain. For example, consider plan (5,4). If a VPI target of 3 is imposed the plan flexibility takes a value of 0.34, whereas at a target value of 5 the flexibility has a higher value of 0.5.

These two features of the trade-off curve relating plan flexibility to VPI target clearly highlight the importance of the combined flexibility-VPI index as a measure for the price of flexibility in planning decisions.

In the case where $F_1(\theta)$ and $F_2(\theta, x_1)$ involve bilinear terms of the uncertain parameters, the trade-off curve will be piecewise continuous function where again each segment is characterized either by different active set or by different VPI expressions. The generation of the trade-off curve in this case involves the solution of problem (F-VPI'), which in this case corresponds to a mixed-integer nonlinear program, parametrically with respect to VPI^T. Alternatively, one could preserve linearity following the approach discussed in Appendix C.2, by taking the maximum value of VPI with respect to the uncertain parameters responsible for the nonlinearities and examine each corresponding region separately. Of course in this case the resulting curve is an approximation of the real case.

5.4.4. Stochastic flexibility-VPI metric

For the case where future uncertainty is described by continuous probability distributional forms, the following combined flexibility-VPI index (for a specific plan, $\bar{x}_1$) is introduced:

$$\text{SF-VPI}(\bar{x}_1) = \int \quad \cdots \quad \int_{\theta \in \mathbf{R}^*} p_D(\theta)\, d\theta$$

$$\mathbf{R}^* = \{\theta \mid \forall\theta \in \mathbf{R} \exists x_2 : B_1 x_1 + B_2(\theta) x_2 \leq b_2(\theta),\ \text{VPI}(\bar{x}_1, \theta) \leq \text{VPI}^T\}$$

$\text{VPI}(\bar{x}_1, \theta)$ defined as in 5.9; VPI^T denotes a target value for the value of perfect information.

In order to compute SF-VPI, a constraint of the following form:

$$\text{VPI}(\bar{x}_1, \theta_1^{q_1}, \theta_2^{q_1 q_2}) - \text{VPI}^T \leq \epsilon \ (\epsilon \geq 0; \text{ a specified tolerance}) \tag{5.23}$$

is included in the stochastic index formulation of Straub and Grossmann (1993) resulting in the following formulation:

Problem (SF-VPI)

$$\text{SF-VPI} = \max\{\frac{\theta_1^U - \theta_1^L}{2} \sum_{q_1=1}^{Q_1} w_1^{q_1} \frac{\theta_2^U(\theta 1) - \theta_2^L(\theta 1)}{2} \sum_{q_2=1}^{Q_2} w_2^{q_2}\, p_D(\theta_1^{q_1}, \theta_2^{q_1 q_2})\}$$

$$s.t.\ B_1 \bar{x}_1 + B_2(\theta_1^L, \theta_2^{(.)}) x_2^{(.)} \leq b_2(\theta_1^L, \theta_2^{(.)})$$

$$B_1 \bar{x}_1 + B_2(\theta_1^U, \theta_2^{(.)}) x_2^{(.)} \leq b_2(\theta_1^U, \theta_2^{(.)})$$

$$\theta_1^{q_1} = 0.5[\theta_1^U(1 + v_1^{q_1}) + \theta_1^L(1 - v_1^{q_1})] \quad q_1 = 1, .., Q_1$$

$$B_1 \bar{x}_1 + B_2(\theta_1^{q_1}, \theta_2^{(Lq_1)}) x_2^{(.)} \leq b_2(\theta_1^{q_1}, \theta_2^{(Lq_1)}) \quad q_1 = 1, .., Q_1$$

$$B_1 \bar{x}_1 + B_2(\theta_1^{q_1}, \theta_2^{(Uq_1)}) x_2^{(.)} \leq b_2(\theta_1^{q_1}, \theta_2^{(Uq_1)}) \quad q_1 = 1, .., Q_1$$

$$\theta_2^{q_1\, q_2} = 0.5[\theta_2^{Uq_1}(1 + v_2^{q_2}) + \theta_2^{Lq_1}(1 - v_2^{q_2})] \quad q_1 = 1, .., Q_1 \quad q_2 = 1, .., Q_2$$

$$\theta_1^{MIN} \leq \theta_1^L \leq \theta_1^U \leq \theta_1^{MAX}$$

$$\theta_2^{MIN} \leq \theta_2^{Lq_1} \leq \theta_2^{Uq_1} \leq \theta_2^{MAX} \quad q_1 = 1, .., Q_1$$

$$\theta_2^{MIN} \leq \theta_2^{(.)} \leq \theta_2^{MAX}$$

$$\text{VPI}(\bar{x}_1, \theta_1^{q_1}, \theta_2^{q_1 q_2}) \leq \text{VPI}^T \quad q_1 = 1, .., Q_1 \quad q_2 = 1, .., Q_2$$

where θ_1^L, θ_1^U and $\theta_2^{L\, q_1}, \theta_2^{U\, q_1}$ are the bounds of plan's feasible region, $\theta_1^{q_1}$, $\theta_2^{q_1 q_2}$ are the quadrature points inside the plan's feasible region, $\theta_2^{(.)}) x_2^{(.)}$ are variables associated with each set of constraints since they must be chosen independently to determine the lower and upper bounds and Q_1, Q_2 are the number of quadrature points considered in θ_1 and θ_2 space respectively.

Since analytical expressions of the value of information is not available, the following iterative procedure is suggested:

Step 0: Solve problem (SF-VPI) without incorporating constraint $\text{VPI}(\bar{x}_1, \theta_1^{q_1}, \theta_2^{q_1 q_2}) \leq \text{VPI}^T$ to evaluate the stochastic flexibility of $\bar{x}_1$ and place the quadrature points inside the feasible region. Set k=1; go to Step 2.

Step 1: Solve problem (SF-VPI) to obtain a value for the SF-VPI^k and a set of quadrature points, $\theta_1^{q_1 k}$, $\theta_2^{q_1 q_2 k}$.

Step 2: Compute the value of information at the quadrature points $(\theta_1^{q_1 k}, \theta_2^{q_1 q_2 k})$. If the target, VPI^T, posed by the decision maker is satisfied; i.e. $\text{VPI}(\bar{x}_1, \theta_1^{q_1 k}, \theta_2^{q_1 q_2 k}) - \text{VPI}^T \leq \epsilon$ where ϵ is a specified tolerance limit, at all quadrature points, stop; the value of stochastic flexibility SF-VPI^k is obtained. Otherwise, go to Step 3.

Step 3: Generate the constraints for the value of information using the expressions from the previous determined quadrature points. Set k=k+1, and go to Step 1.

In the next section, six example problems will be presented in detail to further demonstrate the benefits of using an integrated approach for operational planning under uncertainty.

5.5. Examples

In this section a few example problems are analyzed in the context of the proposed integrated planning framework. The purpose of the first two examples is to demonstrate the use and evaluation procedure of the combined flexibility-VPI metrics. The third planning example is used to present the computational results of the algorithmic procedure and analyze the VPI and EVPI of different production policies. The fourth example involves a long-range planning problem where the first-stage decision is the optimal capacity expansion strategy; the estimation of EVPI aids the decision maker in implementing a plan based on his/her attitude towards risk. The last two examples are problems from the area of process synthesis. In particular, the fourth example corresponds to the synthesis/planning problem presented at chapter 2 where a decision should be made regarding the optimal plant configuration comprising a set of processes. The value of information is used to determine the "price" of additional plant flexibility to accommodate demand fluctuations as well as the relative importance of different processes regarding future plant feasibility. The last example corresponds to the process synthesis problem of a benzene chlorination process (see chapter 2). Discrete and continuous decisions regarding plant configuration and operation are considered.

Example 1

The plant of Figure 4.4 is considered here. The two-stage planning model is as follows where we use the same notation as in chapter 4:

Maximize the expected profit:

$$\begin{aligned}\text{Expected Profit} = {} & 100S_{13} + 80S_{14} + 10I^f_{11} + 15I^f_{12} + 20I^f_{13} \\ & +25I^f_{14} - 10P_{11} - 15P_{12} - 30R_{11} - 35R_{12} \\ & +E_\theta\{\theta\mathbf{1}S_{23} + 80S_{24} + 10I^f_{21} + 15I^f_{22} + 25I^f_{23} + 20I^f_{24} - 10P_{21} \\ & -15P_{22} - 30R_{11} - 35R_{12} - 10I^{in}_{21} - I^{in}_{22} - 30I^{in}_{23} - 30I^{in}_{24}\}\end{aligned}$$

subject to:

$$\left.\begin{aligned} & P_{s1} + I^{in}_{s1} - 0.4R_{s1} - I^f_{s1} = 0 \\ & P_{s2} + I^{in}_{s2} - 0.6R_{s1} - R_{s2} - I^f_{s2} = 0 \\ & I^{in}_{s3} + 0.5R_{s1} - I^f_{s3} - S_{s3} = 0 \\ & I^{in}_{s4} + 0.6R_{s2} - I^f_{s4} - S_{s4} = 0 \end{aligned}\right\} \begin{array}{l}\text{material balances}\\ \text{at stage s}\\ \text{s=1,2}\end{array}$$

$$\left.\begin{aligned} & 90 \le R_{11} \le 150 \\ & 30 \le R_{12} \le 150 \\ & 20 \le R_{21} \le 100 \\ & 30 \le R_{22} \le 150 \end{aligned}\right\} \text{capacity constraints}$$

$$\left.\begin{aligned} & 20 \le P_{11} \le 100 \\ & 30 \le P_{12} \le 200 \\ & 20 \le P_{21} \le 100 \\ & 10 \le P_{22} \le \theta\mathbf{2} \end{aligned}\right\} \text{availability constraints}$$

$$\left.\begin{aligned} & 20 \le S_{13} \le 40 \\ & 20 \le S_{14} \le 85 \\ & 20 \le S_{23} \le \theta\mathbf{3} \\ & 20 \le S_{24} \le 85 \end{aligned}\right\} \text{demand constraints}$$

$$\left.\begin{aligned} & 0 \le I^f_{si} \le 80 \\ & s = 1,2; \;\; i = 1,..,4 \end{aligned}\right\} \text{Inventory constraints}$$

Three uncertain parameters are involved in the description of the model: (i) the sales price of material 3 at the second stage with nominal value 90 \$/unit and deviations 27 \$/unit in both directions, (ii) the availability of material 2 at the second stage with

nominal value 50 units/hr and deviations 10 units/hr in both directions, and (iii) the demand of material 3 at the second stage with nominal value 50 units/hr and deviations 20 units/hr in both directions.

Following the procedure for the solution of F1 subproblem as parametric LP (see Appendix C.1) the expressions illustrated in Table 5.2 are obtained. For the parametric solution of F1 problem a single LP problem is solved at the nominal values of the uncertain parameters consuming 0.08 seconds CPU time where 7 Gaussian elimination steps are required that approximately consume 0.35 seconds in a SPARC IPX machine. Then, a specific plan is examined with values of the first period variables as shown in Table 5.3. Problem F2 is then solved as a parametric LP and the expressions obtained are illustrated in Table 5.4. For the parametric solution of problem F2 a solution of an initial LP at the nominal point and 8 Gaussian eliminations steps are required consuming a total of 0.14 seconds of CPU time in a SPARC IPX machine. The VPI function is determined as the difference between the resulting F1 and F2 expressions as shown in Table 5.5. Problem (F-VPI′) is then solved with the exact nonlinear expressions of VPI function, parametrically with respect to VPI^T resulting in the generation of the points presented in Table 5.6 and illustrated in Figure 5.13 by the piecewise continuous curve. The computation time for the solution of the MINLP problem for a fixed VPI target VPI^T is approximately 10 sec (SPARC IPX). Following the procedure described in the previous section the linear maximum VPI expressions illustrated in Table 5.5 are also obtained. The results of the flexibility-VPI analysis for different values of VPI target using the linear VPI expressions are illustrated in Table 5.6. The computation time for the solution of problem (F-VPI′) for a specific VPI^T is approximately 0.2 sec in SPARC IPX machine. The algorithm for generating the trade-off curve is then applied using the linear maximum VPI expressions and the family of solid line curves shown in Figure 5.13 are obtained. Each of these curves corresponds to a different region of the sales price uncertainty, $\theta 1$. Note, that these approximate curves provide useful information to the decision maker in his attempt to select a plan that succeeds to meet his targets with less computational effort.

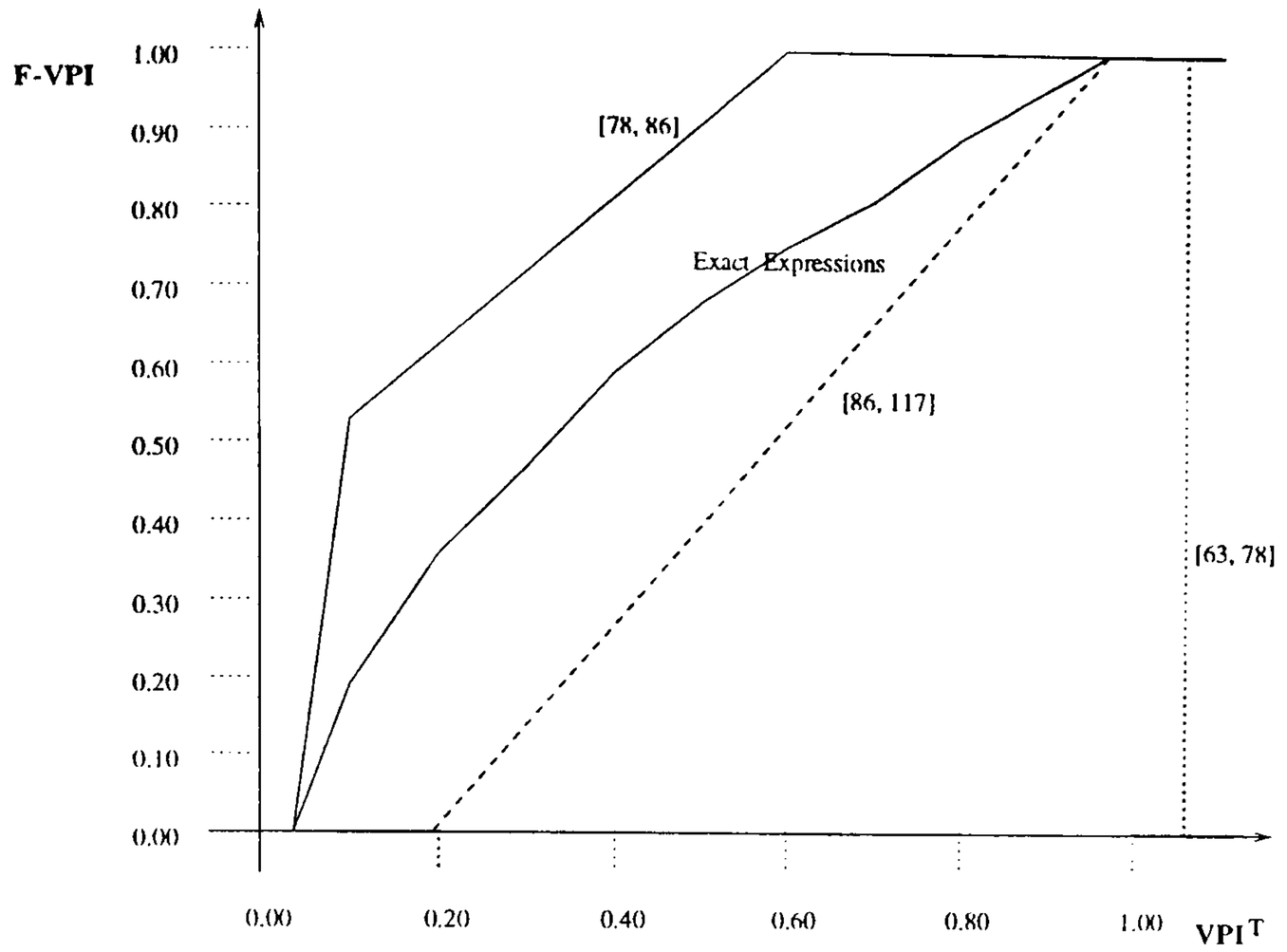


Figure 5.13: Trade-off Curves - Example 1

Expressions of F1	Uncertain parameter's ranges		
	$\theta 1$	$\theta 2$	$\theta 3$
$1426 - 86\theta 3 + \theta 1\theta 3$	$\theta 1 \geq 86$	$\theta 2 \geq 10$	$45 \leq \theta 3 \leq 80$
1066 - 78 $\theta 3$ + $\theta 1\theta 3$	$\theta 1 \geq 78$	$\theta 2 \geq 10$	$15 \leq \theta 3 \leq 45$
$1426 - 86\theta 3 + \theta 1\theta 3$	$\theta 1 \geq 86$		$80 \leq \theta 3 \leq 85$
		$1.2\theta 3 - \theta 2 \leq 85.32$	
$-5884 + 85\theta 1$	$\theta 1 \geq 86$	$\theta 2 \geq 16.68$	$\theta 3 \geq 85$
$-494 + 20\theta 1$	$\theta 1 \leq 78$	$\theta 2 \geq 10$	$\theta 3 \geq 20$
$-2444 + 45\theta 1$	$78 \leq \theta 1 \leq 86$	$\theta 2 \geq 10$	$\theta 3 \geq 45$

Table 5.2: F1 expressions as a function of uncertain parameters - Example 1

Variables	**1st Period Plan**
Sales of material 3	40.00
Sales of material 4	20.00
Purchase of material 1	56.00
Purchase of material 2	152.67
Utilization level of unit 1	140.00
Utilization level of unit 2	33.33

Table 5.3: First-period plan - Example 1

Expressions of F2	Range of uncertain parameters		
	$\theta 1$	$\theta 2$	$\theta 3$
$-815 - 71.67\theta 2 + 0.8\theta 2\theta 1 + 6.67\theta 1$	$\theta 1 \geq 86$	$40 \leq \theta 2 \leq 88$	
		$1.2\theta 3 - \theta 2 \geq 8$	
1388 - 86 $\theta 3$ + $\theta 1\theta 3$	$\theta 1 \geq 86$		$40 \leq \theta 3 \leq 80$
		$1.2\theta 3 - \theta 2 \leq 8$	
$-5494 + 80\theta 1$	$\theta 1 \geq 86$	$\theta 2 \geq 88$	$\theta 3 \geq 80$
$-2054 + 40\theta 1$	$25 \leq \theta 1 \leq 86$	$\theta 2 \geq 40$	$\theta 3 \geq 40$
$-1054 - 25\theta 3 + \theta 1\theta 3$	$\theta 1 \geq 25$	$\theta 2 \geq 40$	$20 \leq \theta 3 \leq 40$
$-1554 + 20\theta 1$	$\theta 1 \geq 25$	$\theta 2 \geq 40$	$\theta 3 \geq 20$

Table 5.4: F2 expressions as a function of uncertain parameters - Example 1

In order to present the geometric interpretation of the combined flexibility-VPI metrics as well as to illustrate their differences we consider here the same problem where only two uncertain parameters are involved: (i) the availability of (raw) material 2 ($\theta 1$) and the demand of (product) material 3, following normal probability distribution functions of the form N(50,5) and N(50, 10), respectively ($\Delta\theta 1^+ = \Delta\theta 1^- = 10$ and $\Delta\theta 2^+ = \Delta\theta 2^- = 20$ for 95.46% level of confidence).

For the first-stage decision shown in Table 5.3, the evaluation of the stochastic flexibility-VPI metric for different VPI^T values results in the values presented in Table 5.7. For a specific VPI^T, for example VPI^T=300, the combined metric suggests that for $34.4 \leq \theta 1 \leq 70$ and $40 \leq \theta 2 \leq 60$ demand and availability variations can be ignored and instead a mean value can be used in order to determine future plant operation. Lower target VPI^T values reveal an increasing risk-aversion decision making: the fraction of the feasible region where uncertainty can be substituted by a mean value decreases and consequently further control of future plant operation according to uncertainty realization is required. This is also pictorially shown in Figure 5.14 in the space of the two uncertain parameters, where the shaded areas indicate the part of the feasible region where a mean value can be used (for two different VPI^T target values).

For comparison, the combined "deterministic" flexibility-VPI metric has also been evaluated for different values of VPI^T (see Table 5.7) - the results clearly show that the SF-VPI metric provides significantly less conservative estimates.

Expressions of VPI (exact expressions)	Uncertain parameter's ranges		
	$\theta 1$	$\theta 2$	$\theta 3$
$2118 - 53\theta 3$	$\theta 1 \geq 86$	$\theta 2 \geq 40$	$20 \leq \theta 3 \leq 40$
-322 + 8 $\theta 3$	$\theta 1 \geq 86$	$\theta 2 \geq 10$	$40 \leq \theta 3 \leq 45$
		$1.2\theta 3 - \theta 2 \leq 8$	
38	$\theta 1 \geq 86$	$\theta 2 \geq 10$	$45 \leq \theta 3 \leq 80$
		$1.2\theta 3 - \theta 2 \leq 8$	
$-528.67 - 25.83\theta 2 + 39\theta 3$ $(251.33 - 78\theta 3 + 71.67\theta 26.67\theta 1 +$ $\theta 1\theta 3 - 0.833\theta 2\theta 1)$	$\theta 1 \geq 86$	$40 \leq \theta 2 \leq 88$	$40 \leq \theta 3 \leq 45$
		$1.2\theta 3 - \theta 2 \geq 8$	
$-168.67 - 25.83\theta 2 + 31\theta 3$ $(611.33 - 86\theta 3 + 71.67\theta 2 - 6.67\theta 1+$ $\theta 1\theta 3 - 0.833\theta 2\theta 1)$	$\theta 1 \geq 86$	$40 \leq \theta 2 \leq 88$	$45 \leq \theta 3 \leq 80$
		$1.2\theta 3 - \theta 2 \geq 8$	
$-2444 + 31\theta 3$ $(6918 + 31\theta 3 + \theta 1\theta 3)$	$\theta 1 \geq 86$	$\theta 2 \geq 88$	$80 \leq \theta 3 \leq 85$
		$1.2\theta 3 - \theta 2 \leq 85.32$	
193 $(5\theta 1)$	$\theta 1 \geq 86$	$\theta 2 \geq 88$	$\theta 3 \geq 85$
$-168.67 - 25.83\theta 2 + 31\theta 3$ $(611.33 - 86\theta 3 + 71.67\theta 2 - 6.67\theta 1+$ $\theta 1\theta 3 - 0.833\theta 2\theta 1)$	$\theta 1 \geq 86$	$40 \leq \theta 2 \leq 88$	$80 \leq \theta 3 \leq 85$
		$8 \leq 1.2\theta 3 - \theta 2 \leq 85.32$	
$2466.33 - 25.83\theta 2$ $(-6694.77 + 78.3\theta 3 - 0.8\theta 1\theta 2)$	$\theta 1 \geq 86$	$40 \leq \theta 2 \leq 88$	$\theta 3 \geq 85$
		$1.2\theta 3 - \theta 2 \geq 8$	
$2118 - 53\theta 3$	$78 \leq \theta 1 \leq 86$	$\theta 2 \geq 40$	$20 \leq \theta 3 \leq 40$
$-322 + 8\theta 3$ $(3118 - 78\theta 3 - 40\theta 1 + \theta 1\theta 3)$	$78 \leq \theta 1 \leq 86$	$\theta 2 \geq 40$	$40 \leq \theta 3 \leq 45$
38 $(5\theta 1)$	$78 \leq \theta 1 \leq 86$	$\theta 2 \geq 40$	$\theta 3 \geq 45$
1058 $(20\theta 1)$	$25 \leq \theta 1 \leq 78$	$\theta 2 \geq 40$	$\theta 3 \geq 40$
1058 $(20\theta 1 - \theta 3\theta 1)$	$25 \leq \theta 1 \leq 78$	$\theta 2 \geq 40$	$20 \leq \theta 3 \geq 40$
1058	$\theta 1 \leq 25$	$\theta 2 \geq 40$	$\theta 3 \geq 20$

Table 5.5: VPI expressions as a function of uncertain parameters - Example 1

VPI target	Combined Flexibility-VPI Index with the exact VPI expressions	Approximate Combined Flexibility-VPI Index
200	0.359	0.0
500	0.675	0.0
1000	1.0	0.0
1100	1.0	1.0
1200	1.0	1.0

Table 5.6: Results for Flexibility-VPI analysis - Example 1

VPI^T	30	40	50	100	200	300	400	500	600
F-VPI	0	0.537	0.547	0.59	0.69	0.78	0.88	0.97	1
SF-VPI	0.13	0.908	0.912	0.93	0.959	0.98	0.996	1.0	1.0

Table 5.7: Combined metrics - Example 1

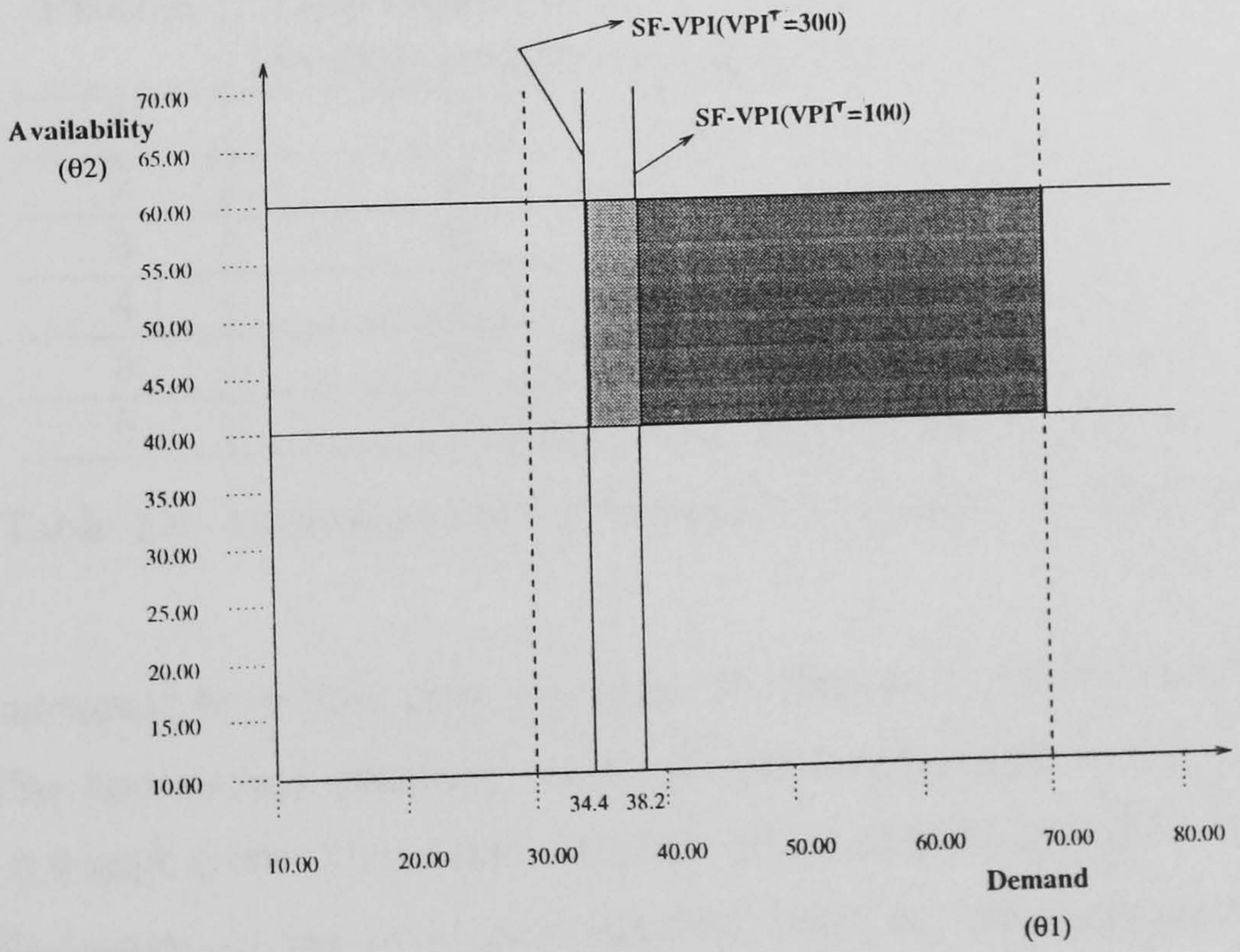


Figure 5.14: Combined metrics - Example 1

Example 2

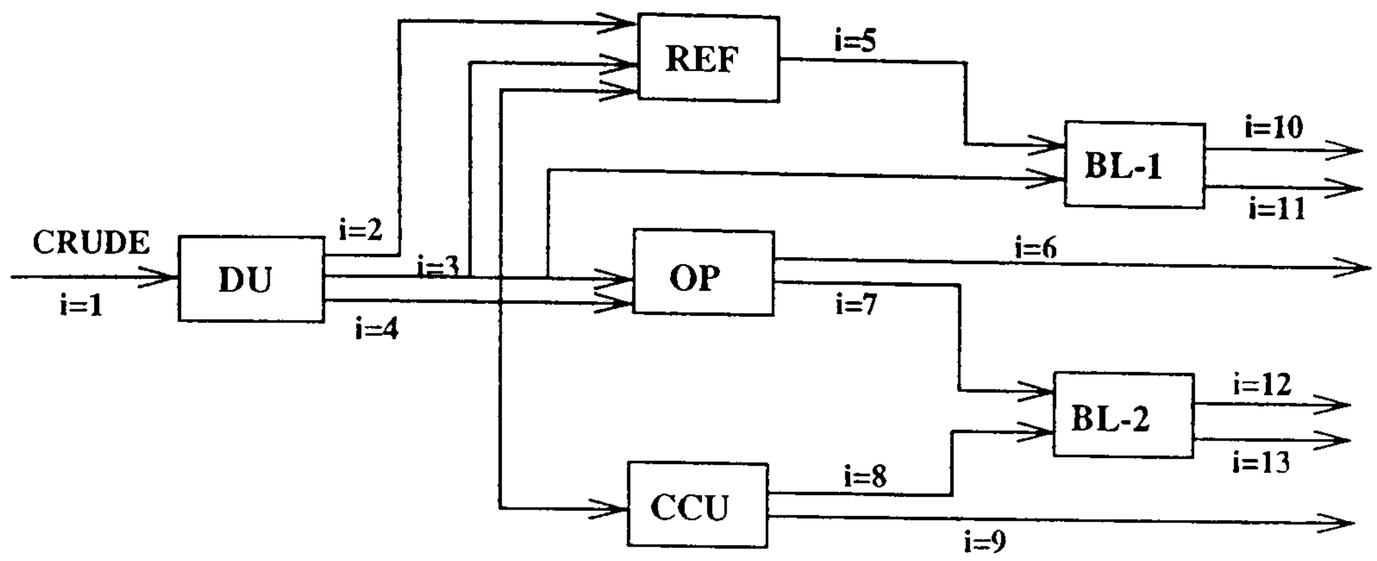


Figure 5.15: Chemical Complex - Example 2

The chemical complex that is examined here, corresponds to a simplified refinery plant, shown in Figure 5.15 which involves 6 processes: namely, a crude distillation unit (DU), a reformer (REF), an olefins plant (OP), a cat cracker unit (CCU) and blending operations (BL-1, BL-2), as well as appropriate material storage facilities. It also involves 13 materials (i=1,..,13) which correspond to raw materials, intermediates and final products.

Process	Operating cost at the first time period	Operating cost at the second time period
1	50	50
2	30	30
3	40	40
4	45	45
5	10	10
6	10	10

Table 5.8: Economic data of chemical processes - Example 2

It is assumed here that only one type of crude is processed through the distillation unit. The two-period planning model is generated based on the data presented in Tables 5.8, 5.9 and 5.10. The model involves 104 inequalities and 52 equalities in 78 unknowns. Elimination of the inventory variables leads to 104 inequalities with 26 free variables, the utilization level of each process and the levels of purchase and sale of each material during the first and second time period. It is also assumed that there is no inventory at the beginning of the first period.

Four uncertain parameters are involved in the description of the model: (i) the availability of the crude at the second time period with nominal value of 70 units/hr and

Material i	Price of material i	Value of final inventory of material i	Purchase price of material i
1	-	10	10
2	-	20	-
3	-	15	-
4	-	10	-
5	-	15	-
6	200	20	-
7	-	20	-
8	-	10	-
9	160	25	-
10	120	10	-
11	120	15	-
12	200	20	-
13	160	20	-

Table 5.9: Economic data of materials for the first time period for Example 2

deviations 10 units/hr in both directions, (ii) the level of demand of material 13 at the second time period with nominal value of 80 units/hr and deviation 20 units/hr in both directions, and (iii) the levels of prices of materials 10 and 6 respectively during the second time period with nominal values 160 and 120 \$/unit respectively and corresponding deviations 40 and 20 \$/unit.

Applying the procedure for the solution of F1 subproblem as a parametric LP the expressions illustrated in Table 5.11 are obtained. The computation time for the parametric solution of F1 is approximately 0.58 seconds of a SPARC IPX machine. Then, two different plans are selected for evaluation with values of the first period variables as shown in Table 5.12. F2 subroblems are then solved as parametric LP problems and the analytical expressions obtained for each of the two plans are displayed in Tables 5.13 and 5.14 respectively. The computation times for these problems are approximatelly 0.30 seconds of a SPARC IPX machine. The VPI function is then determined as the difference between the objectives of F1 and F2 subproblems and is used for the determination of the combined flexibility-VPI index. The results of the above analysis for different values of VPI target are illustrated in Table 5.15. The final MILP problem (F-VPI′) for a specific VPI^T is solved using SCICONIC and takes approximately 0.45 sec of a SPARC IPX machine. Note that regarding plan I there are significant trade-offs between the VPI target value and the combined flexibility-VPI index, whereas plan II remains totally inflexible. These

trends are further shown in the trade-off curves depicted in Figure 5.16.

Although the purpose of this example is to illustrate the computational requirements for the evaluation of the combined flexibility-VPI metric, one could notice that comparing the two plans (plan I and II) plan I is definitely a choise of a risk-taking decision maker since by implementing this plan no further control of operating variables is reqiuired i.e. second-stage planning can be based on a mean value of uncertain parameters, whereas, the selection of plan II would require future adjustment of operating conditions with respect to uncertain parameter realization depending on decision maker's attitude towards risk.

Material i	Price of material i	Value of starting inventory of material i	Value of final inventory of material i	Purchase price of material i
1	-	10	40	10
2	-	20	80	-
3	-	15	60	-
4	-	10	40	-
5	-	15	60	-
6	200	15	80	-
7	-	20	80	-
8	-	10	40	-
9	160	25	80	-
10	160	15	60	-
11	120	15	60	-
12	220	20	80	-
13	200	25	80	-

Table 5.10: Economic data of materials for the second time period - Example 2

Expressions of F1	Uncertain parameter's ranges			
	$\theta 1$	$\theta 2$	$\theta 3$	$\theta 4$
$2123.65 + 56.42\theta 3 + 30\theta 1 + 3.84\ \theta 2 + 0.192\ \theta 2\ \theta 3$	$\theta 1 \leq 388.7$	$15 \leq \theta 2 \leq 165$	$63.4 \leq \theta 3 \leq 80$	$\theta 4 \geq 10$
$6637.29 + 30\ \theta 1 + 19.2\ \theta 2$	$\theta 1 \leq 388.7$	$15 \leq \theta 2 \leq 165$	$63.4 \leq \theta 3 \leq 80$	$\theta 4 \geq 10$
$-7579.3 + 209.5\theta 3 + 30\theta 1 + 16\theta 2$	$\theta 1 \leq 1061.5$	$15 \leq \theta 2 \leq 165$	$60.9 \leq \theta 3 \leq 63.4$	$\theta 4 \geq 10$
$-8063.9 + 217.5\theta 3 + 30\theta 1 + 16\theta 2$	$\theta 1 \leq 1088$	$15 \leq \theta 2 \leq 165$	$56.3 \leq \theta 3 \leq 60.9$	$\theta 4 \geq 10$

Table 5.11: F1 expressions as a function of uncertain parameters - Example 2

Variables	**PLAN I**	**PLANII**
Sales of material 9	23.09	26.08
Sales of material 10	27.09	28.80
Sales of material 6	5.00	5.00
Sales of material 11	5.40	7.20
Sales of material 12	5.40	5.40
Sales of material 13	13.80	15.90
Purchase of material 1	170.00	170.00
Utilization level of unit 1	150.00	150.00
Utilization level of unit 2	42.33	45.00
Utilization level of unit 3	11.02	14.69
Utilization level of unit 4	20.00	22.71
Utilization level of unit 5	33.86	36.00
Utilization level of unit 6	7.71	10.28

Table 5.12: Two alternative first period plans - Example 2

Expressions of F2 for plan I	Uncertain parameter's ranges			
	$\theta 1$	$\theta 2$	$\theta 3$	$\theta 4$
$2242.5 + 46.37\theta 3 + 30\theta 1 +$ $5.55\ \theta 2 + 0.192\ \theta 2\ \theta 3$	$\theta 1 \leq 361.6$	$\theta 2 \geq 15$	$63.4 \leq \theta 3 \leq 80$	$\theta 4 \geq 10$
			$0.21\theta 3 - \theta 4 \leq 2.6$	
$5952.65 + 30\ \theta 1 + 20.9\ \theta 2$	$\theta 1 \leq 361.6$	$\theta 2 \geq 15$	$\theta 3 \geq 80$	$\theta 4 \geq 14.2$
$2593.55 + 18.02\theta 3 + 135\theta 4 + 30\theta 1$ $5.55\ \theta 2 + 0.192\ \theta 2\ \theta 3$	$\theta 1 \leq 361.6$	$\theta 2 \geq 15$	$63.4 \leq \theta 3 \leq 80$	$\theta 4 \geq 10$
			$2.6 \leq 0.21\theta 3 - \theta 4 \leq 82.6$	
$1567.54 + 57.02\theta 3 + 30\theta 1$ $- 14.73\ \theta 2 + 0.512\ \theta 2\ \theta 3$	$\theta 1 \leq 361.6$	$\theta 2 \geq 15$	$60.00 \leq \theta 3 \leq 63.4$	
			$0.21\theta 3 - \theta 4 \leq 2.6$	
$1918.57 + 28.67\theta 3 + 30\theta 1$ $- 14.73\ \theta 2 + 0.512\ \theta 2\ \theta 3 + 135\theta 4$	$\theta 1 \leq 361.6$	$\theta 2 \geq 15$	$60.00 \leq \theta 3 \leq 63.4$	$\theta 4 \geq 10$
			$2.6 \leq 0.21\theta 3 - \theta 4 \leq 82.6$	

Table 5.13: F2 expressions as a function of θ for plan I - Example 2

Expressions of F2 for plan II	Uncertain parameter's ranges			
	$\theta 1$	$\theta 2$	$\theta 3$	$\theta 4$
$2825.75 + 46.37\theta 3 + 30\theta 1 +$ $3.84\ \theta 2 + 0.192\ \theta 2\ \theta 3$	$\theta 1 \leq 361.6$	$\theta 2 \geq 15$	$70 \leq \theta 3 \leq 80$	
			$0.21\theta 3 - \theta 4 \leq 4.7$	
$6582.1 + 30\ \theta 1 + 19.2\ \theta 2$	$\theta 1 \leq 361.6$	$\theta 2 \geq 15$	$\theta 3 \geq 80$	$\theta 4 \geq 12.1$
$3460.22 + 18.02\theta 3 + 135\theta 4 + 30\theta 1$ $3.84\ \theta 2 + 0.192\ \theta 2\ \theta 3$	$\theta 1 \leq 361.6$	$\theta 2 \geq 15$	$70 \leq \theta 3 \leq 80$	
			$4.7 \leq 0.21\theta 3 - \theta 4 \leq 84.7$	
$4902.3 + 30\theta 1 + 135\theta 4 + 19.2\theta 2$	$\theta 1 \leq 361.6$	$\theta 2 \geq 15$	$\theta 3 \geq 80$	$10 \leq \theta 4 \leq 12.1$

Table 5.14: F2 expressions as a function of θ for plan II - Example 2

VPI target	Combined Flexibility-VPI index	
	PLAN I	PLAN II
200	0.0	0.0
420	0.066	0.0
450	0.365	0.0
500	0.863	0.0
520	1.0	0.0

Table 5.15: Results of Flexibility-VPI analysis - Example 2

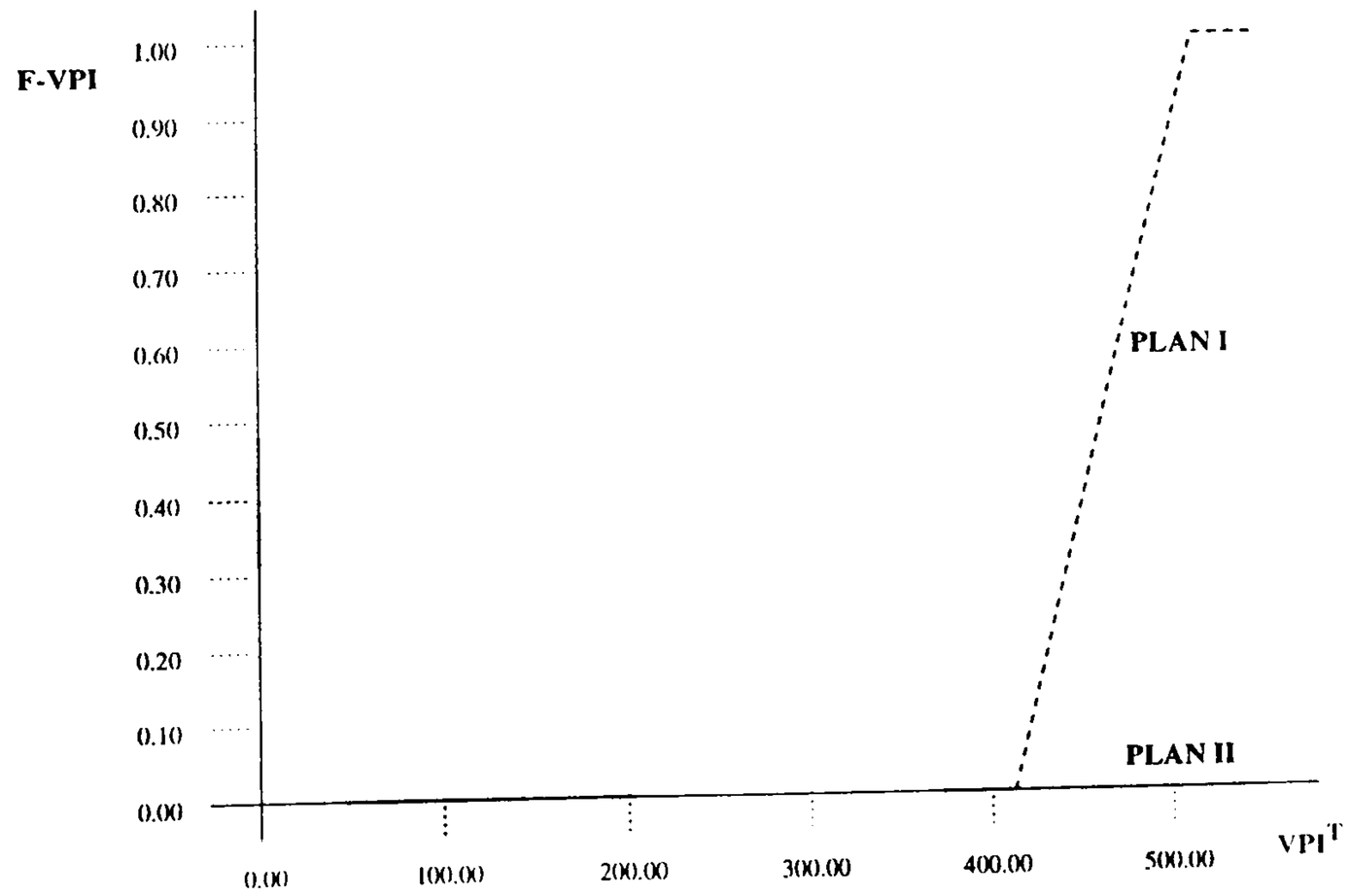


Figure 5.16: Trade-off Curves - Example 2

Example 3

Consider again here the small-scale chemical complex of Figure 5.8. The implementation of the proposed approach leads to the decision of producing 4.8 units of product during the first period, which has the maximum expected profit of 16.6 units (see also Figure 5.17). The optimal production policy assures future (second-period) demand satisfaction within the range of $3.8 \leq \theta \leq 7$.

Note that a more flexible production policy (see Figures 5.18 and 5.19) which can accommodate the whole demand range ($x_1 = 4$) results in a smaller expected profit, EP=16 units. Also note that the solution at the mean value of demand ($x_1 = 5$) has lower expected profit EP=16.4 units and smaller feasible region ($4 \leq \theta \leq 7$) compared with the optimal production; i.e. the production of additional units (more than the optimal 4.8 units) at the first period is neither profitable nor can improve system's flexibility. Figure 5.19 clearly illustrates this trend - there is an optimal balance between expected profit and plan flexibility.

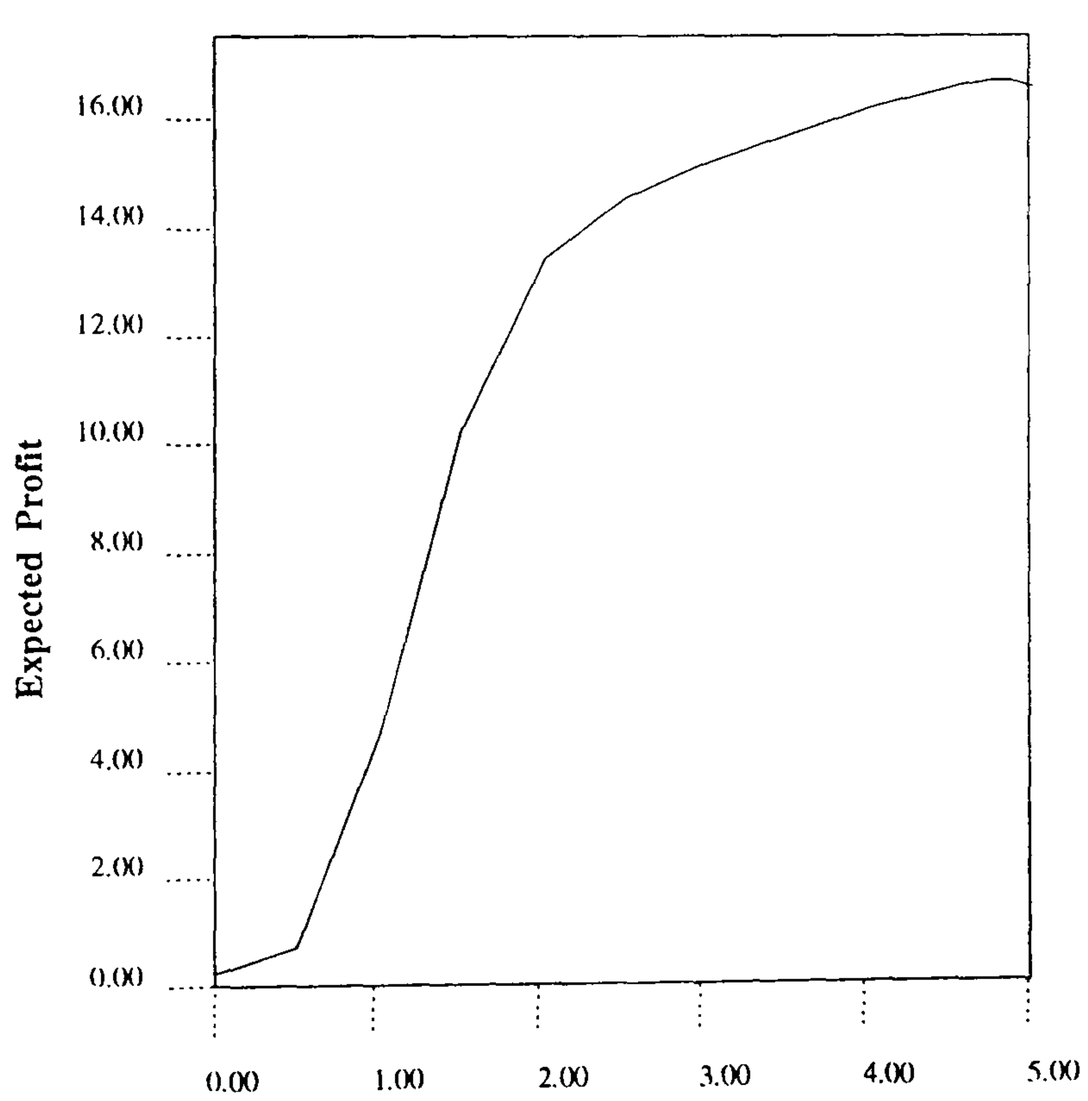


Figure 5.17: Expected profit for different demand levels - Example 3

Figure 5.20 shows the value of information as a function of the uncertain demand for different production plans. First note that for the optimal production the value of information is relatively low, implying small profit gains of determining future production

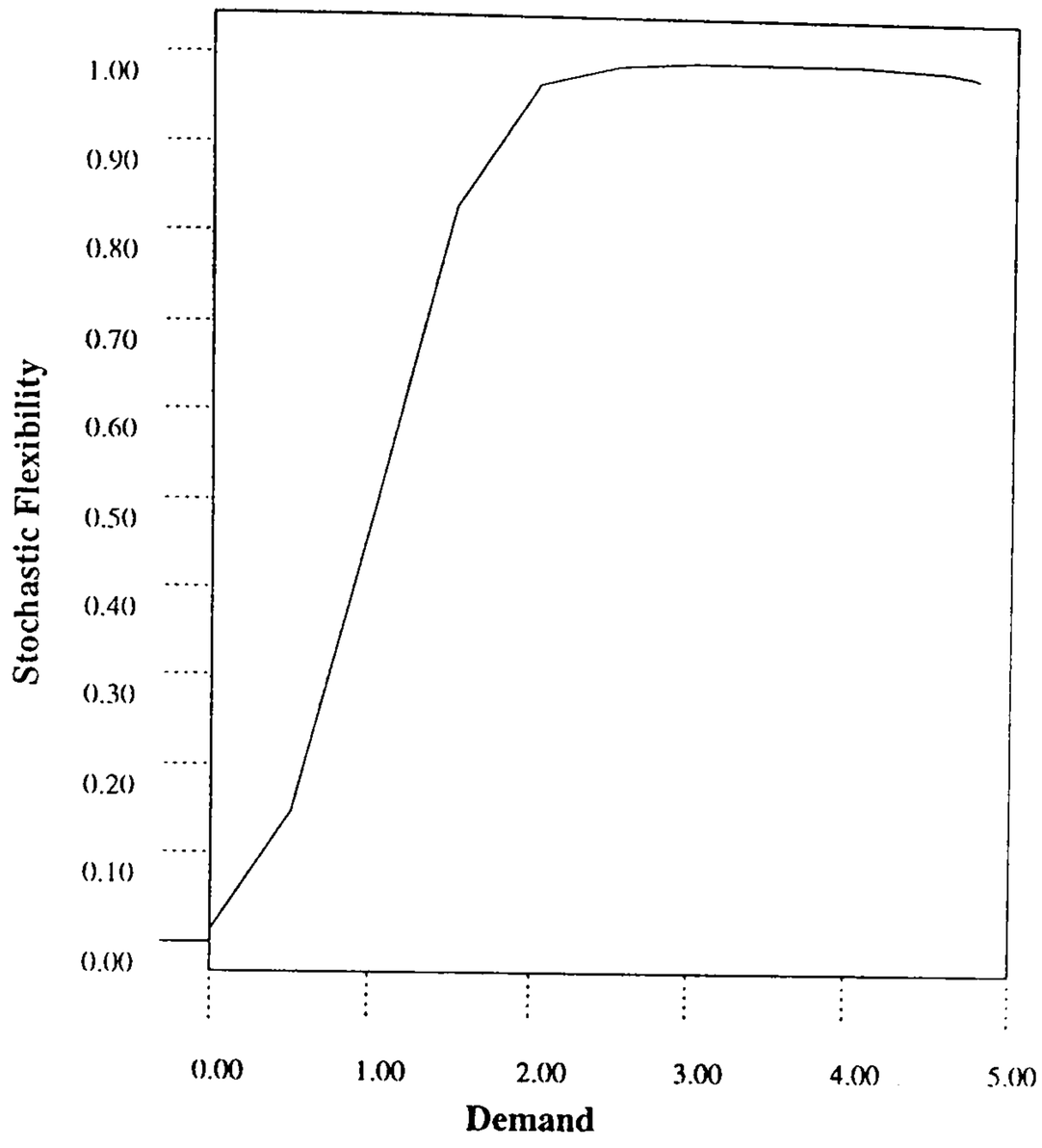


Figure 5.18: Stochastic Flexibility versus demand - Example 3

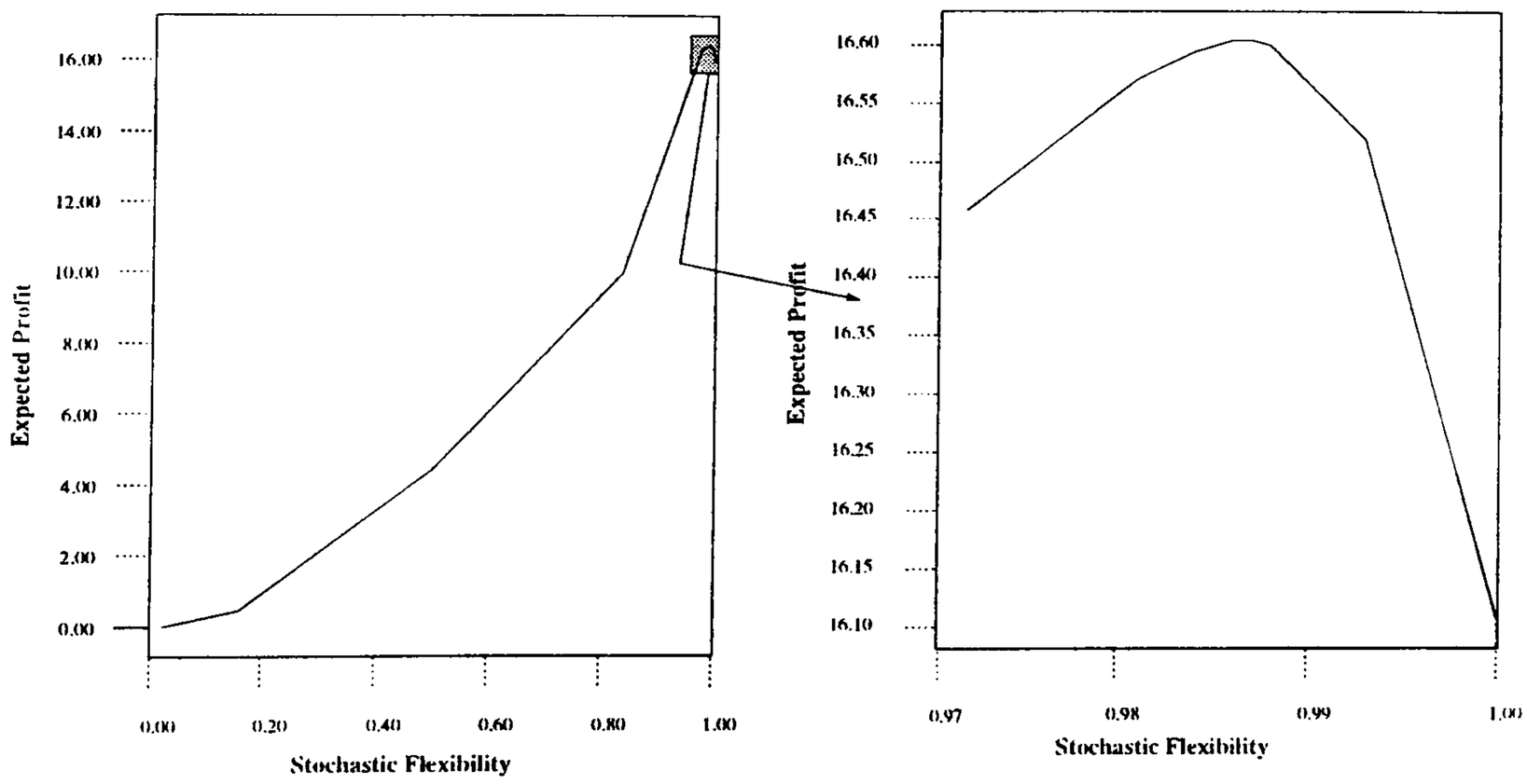


Figure 5.19: Expected profit vs Stochastic Flexibility - Example 3

contingent to demand realizations. It can be also noticed that as demand increases until the value of 4.1 units the value of information also increases: knowing the value of demand will result in a higher profit for large demand value is or in other words the opportunity loss is larger.

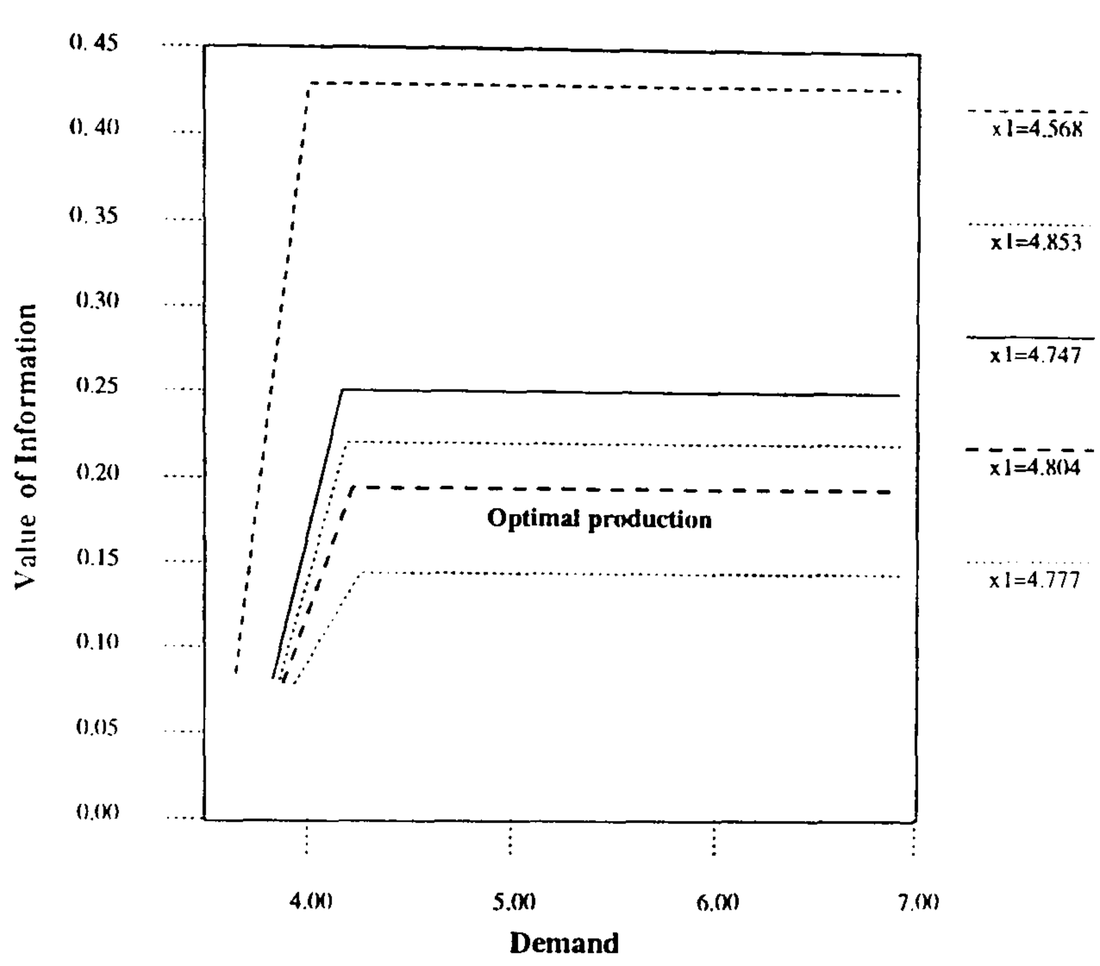


Figure 5.20: Value of Information versus demand - Example 3

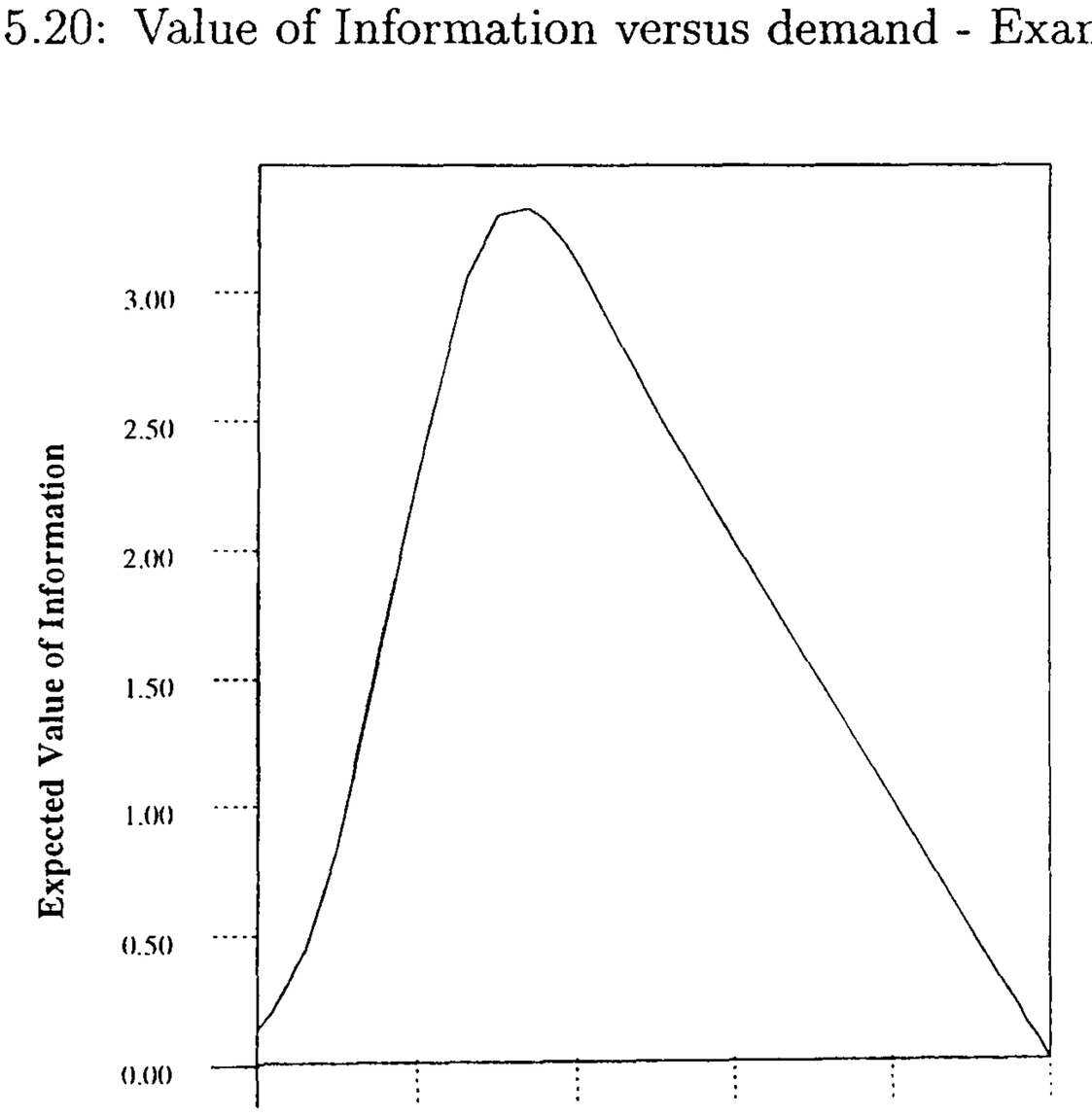


Figure 5.21: Expected Value of Information vs. first-stage decision - Example 3

Comparing different production policies (see also Figure 5.21) as x_1 increases the expected value of information increases since opportunity losses are worth incurring. Con-

sequently, it is appealing to increase profit by producing more; however, as x_1 increases above a threshold value, the value of information becomes less valuable since opportunity losses are smaller by not meeting demand fluctuations. Furthermore, it is interesting to compare two alternative plans; the production of 2 and 5 units, respectively. Note that there are almost equally profitable and flexible; yet, their difference in EVPI values (EVPI($x_1 = 2$)= 3.1, EVPI($x_1 = 5$)= 0.0) reveals that the production of 5 units involves no opportunity loses (and consequently would be selected by a risk averse decision maker).

Example 4

The production network of Figure 4.6 is considered here. The demand of both products as well as the availability of raw material are considered as uncertain parameters following normal probability distributions N(20,2.5), N(15,2.5) and N(40.2.5), respectively. The two-stage stochastic planning problem (see section 4.4) involves as a first-stage decision the optimal capacity expansion of process 1 (becoming available at the second stage), and as second-stage decision the operating variables, purchase of raw material, sales of products and a possible capacity expansion of process 2.

The proposed algorithm requires 9 iterations to converge to the optimal capacity expansion of 12.6 units having a maximum expected profit of 1245.3 units as illustrated in Figure 5.22. Considering 5 quadrature points for each one of the three uncertain parameters and using GAMS/SCICONIC for the solution of the required MILP problems, 48.4 CPU s in SPARCstation 10 were required with almost all of the time (48.2 s) spent at the solution of feasibility and profit maximization subproblems and 0.2 s at the solution of master problem. The evaluation of the expected value of information for different capacity expansion policies requires the solution of one additional problem at each quadrature point (37.5 CPU s). The results are shown in Figure 5.23.

Note that, for small values of capacity expansions as capacity increases EVPI decreases moving towards the optimal wait-and-see decision. However, above a threshold capacity of 11 units the opportunity cost of capacity shortage increases overcoming the investment cost and in turn EVPI rises. The breakeven point occurs at the capacity expansion of 11 units - very close to the optimal capacity expansion with maximum expected profit which has an EVPI of 230 units. Of course this trend is case-dependent - mainly influenced by the magnitude of capital costs and product prices.

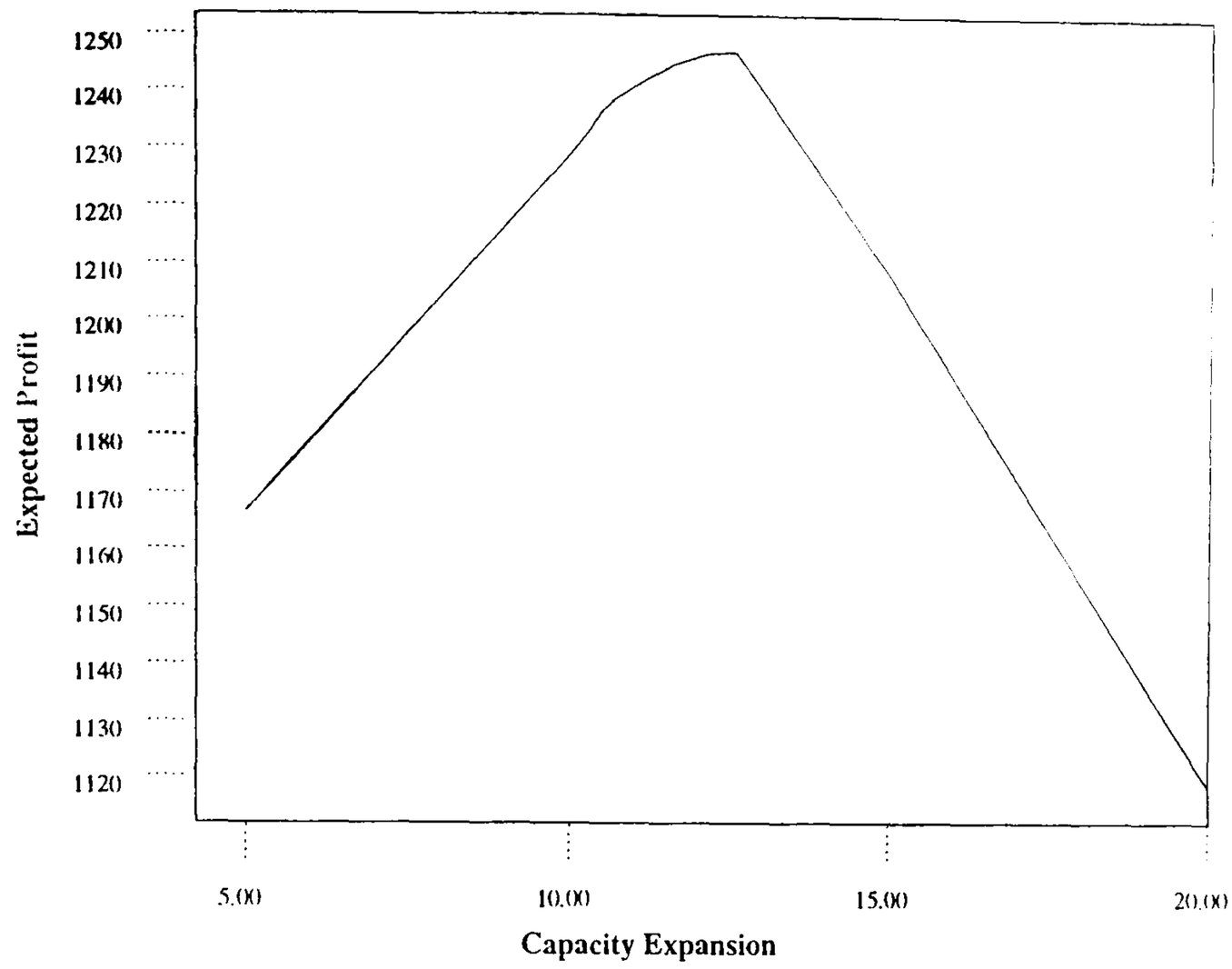


Figure 5.22: Expected Profit vs. Capacity expansion - Example 4

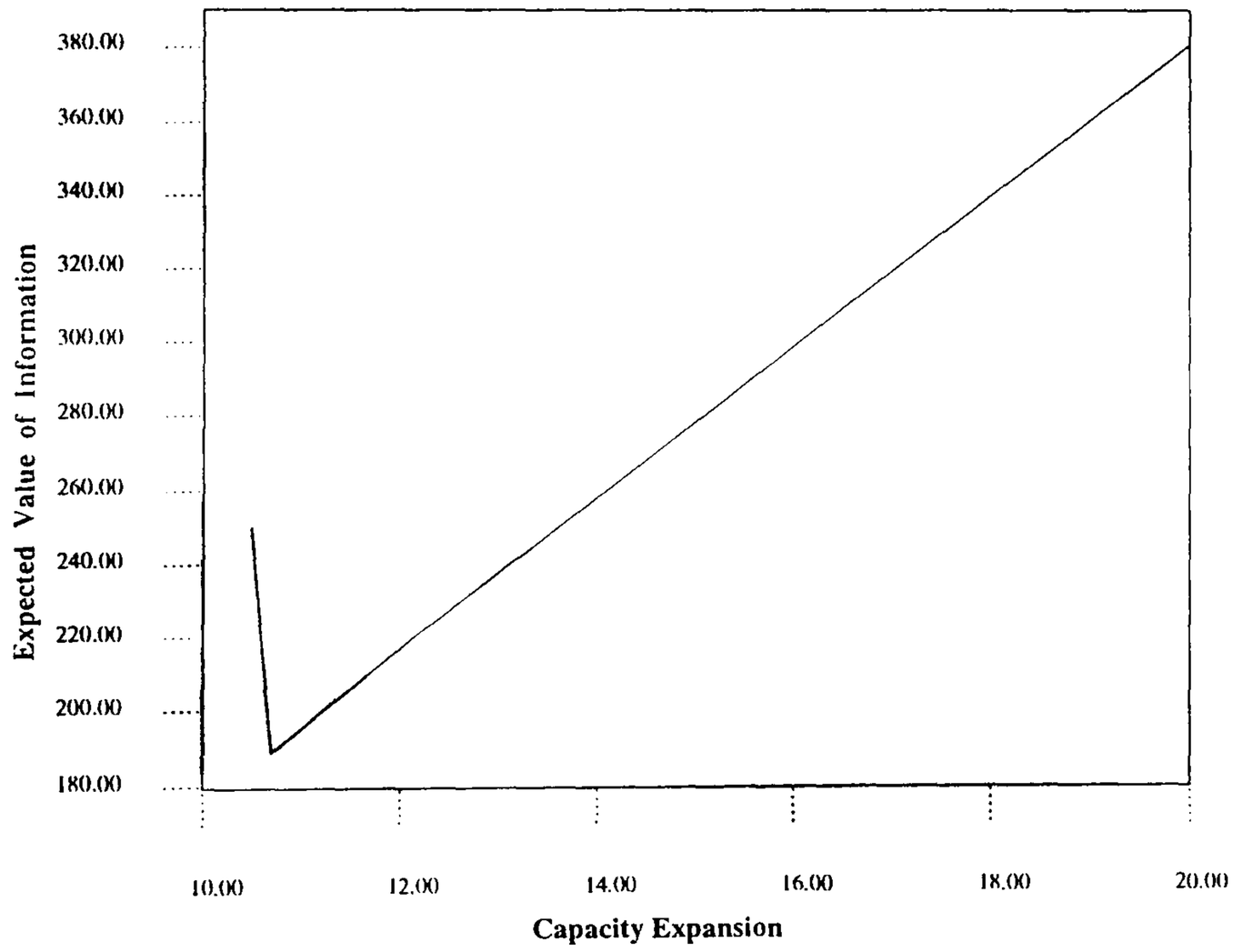


Figure 5.23: EVPI vs. Capacity expansion - Example 4

Example 5

In this example the production of chemical C is considered in the production system shown in Figure 2.11. The mathematical formulation of the problem and the model parameters are given in section 2.4. The current level of the demand of product C is considered known with its future level be forecasted as a random variable following a normal distribution function N(17.5, 2.5). Here the decision maker has to identify an optimal plant structure from a number of possible alternatives (for example to install all three processes, any combination of two, etc).

The results of the implementation of the proposed integrated planning algorithm are summarized in Tables 5.16 and 5.17. Proper balance of economic and feasibility targets is achieved resulting in structure (1,1,0), initially processes 2 and 3 for the production of B from A, as the optimal plant configuration with expected profit of 3144.5 which can accommodate future demand variations up to 26 units. For comparison, the problem was solved via a multiperiod/scenario approach by placing a 5 point quadrature grid inside the entire demand range $T(\theta) = \{\theta \mid \bar{\theta} - 4\sigma \leq \theta \leq \bar{\theta} + 4\sigma\} = \{7.5, 27.5\}$, weighting by its corresponding probability. The optimal decision in this case is to install all three processes for the production of B from A. Table 5.17 depicts that the latter has a lower expected profit despite being more flexible.

	ITERATION (6 CPUs-SPARCstation 10)		
	1	2	3
Upper Bound	5798.65	3884.5	3144.49
Lower Bound	2149.98	3144.49	3144.49
Structure	(1,0,1)	(1,1,0)	(1,1,1)
Expected profit	2149.98	3144.49	3082.63
Feasible region	$7.5 \leq \theta \leq 23.3$	$7.5 \leq \theta \leq 26$	$7.5 \leq \theta \leq 27.5$
Stochastic Flexibility	0.928	0.968	1
Expected Value of Information	845.9	0.05	211.7

Table 5.16: Convergence of the Algorithm - Example 5

Figure 5.24 (together with Table 5.17) displays the value of information as a function of the uncertain demand for different plant structures. Note that for the optimal structure (1,1,0) and for demand values between 12 and 26 units the expected opportunity loss is zero (VPI=0) implying that in fact decisions here coincide with wait-and-see de-

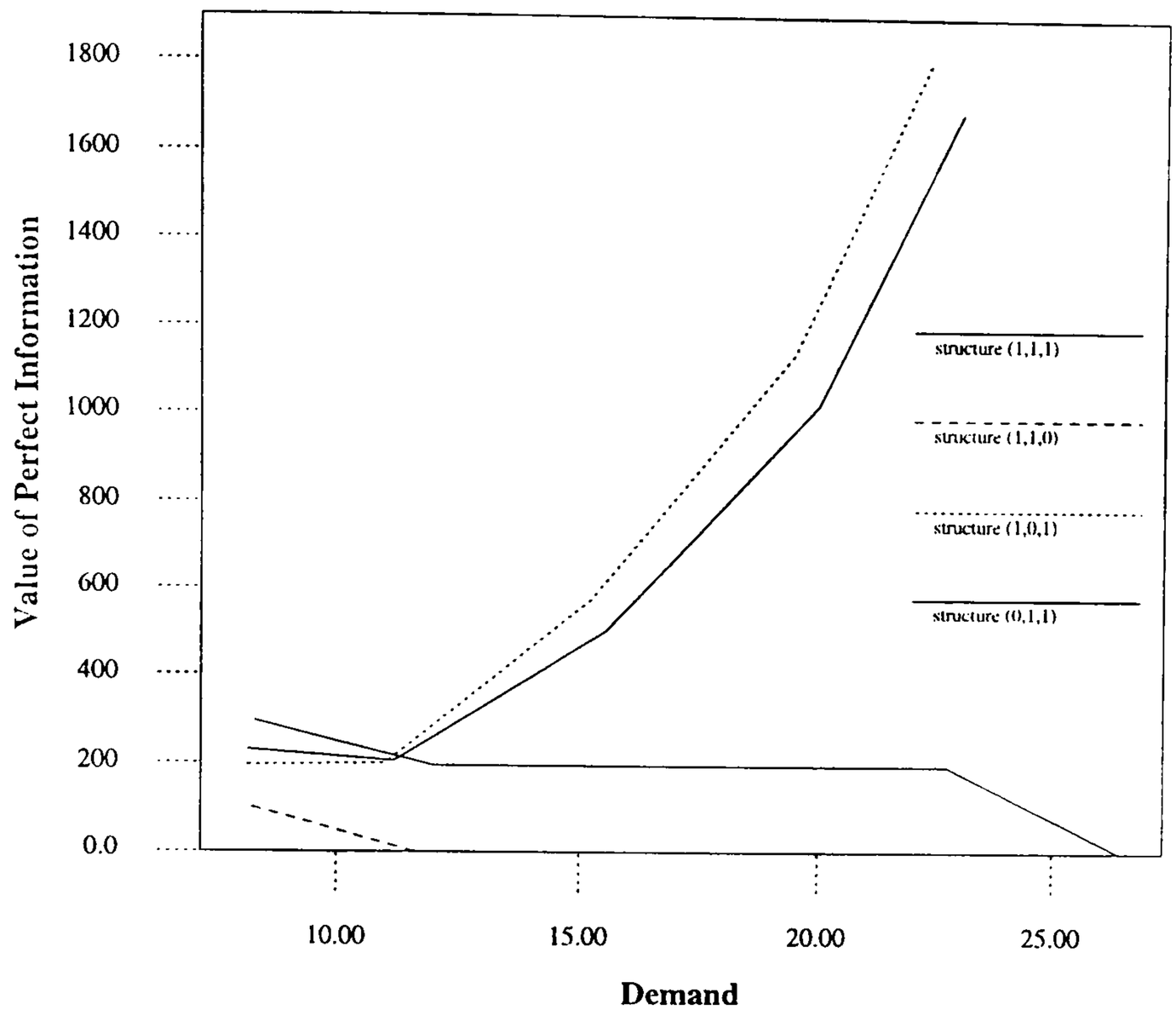


Figure 5.24: Value of Perfect Information for different structures - Example 5

Structure	Stochastic Flexibility (SF)	Feasible Region	Expected Profit (EP)	Expected Value of Information (EVPI)
(1,1,1)	1.0	$7.5 \leq \theta \leq 27.5$	3082.6	211.7
(1,1,0)	0.968	$7.5 \leq \theta \leq 26$	3144.5	0.05
(1,0,1)	0.928	$7.5 \leq \theta \leq 23.3$	2149.9	845.9
(0,1,1)	0.936	$7.5 \leq \theta \leq 23.9$	2310.4	710.7
(1,0,0)	0.242	$7.5 \leq \theta \leq 15.8$	470.2	73.3
(0,1,0)	0.328	$7.5 \leq \theta \leq 16.5$	712.8	89.4
(0,0,1)	0.104	$7.5 \leq \theta \leq 14.4$	-205.3	209.6

Table 5.17: Summary of results - Example 5

cisions - subsequently, we can replace uncertainty in this range by a corresponding mean value ($\bar{\theta}$= 17.4); however, for demand values between 7.5 and 12 units it is worth monitoring future operating decisions regarding process utilization levels, sales of product and raw material purchase to follow demand realizations. To exploit this fact further we have evaluated the expected revenue within the demand range (7.5-12) for two alternative policies, policy A in which we control operating variables to meet the demand, and policy B by considering the mean value of demand (10.4). This results in expected revenue values of 33.14 for policy A and 12.44 for policy B, respectively which clearly confirms the need for monitoring future action.

Note also that for the two "dominant" plant configurations, structures (1,1,0) and (1,1,1) respectively, as demand increases the value of information decreases: for low demand there is no pressure for selecting a structure that can accommodate high demand values. As demand increases this certainly is not true: in this case, the dominant structures approach the solution of the correspond wait-and-see problems thus involving low opportunity losses (in fact, the optimal structure as mentioned above, matches exactly the wait-and-see solution for demand values above 12 units). Of course, this is not unexpected, since as shown in Table 5.17, these structures can accommodate almost the entire demand range - information about future demand increase is not so critical.

In contrast, for two suboptimal structures, (1,0,1) and (0,1,1), the value of information increases as demand increases - for high demand values. This is due to the incapability of the latter structures to handle increasing demand orders - here, the information about future demand increase is indeed critical.

Finally, Figure 5.25, which shows the expected value of perfect information in terms of plan flexibility, reveals another interesting trend. As EVPI decreases the increase of plan flexibility is well justified; however, increase of EVPI implies that extra plan flexibility may not be desired. Although it is worth paying for additional feasibility (larger demand range) until a value of 0.968 (corresponding to the optimal structure (1,1,0)) with zero EVPI, the installation of an additional unit (process 3) to enable further demand feasibility is not really worthwhile.

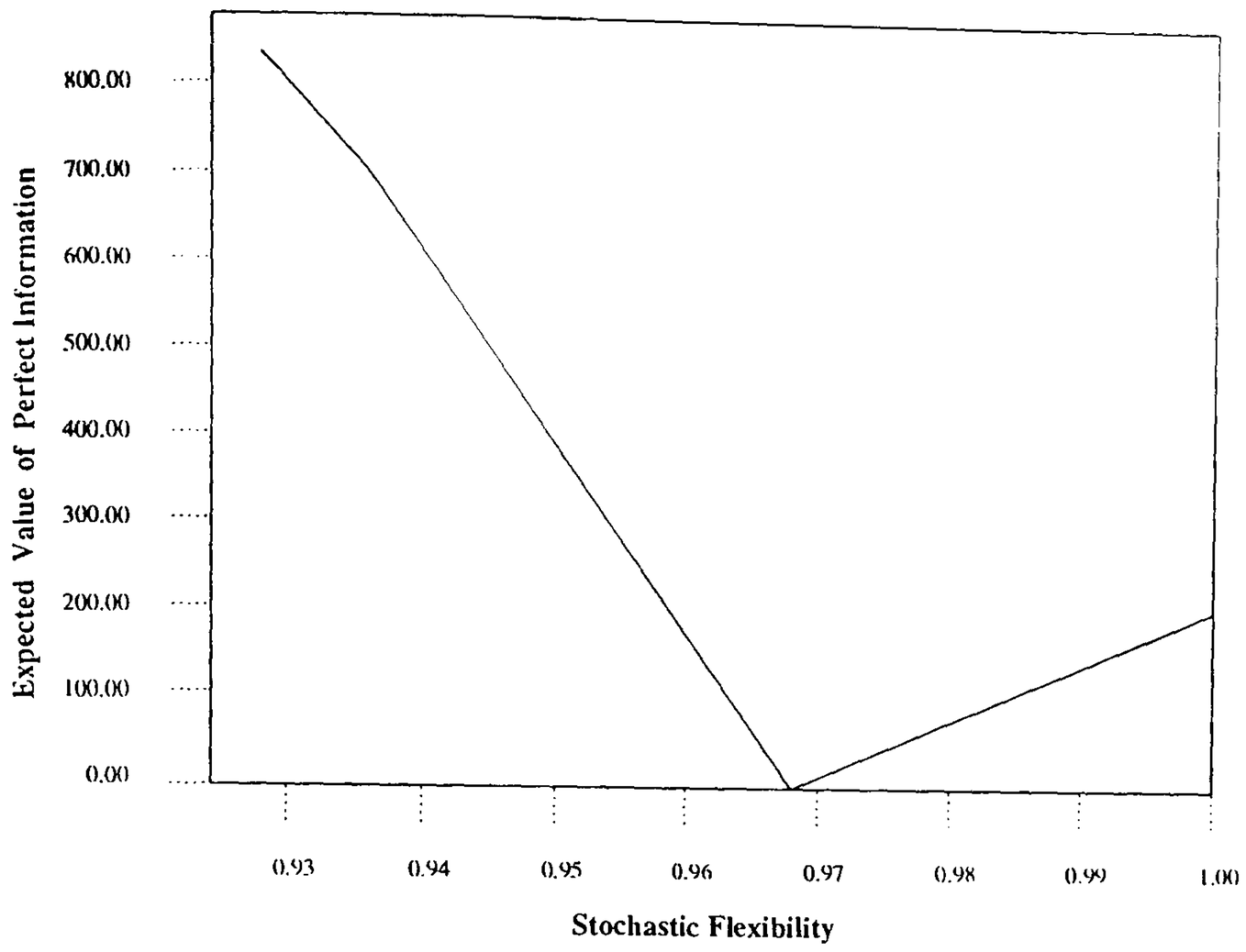


Figure 5.25: EVPI vs. SF - Example 5

Example 6

The two-stage stochastic design problem of the benzene chlorination process (Figure 2.14) is examined here. Figure 5.27 shows the results of the solution of the wait-and-see and here-and-now profit models as a function of purity for different demand levels. Note that as purity increases the solutions of the wait-and-see and here-and-now models coincide for different demand cases - this trend becomes even more prevailing as demand increases: plants with excess capacity become more attractive since high purity and demand levels result in high revenues (this will of course be affected by the magnitude of the corresponding capital cost). For a given demand and purity requirements of 55 kmol/hr and 0.985 (chlorobenzene molar fraction), the optimal solution of the wait-and-see model corresponds to the installation of three reactors of 3.7, 4.2 and 4.4 m^3 followed by a single distillation unit with an annual profit of $ 7.2E5. On the other hand, the optimal solution of the two-stage approach (of three reactors followed by two distillation units) has a corresponding annual profit of $ 6.9E5. The difference of 30,000 $/year represents the price of uncertainty, i.e. the amount of money lost due to the fact that information regarding uncertainty in future demand and purity is not available at the first-stage.

For the optimal structure, the Value of Perfect Information as a function of demand level for different purity requirements is shown in Figure 5.28. Note that VPI declines as demand and purity levels increase - at low demand and purity levels the oppor-

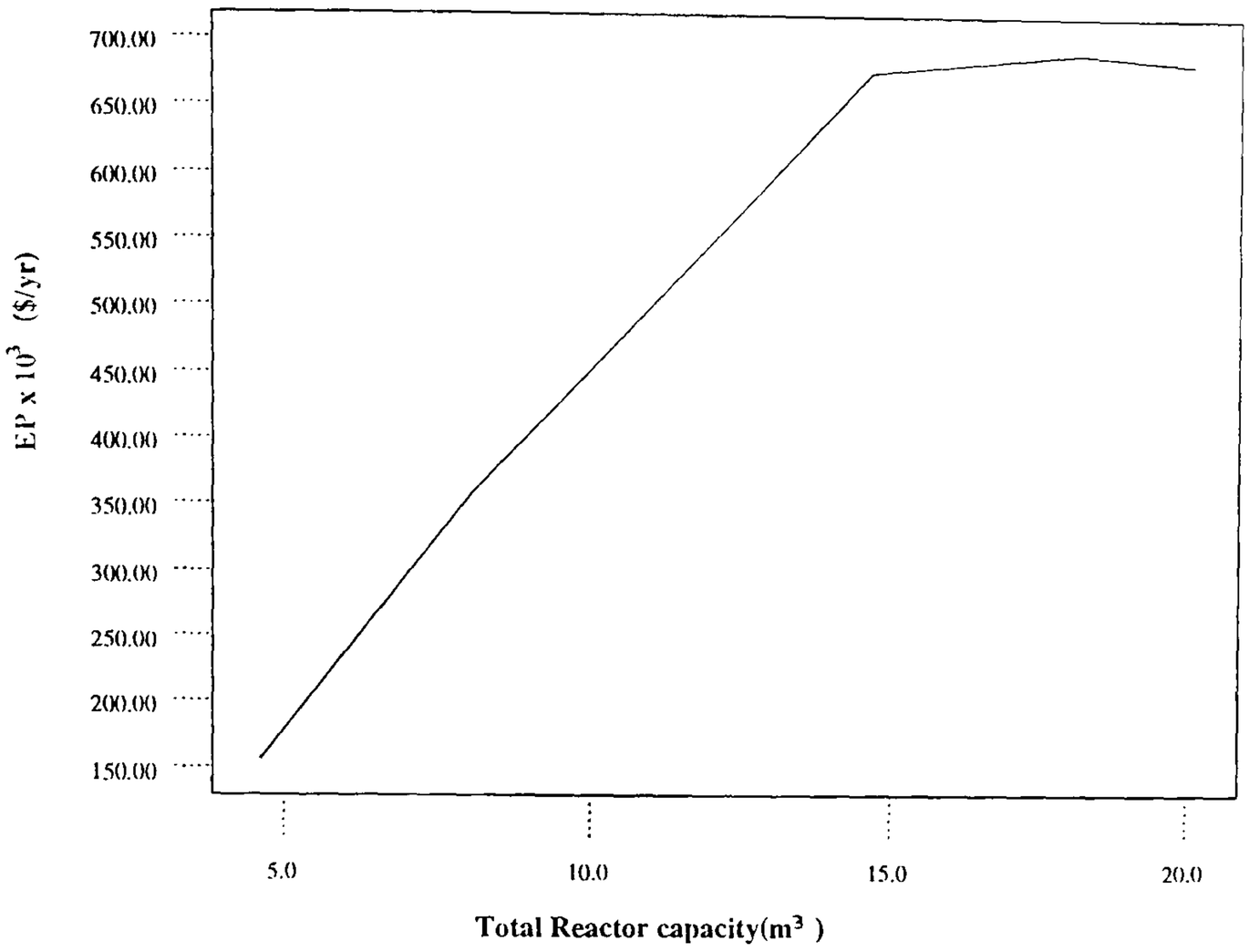


Figure 5.26: Expected profit vs. Reactor capacity - Example 6

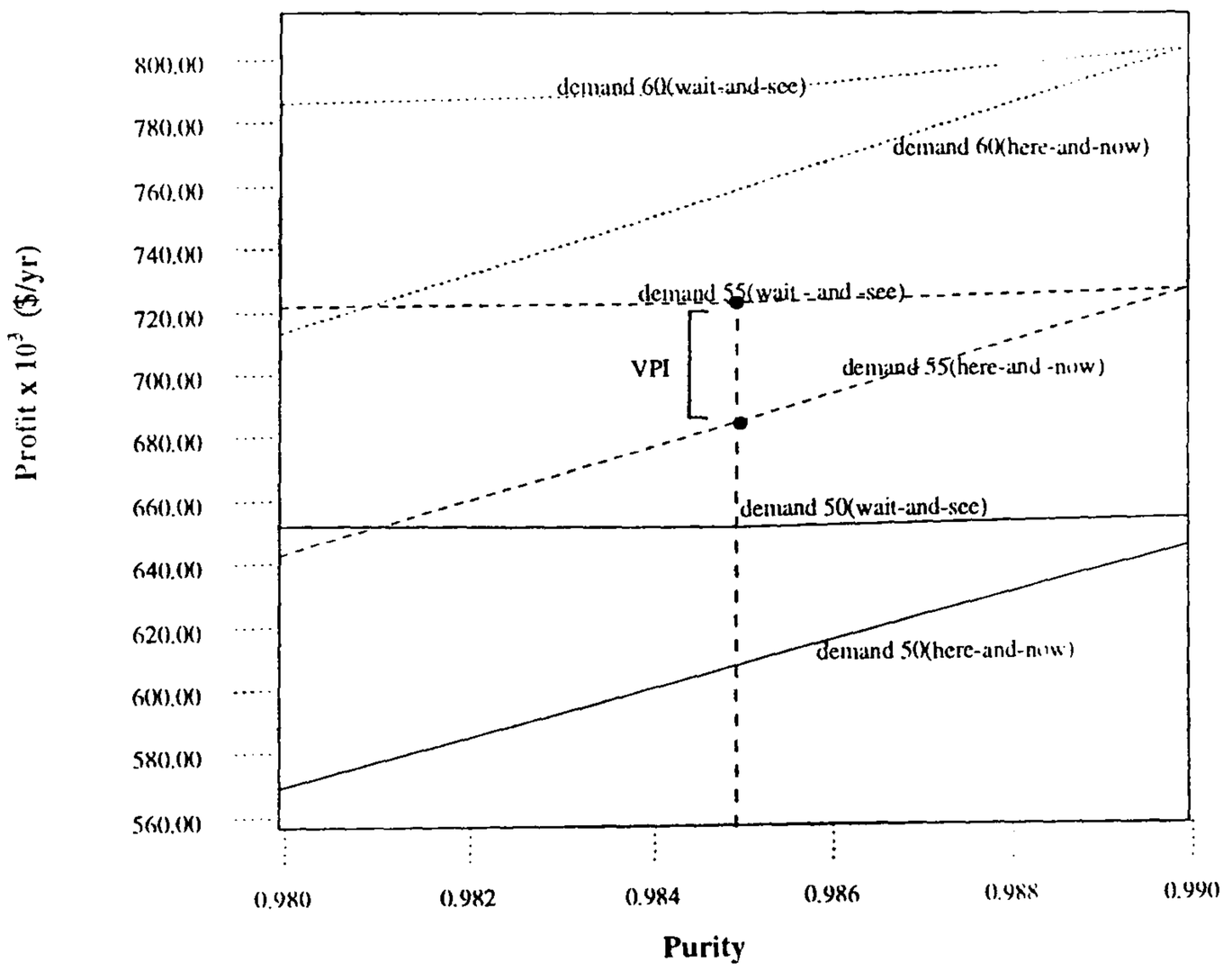


Figure 5.27: Wait-and-see and Here-and now profit vs. purity - Example 6

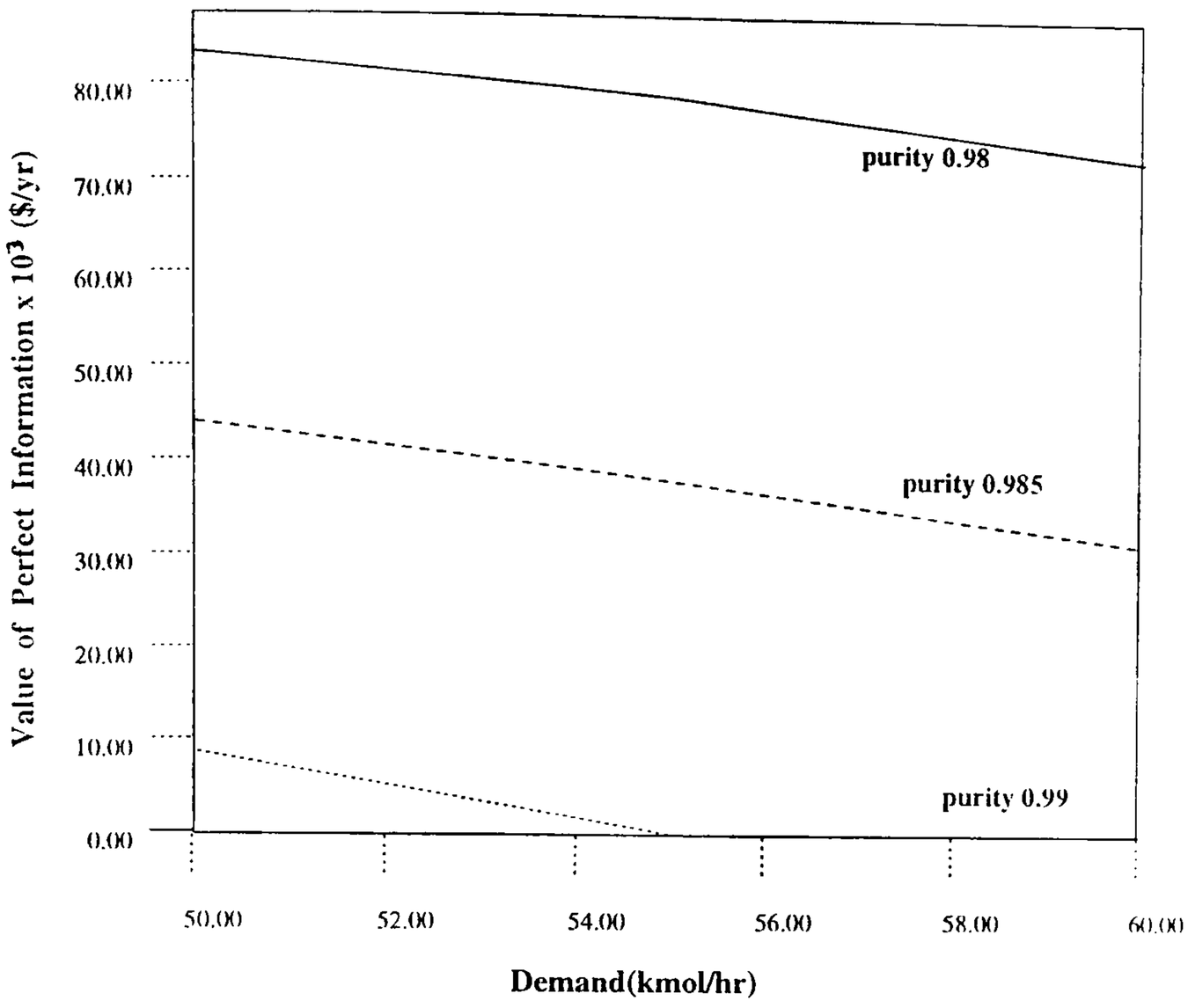


Figure 5.28: Value of Perfect Information for Optimal Plant - Example 6

tunity cost of capacity shortage is larger than the required capital cost; the risk of building up excess capacity is worth justified. Note also that for a purity of 0.99 VPI takes a value of zero for demand levels above a threshold value of 55kmol/hr - the demand range [55,60] can be substituted by a mean value without affecting any optimal two-stage policy (since it will coincide with the wait-and-see solution).

The consideration of a different plant configuration is examined in Figures 5.29 and 5.30. This configuration, which corresponds to the optimal solution of the wait-and-see model for a demand value of 50 kmol/hr and a purity of 0.98 (chlorobenzene molar fraction), involves three reactors in series of sizes 3.5, 3.5 and 4.9 m^3 respectively, followed by a single distillation column. Figure 5.29 reveals that in this case the Value of Perfect Information, unlike the optimal structure, increases as demand and purity levels increase: the opportunity cost here keeps on increasing signifying that capacity expansion might be desired. The evaluation of the Expected Value of Perfect Information for this plant further supports this evidence - the resulting EVPI of 3.0E5 is almost twice the corresponding EVPI of the optimal two-stage plant with a value of 1.6E5! The need for capacity expansion is clearly shown in Figure 5.30, which compares the VPI values as a function of purity for demand level of 50 kmol/hr with and without the consideration of an extra distillation column. It is interesting to note that, although at low purity levels the introduction of a second column results in higher VPI (compared to the single unit case),

as purity increases above a threshold value of 0.985 the trend is reversed: a decision not to install a second distillation column at high purity specification has large opportunity cost since the revenues from the increased product prices overcome the associated investment cost.

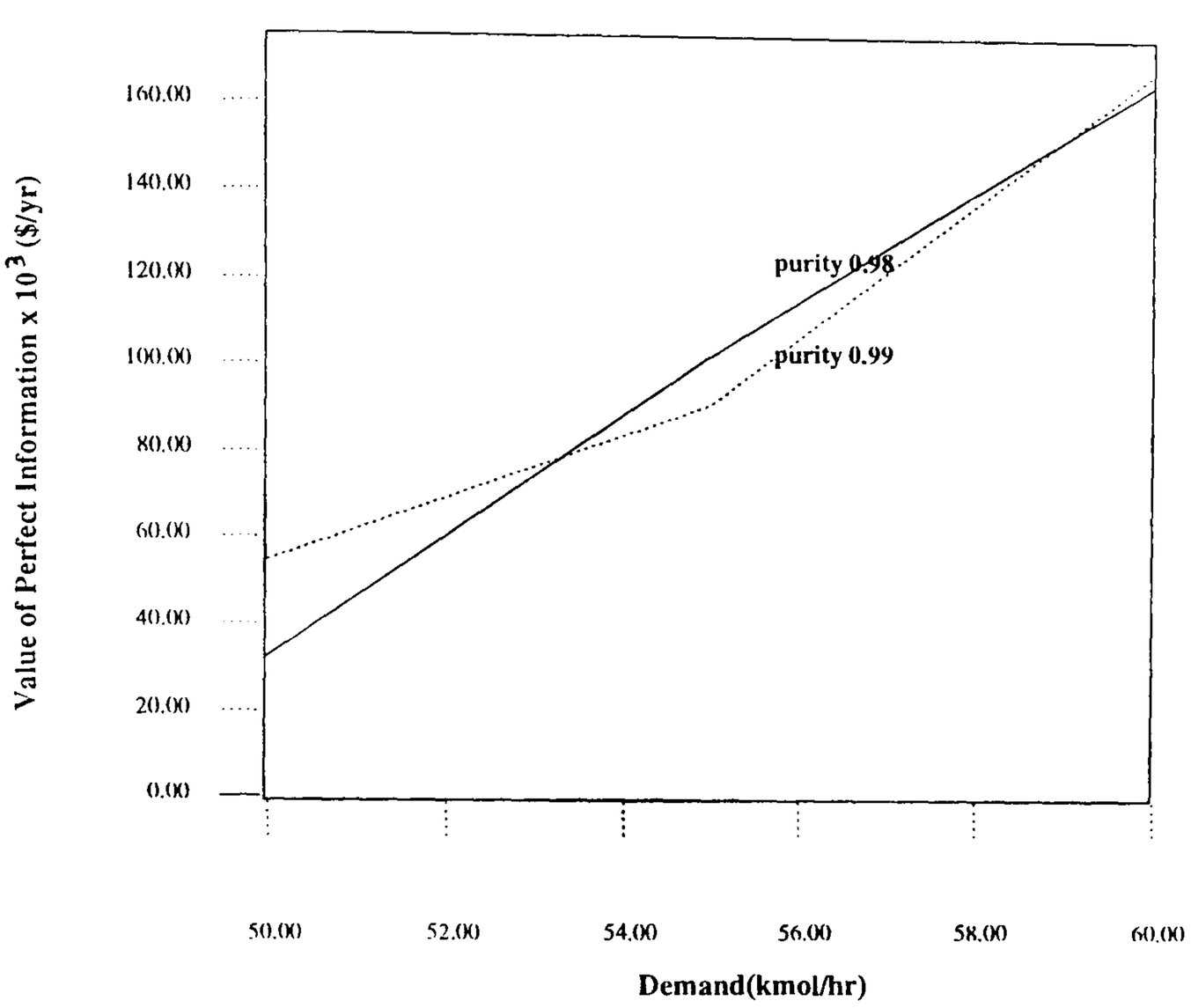


Figure 5.29: VPI results for a different plant - Example 6

5.6. Summary

The role of uncertainty in operational planning has been analyzed in this chapter through the considerations of future plan feasibility and value of perfect information. The integrated planning strategy proposed offers a decision analysis tool which can be especially useful in capacity expansion projects. In such situations, expected profit and future feasibility frequently have to be balanced with the decision maker's attitude towards risk. As the example problems have demonstrated, the information obtained by applying theses tools are complementary to existing planning algorithms by providing insight and quantitative interpretation regarding future outcomes. In some cases, these tools enable the identification of conditions under which the transformation of the stochastic two-stage problem into a deterministic equivalent is indeed feasible - an issue that obviously deserves further attention when dealing with process engineering problems under uncertainty.

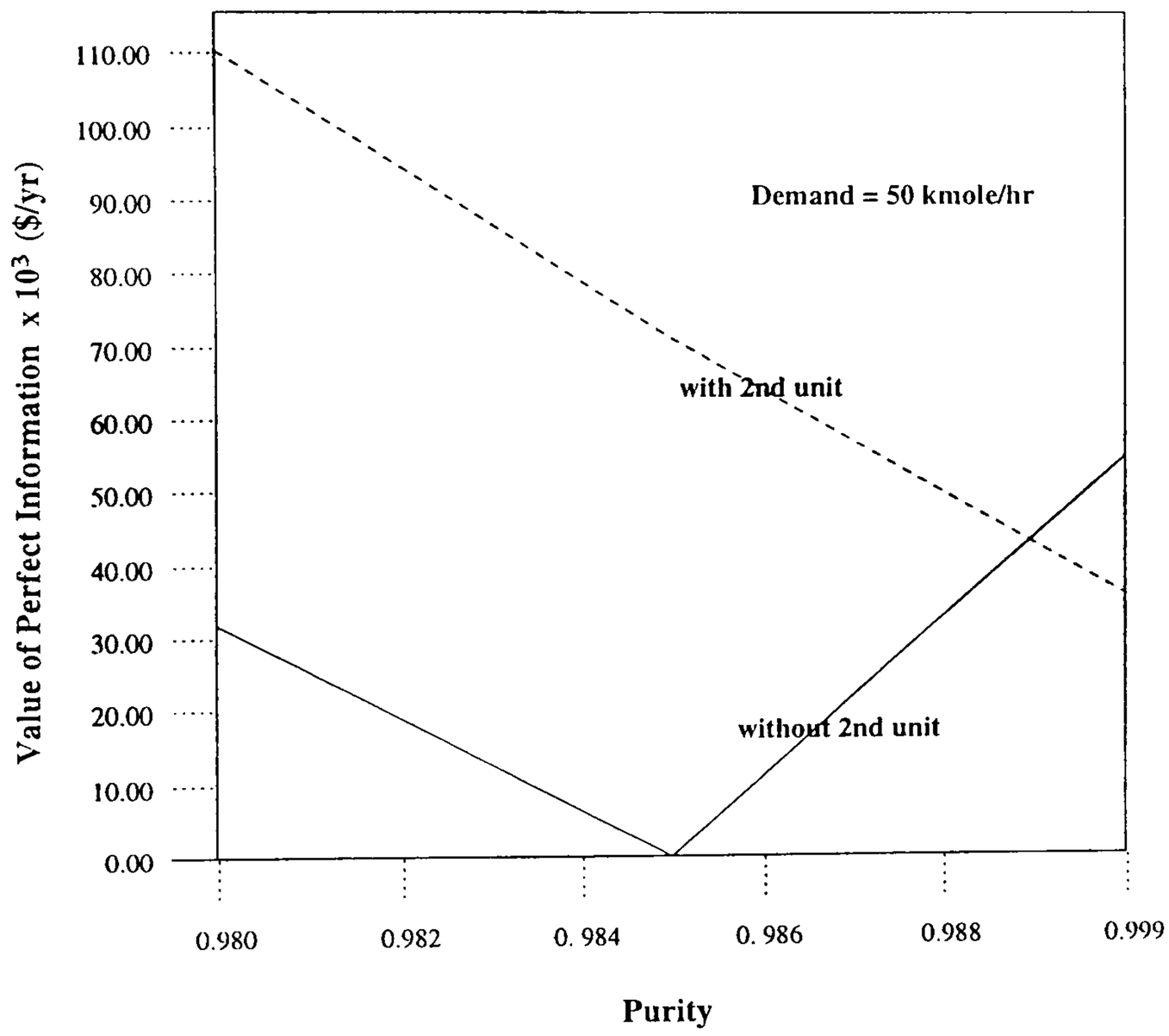


Figure 5.30: VPI results for a different plant in example 6 - the consideration of a second distillation column

Chapter 6

Conclusions and Future Directions

6.1. Conclusions

This thesis has been concerned with the aspects of uncertainty in process engineering problems. Issues related to uncertainty modelling, uncertain parameter classification, stochastic programming formulation as well as algorithmic developments have been considered.

In chapter 2, a unified framework was presented for the representation, mathematical formulation and solution of process engineering problems under uncertainty. In particular, modelling issues regarding uncertainty classification i.e. deterministic and stochastic uncertain parameters, and design objectives with respect to feasibility, i.e. fixed degree of flexibility - optimal degree of flexibility, were formally introduced within a comprehensive multiperiod/stochastic two-stage optimization formulation with the aim to determine a design/plan which maximizes an expected profit criterion at an optimal level of feasibility. A novel decomposition solution strategy was developed, featuring an iterative scheme involving the successive solution of feasibility subproblems, to depict the feasible region of operation in the space of uncertain parameters for a given set of design variables, profitability subproblems to approximate the profit function at the appropriate placed with the feasible region quadrature points and a master subproblem, specially constructed based on dual information of the feasibility and profitability subproblems, to return a new set of design variables. The algorithm was shown to be applicable to different types of problems, such as process synthesis/design under uncertainty, batch plant design/scheduling models, planning and capacity expansion formulations.

In chapter 3, batch plant design/scheduling models involving uncertainty in (i) processing times and size factors, reflecting process variability and model inaccuracy, and (ii) product demands, reflecting changing market conditions and/or variations of forecasted customer orders were studied in detail in view of the developments presented in chapter 2. A conceptual two-stage stochastic programming formulation is proposed with an objective function comprising investment costs, expected revenues from product sales and a penalty term accounting for expected losses due to unfilled orders. The formulation, featuring a relaxation of the feasibility requirement with respect to uncertain demand, conceptually allows for economic optimality and plant feasibility to be performed simultaneously. Furthermore, the exploitation of the special structure of the problem enables the transformation of the initial two-stage (embedded) stochastic formulation to a single optimization problem. It was shown that (i) the proposed formulation captures the various decision making policies towards demand satisfaction in a unified way, (ii) for the case of discrete equipment sizes and despite the use of general continuous probability distribution functions to describe the uncertainty, linearity of the model is preserved allowing detailed scheduling models to be included directly in the optimization model, and (iii) for the case of continuous equipment sizes, a careful exploitation of the model structure allows for the development of an efficient global optimization procedure based on the recent developments of global optimization solution approach presented by Floudas and Viswesvaran (1990, 1993).

In chapter 4, the problem of planning under uncertainty was addressed. Short term production planning with time horizon of few weeks or months as well as long-range planning including capacity expansion options were considered. Based on the postulation of general probability distribution functions describing process uncertainty (i.e. product demands and prices, raw material availabilities) a two-stage stochastic programming formulation was developed where the objective is to determine an optimal production plan (i.e. process utilization levels, purchases and sales of materials) and/or an optimal capacity expansion policy that maximize an expected profit while considering future plant feasibility. Along the lines of the approach presented in chapter 2, a decomposition based optimization approach was proposed, where planning decisions are taken by coupling economic optimality and plan feasibility without requiring an "a priori" discretization of the uncertainty. Results from the implementation of the proposed approach were presented in section 4.4. for a few example problems. Although the size of the examples is small they have been used to illustrate the proposed approach. The potential of using parallel

solution algorithms opens the possibility of dealing with much larger problems especially as the number of uncertain parameters is concerned, since the amount of additional computations for the introduction of one more uncertain parameter is considerable.

In chapter 5, the decision making process under uncertain environment was studied from the point of view of analyzing the potential decisions based on decision maker attitude towards risk. The value of perfect information (VPI) defined by the difference between the two alternative behavioral models of decision making under uncertainty, namely the *here-and-now* and the *wait-and-see* models was used to quantify the "price" of uncertainty or in other words to assess the amount, in economic grounds, that the decision maker is willing to pay to resolve some uncertainty. Very little work has been published in the chemical engineering community, mostly been focussed on analyzing different capacity expansion policies. In chapter 5, considerations of future plan feasibility, different attitudes towards risk, along with expected profit criteria were integrated in supporting the decision making of developing an optimal planning strategy. It was shown that the estimation of the VPI can be effectively incorporated within the planning framework presented in chapter 4. Combined metrics were also introduced to represent the relation between flexibility and the value of information in an attempt to quantify and access the importance of uncertainty in planning decisions. A number of example problems were discussed in detail in section 5.5 to illustrate some potential advantages of such an integrated approach to planning under uncertainty.

Summarizing, the major contributions of this thesis are the following:

1. The consideration of uncertain parameters in a unified multiperiod/stochastic two-stage programming formulation based on the uncertainty classification to deterministic and stochastic uncertain parameters, and design objectives with respect to feasibility, i.e. fixed degree of flexibility - optimal degree of flexibility.

2. The development of an efficient solution procedure for the resulting problem formulation featuring the following characteristics: (i) simultaneous consideration of economic optimality and plant feasibility, (ii) highly parallel structure enabling enhancement of computational performance, (iii) ability to deal with different process engineering problems under uncertainty.

3. The exploitation of the batch plant problem special structure and characteristics which enables (i) the representation of process uncertainty in a unified framework.

(ii) the transformation of the two-stage stochastic programming formulation to a single optimization problem and (iii) the efficient solution of the resulting formulation for the cases of continuous and discrete equipment sizes.

4. The derivation of flexible production plans and capacity expansion policies based on maximization of the expected profit.

5. The introduction of quantitative measures for the "price" of the uncertainty based on the concept of value of perfect information which provides the tools for accessing the decision maker's attitude towards risk and analyzing the effects of uncertainty in decision making process.

6.2. Recommendations for Future work

Based on the ideas suggested in this thesis and along the lines of the presented developments, a number of points have been raised that require further investigation and can lead to interesting extensions of this work.

From the modelling point of view:

(i) it is interesting to investigate the idea of feasibility relaxation for the case of multiproduct/multipurpose plants operating in continuous mode where the binary variables within the deterministic model lead to non-compact feasible regions. Preliminary results have been already obtained revealing similar behaviour with batch plants which enables the transformation of the two-stage stochastic formulation to a single optimization problem.

(ii) the two-stage stochastic model formulation was employed to incorporate uncertainty aspects based on the nature of the design/planning problem where having selected the first stage decision variables (design/plan) the objective of the second stage is to optimize system operation within the feasible region of the plant. However, different stochastic models have to be exploited to suit the needs of different problems - for example, chance-constraint programming could be suitable for the case when you have to meet the constraints within a specified probability as is the case in the design of telecommunication networks.

From the computational point of view:

(i) as it was discussed earlier, one drawback of the proposed approach is its potentially high computational requirements. Nevertheless, as it was pointed out in chapter 2

the algorithm features a highly distributed structure since most optimization tasks can be performed independently i.e. the feasibility problems of θ_2 after the determination of quadrature points at θ_1 and the profit maximization after the collocation of quadrature points within the feasible region. This calls for the use of parallel and distributed computing systems which will enable the efficient implementation of the proposed approaches in real large scale problems by improving its computational efficiency

(ii) since the computational effort for the proposed algorithmic procedure increases mainly with respect to the uncertain parameters, aggregation techniques based on sensitivity and behaviour analysis could be used to reduce either the number of uncertain parameters or the range of uncertain parameter variations based on the effect of uncertainty at the objective function. The results of section 5.5 suggest the VPI analysis as a tool to limit the uncertain parameter range.

Regarding global optimization analysis:

(i) the proposed approach guarantees global optimality for the case of convex models. However, nonconvex models are very often encountered in real life. Moreover, along the lines of chapter 3, the uncertainty incorporation often leads to the introduction of nonconvexities. For these cases the proposed approach can lead to local optimum. If one decides to pursue the optimization to locate the global solution, more efficient methods for updating the upper bound need to be employed following the ideas of the global optimization algorithm presented in chapter 3 for the case of batch plant design with continuous equipment sizes

(ii) based on the bilevel nature of the decision making procedure under uncertainty a different solution approach would be to develop global optimization algorithms by exploiting the special structure of bilevel problem. Some promising results have been obtained for the case of linear and quadratic programming problems (Visweswaran et al. 1995).

Finally, for the case of batch plant design and scheduling:

(i) modelling issues regarding the design/scheduling problem formulation especially in view of the level of aggregation with which scheduling is considered at the design stage,

(ii) decision policies in the precense of uncertain parameters, i.e. planning for a robust

schedule or consider schedule patterns to change with respect to uncertainty realization,

(iii) the reduction of the number of the uncertain parameters, based on the relative quantitative accessment of their impact on optimal decisions.

References

Beale, E.M.; Forrest, J.J.H.; Taylor, C.J. Multi-time-period Stochastic Programming, *Stochastic Programming*; Academic Press: New York, 1980.

Bienstock, D.; Shapiro, J. F. Optimizing Resource Acquisition Decisions by Stochastic Programming. *Manag. Sci.* **34**, 215, (1988).

Birge J. R., The Value of the Stochastic Solution in Stochastic Linear Programs with Fixed Recourse. *Math. Prog.* **24**, 314 (1982).

Birge J. R., Aggregation Bounds in Stochastic Linear Programming. *Math. Prog.* **25**, 31 (1985).

Birge J. R. and R. Wets, Sublinear Upper Bounds for Stochastic Programs with Recourse. *Math. Prog.* **43**, 131 (1989).

Birewar, D.B. and I.E. Grossmann, Incorporating Scheduling in the Optimal Design of Multiproduct Plants. *Comput. Chem. Engng.* **13**, 141 (1989).

Bloom, J. A. Solving an Electricity Generating Capacity Expansion Planning Problem by Generalized Benders Decomposition. *Oper. Res.*, **31**, 84, (1983).

Borison, A. B.; Morris, P. A.; Oren, S. S. A State-of-the World Decomposition Approach to Dynamics and Uncertainty in Electric Utility Generation Expansion Planning. *Oper. Res.* **32**, 1052, (1984).

Brauers, J.; Weber, M. A New Method of Scenario Analysis for Strategic Planning. *Jl. of Forecasting* **7**, 31-47, (1988).

Clay, R.L. and I.E. Grossmann, Optimization of Stochastic Planning Models Trans. IChemE, **72**, Part A (1994).

Dantzig G. B., Decomposition Techniques for Large-Scale Electric Power Systems Planning Under Uncertainty. *Annals of Operations Research* (1989).

Davis, M.H.A.; Dempster, M.H.A.; Sethi, S.P.; Vermes, D. Optimal Capacity Expansion Under Uncertainty. *Adv. Appl. Prob.* (1986).

Dempster, M.A.H., The expected value of Perfect Information in the Optimal Evolution of Stochastic Systems. *Stochastic differential systems* Proceedings of the 3rd IFIP-WG 7/1 Working Conference, Visegrad, Hungary (1980).

Edgar, T.F.; Himmelblau, D.M. *Optimization of Chemical Processes*; McGraw Hill: New York, 1988.

Faqir, N.M. and I.A. Karimi, Optimal Design of Batch Plants with Single Production Routes. *Ind. Eng. Chem. Res.*, **28**, 1191, (1989).

Faqir, N.M. and I.A. Karimi, Optimal Design of Batch Plants with Multiple Production Routes. *FOCAPD Proceedings*, Elsevier: Amsterdam, (1990).

Fichtner, G., H.J. Reinhart and D.W.T. Rippin, The Design of Flexible Chemical Plants by the Application of Interval Mathematics, *Comput. Chem. Engng.*, **14**, 1311, (1990).

Floudas, C.A. and I.E. Grossmann, Synthesis of Flexible Heat Exchanger Networks with Uncertain Flowrates and Temperatures. *Comput. chem. Engng.*, **11**, 319 (1987).

Floudas, C.A. and V. Visweswaran, A global optimization algorithm (GOP) for certain classes of nonconvex NLPs-I. Theory. *Comput. chem. Engng.*, **14**, 1379 (1990).

Floudas, C.A. and V. Visweswaran, Primal-Relaxed Dual Global Optimization Approach. J. Opt. Theory Applic., **2**, 187-225 (1993).

Friedman, Y.; Reklaitis, G.V. Flexible Solutions to Linear Programs under Uncertainty : Inequality Constraints. *AIChE Jl*, **21**, 77-83 (1975).

Geoffrion, A.M., Generalized Benders Decomposition. *J. Opt. Theory Applic.*,

10, 237 (1972).

Grigoriadis, M.D., A projective method for structured nonlinear programs. *Math. Prog.*, **1**, 321 (1971).

Grossmann I.E. and K.P. Halemane, Decomposition Strategy for Designing Flexible Chemical Plants. *AIChE Jl*, **28**, 686 (1982).

Grossmann, I.E. and C.A. Floudas, Active Constraint Strategy for Flexibility Analysis in Chemical Processes. *Comput. chem. Engng.*, **11**, 675-693 (1987).

Grossmann, I.E., K.P. Halemane and R.E. Swaney, Optimization Strategies for Flexible Chemical Processes. *Comput. chem. Engng.*, **7**, 439-462 (1983).

Grossmann, I.E. and R.W.H. Sargent, Optimum design of chemical plants with uncertain parameters. *AIChE Jl*, **24**, 1021-1028 (1978).

Grossmann, I.E. and D.A.Straub, Recent Developments in the Evaluation and Optimization of Flexible Chemical Processes. *Computer-Oriented Process Engineering* edited by L. Puigjaner and A. Espuña. Amsterdam (1991).

Halemane, K.P. and I.E. Grossmann, Optimal Process Design under Uncertainty. *AIChE Jl*, **29**, 425 (1983).

Himmelblau, D.M.; Bickel, T.C. Optimal Expansion of Hydrodesulfurization Process. *Comput. Chem. Engng.* **4**, 101, (1980).

Ierapetritou, M.G.; Pistikopoulos, E.N.; Floudas, C.A. Operational Planning Under Uncertainty. *Comput. Chem. Engng.* **18S**, S259, (1994a).

Ierapetritou, M.G. and E.N. Pistikopoulos, Simultaneous Incorporation of Flexibility and Economic risk in Operational Planning under Uncertainty. *Comput. chem. Engng.* **18**, 163-189 (1994b).

Ierapetritou, M.G. and E.N. Pistikopoulos, A Novel Optimization Approach of

Stochastic Planning Models. *Ind. Eng. Chem. Res.* (1994c).

Ierapetritou, M.G. and E.N. Pistikopoulos, Batch plant design and Operations under Uncertainty. Submitted for publication (1995).

Ierapetritou, M.G., J. Acevedo and E.N. Pistikopoulos, 1994. "An Optimization Approach for Process Engineering Problems Under Uncertainty" Submitted for publication.

Jimenez, A. G.; Rudd, D.F. Use of a recursive mixed-integer programming model to detect an optimal integration sequence for the Mexican petrochemical industry. *Comput. Chem. Engng.* **11**, 291, (1987).

Kubic, W.L. and F.P. Stein, A theory of design reliability using probability and fuzzy sets. *AIChE Jl*, **34**, 583 (1988).

Luss, H. Operations Research and Capacity Expansion Problems: A Survey. *Oper. Res.* **30**, 907 (1982).

Manne, A.S. Waiting for the Breeder. *Rev. Econ. Stud. (Symp.)*, 47-65 (1974).

Merkhofer, M.W., The Value of Information Given decision Flexibility. *Management Sci.* **23**, 716-727 (1977).

Modiano, E.M. Derived Demand and Capacity Planning Under Uncertainty. *Oper. Res.* **35**, 185-197 (1987).

Pai, C.C.D. and R.R. Hughes, Strategies for formulating and solving two-stage problems for process design under uncertainty. *Comput. chem. Engng.* **11**, 695-706 (1987).

Papageorgaki, S. and G.V. Reklaitis. Optimal Design of Multipurpose batch Plants 1. problem Formulation. *Ind. eng. Chem. Res.* **15**, 451, (1990).

Papalexandri K. and E.N. Pistikopoulos, An MINLP Retrofit Approach for Im-

proving the Flexibility of Heat Exchanger Networks. *Annals of Operations Research* **42**, (1993).

Paules, G.E. and C.A. Floudas, Stochastic Programming in Process Synthesis: A Two-Stage model with MINPL Recourse for Multiperiod Heat-Integrated Distillation sequences. *Comput. chem. Engng.*, **16**, 189-210 (1992).

Pereira M.V.F. and L.M.V.G. Pinto, Multi-stage stochastic optimization applied to energy planning. *Math. Prog.* **52**, 359-375 (1991).

Pistikopoulos, E.N. and M.G. Ierapetritou, A Novel Approach for Optimal Process Design Under Uncertainty. Accepted for publication *Comput. chem. Engng.* (1995).

Pistikopoulos, E.N. and I.E. Grossmann, Optimal Retrofit Design for Improving Process Flexibility in Linear Systems. *Comput. chem. Engng.* **12**, 719-731 (1988a).

Pistikopoulos, E.N. and I.E. Grossmann, Stochastic Optimization of Flexibility in Retrofit Design of Linear Systems. *Comput. chem. Engng.* **12**, 1215-1227 (1988b).

Pistikopoulos, E.N. and I.E. Grossmann, Optimal Retrofit Design for Improving Process Flexibility in nonlinear Systems: -I. Fixed degree of Flexibility. *Comput. chem. Engng.* **13**, 1003-1016 (1989a).

Pistikopoulos, E.N. and I.E. Grossmann, Optimal Retrofit Design for Improving Process Flexibility in nonlinear Systems: -II. Optimal Level of Flexibility. *Comput. chem. Engng.* **13**, 1087 (1989b).

Pistikopoulos, E.N. and T.A. Mazzuchi, A Novel Flexibility Analysis Approach for Processes with Stochastic Parameters. *Comput. chem. Engng.*, **14**, 991-1000 (1990).

Pistikopoulos, E.N. and T.V. Thomaidis, Towards a Design Framework for Flexibility, Reliability and Maintenance. Presented at AIChE Meeting, Miami Beach (1992).

Raiffa, H. Decision Analysis. Addison-Welsey, Reading, Mass (1968).

Reinhart, H.J. and D.W.T. Rippin, The design of flexible batch chemical plants. *Annual AIChE Mtg*, Paper No 50e, New Orleans (1986).

Reinhart, H.J. and D.W.T. Rippin, Design of flexible multi-product plants. A new procedure for optimal equipment sizing under uncertainty. *Annual AIChE Mtg*, Paper No 92f, Houston (1987).

Reklaitis, G.V. Progress and Issues in Computer-Aided Batch Process Design. FOCAPD Proceedings, Elsevier: New York (1990).

Rippin, D.W.T. Batch Process Systems Engineering: A Perspective and Prospective Review, *Comput. Chem. Engng.*, **17**, S1-S13, (1993).

Rotstein, G.E., R. Lavie and D.R. Lewin, Synthesis of Flexible and Reliable Short-Term batch production Plans. Submitted for publication (1994).

Saboo, A.K., M. Morari and D.C. Woodcock, Design of Resilient Processing Plants - VIII. A Resilience Index for Heat Exchanger Networks. *Chem. Engng Sci.* **40**, 1553-1565 (1983).

Sahinidis, N.V.; Grossmann, I.E.; Fornari, R.E; Chathrathi, M. Optimization Model for Long-Range Planning in Chemical Industry. *Comput. Chem. Engng.* **9**, 1049 (1989).

Sahinidis, N.V. and I.E. Grossmann, Convergence Properties of Generalized Benders Decomposition. *Comput. chem. Engng.*, **15**, 481, (1991).

Schmutzler, A. Flexibility and Adjustment to Information in Sequential Decision Problems: A Systematic Approach. Lectures Notes in Economics and Mathematical Systems, Springer-Verlag (1991).

Shah, N. and C.C.Pantelides, Optimal Long-Term Campaign Planning and Design of Batch Operations. *Ind. eng. Chem. Res.* **30**, 2308, (1991).

Shah, N. and C.C.Pantelides,Design of Multipurpose batch Plants with Uncer-

tain Production Requirements, *Ind. eng. Chem. Res.* **31**, 1325, (1992).

Shimizu, Y. Application of flexibility analysis for compromise solution in large-scale linear systems. *Jl of Chem. Engng of Japan*, **22**, 189-193, (1989).

Shimizu, Y.; Takamatsu, T. Application of mixed-integer linear programming in multiterm expansion planning under multiobjectives. *Comput. Chem. Engng.* **9**, 367, (1985).

Straub, D.A. and I.E. Grossmann, Integrated Stochastic Metric of Flexibility for systems with Discrete state and Continuous Parameter Uncertainties. *Comput. chem. Engng.* **9**, 967-985 (1990).

Straub, D.A. and I.E. Grossmann, Evaluation and optimization of stochastic flexibility in multiproduct batch plants. *Comput. chem. Engng.* **16**, 69 (1992).

Straub, D.A. and I.E. Grossmann, Design Optimization of Stochastic Flexibility. *Comput. Chem. Engng.*, **17**, 339 (1993).

Subrahmanyam, S., J.F. Pekny and G.V. Reklaitis, Design of Batch Chemical Plants under Market Uncertainty. *Ind. eng. Chem. Res.* **33**, 2688, (1994).

Suhami, I. and R.S.H Mah, Optimal Design of Multipurpose Batch Plants. *Ind. eng. Chem. Process. Des. Dev.* **21**, 94, (1982).

Swaney, R.E. and I.E. Grossmann, An Index for Operational Flexibility in Chemical Process Design - Part I : Formulation and Theory. *AIChE Jl* **31**, 621-630 (1985).

Varvarezos, D.K. I.E. Grossmann and L.T. Biegler, An Outer-Approximation method for Multiperiod Design Optimization. *Ind. Eng. Chem. Res.* **31**, 1466 (1992).

Vaselenak, J.A.; I.E. Grossmann and A.W. Westerberg, An Embedding Formulation for the Optimal Scheduling and Design of Multipurpose Batch Plants. *Ind. Chem. Res.* **26**, 139, (1987).

Visweswaran, V. and C.A. Floudas, A global optimization algorithm (GOP) for certain classes of nonconvex NLPs-II. Application of theory and test problems. *Comput. chem. Engng.*, **14**, 1419 (1990).

Visweswaran, V. and C.A. Floudas, New Properties and Computational Improvement of the GOP Algorithm for Problems with Quadratic Objective Functions and Constraints. J. Opt. Theory Applic., **3**, 439-462 (1993).

Voudouris, V.T. and I.E. Grossmann, Mixed-Integer Linear Programming Reformulations for Batch Process Design with Discrete Equipment Sizes. *Ind. Eng. Chem. Res.*, **31**, 1315 (1992).

Walkup, D.W. and R. Wets, Stochastic Programs with Recourse. *SIAM J. Appl. Math.* **14**, 1143 (1970).

Wallace S. W., A piecewise linear upper bound on the network recourse function. *Math. Prog.* **38**, 133 (1987).

Wellons, H.S.; Reklaitis, G.V. The design of multiproduct batch plants under uncertainty with staged expansion. *Comput. Chem. Engng.* , **13**, 115-126, (1989).

Additional References

Acevedo J.; Ierapetritou M. G.; Pistikopoulos E.N. Computational studies of Stochastic Optimization for Process Synthesis under Uncertainty. *Manuscript in preparation* (1995).

Barbosa-Póvoa A.P.; Macchietto S. Detailed Design of Multipurpose batch Plants. *Comput. chem. Engng.* **18**, 1013 (1994).

Carnahan, B.; Luther H.A.; Wilkes J.O. Applied Numerical Methods. New York: Wiley (1969).

Fathi-Afshar, S. The Analysis of Uncertainty in Hierarchical Planning Systems. *Technical Progress Report* (1987).

Gassmann H.I. MSLiP: A Computer Code for the Multistage Stochastic Linear Programming Problem. *Math. Prog.* **47**, 407 (1990).

Kokossis, A.C.; Floudas C.A. Synthesis of Isothermal Reactor-Separator-recycle Systems. *Chem. Eng. Sc.* **46**, 1361 (1991).

Lasserre, J.B.; Roubellat F. Measuring Decision Flexibility in Production Planning. *IEEE Trans. on Automatic Control* **30**, 447-452 (1985).

Lustig, I.J.; Mulrey J.M.; Carpenter T.J. Formulating Two-Stage Stochastic Programs for Interior point methods. *Oper. Res.* **39**, 757 (1991).

Picaseno-Gamiz, J. and G.R. Sullivan, An Optimization Strategy for Multiperiod Scheduling Problems. *AIChE annual Mtg*, Washington, (1988).

Pistikopoulos, E.N.;Mazzuchi T.A.; Van Rijn C.F. Flexibility, Reliability & Availability of manufacturing processes: a unified approach. *Comp. Appl. in Chem. Eng. Elsevier*, (1990).

Sahinidis, N.V.; Grossmann I.E. Reformulation of multiperiod MILP model for

planning and Scheduling of Chemical processes. *Comput. chem. Engng.* **15**, 255 (1991b).

Sahinidis, N.V.; Grossmann I.E. Reformulation of multiperiod MILP model for the capacity expansion of Chemical processes. *Oper. Res.* **40**, S127 (1992).

Shah N.; Pantelides C.C.; Sargent R.W.H. Optimal Periodic Scheduling of Multipurpose Batch Plants. *Ann. Oper. Res.* **42**, 193, (1993).

Wets, R.J.B. The Aggregation Principle in Scenario Analysis and Stochastic Optimization. *Technical report* Department of Mathematics, University of California (1988).

Appendix A

A.1. Equivalence of problems (2.10) and (2.11) for fixed design variables

By fixing the design variables d problems (B1) and $(B2^{q_1}, q_1 = 1, .., Q_1)$ can be solved independently resulting in the evaluation of the feasible region of design. The solution of (B1) and $(B2^{q_1})$ yields also the active constraints and their corresponding Lagrange multipliers. Consequently, the KKT conditions can be simplified as follows (shown here for (B1) problem):

$$\left.\begin{array}{l} f_{1A}^{U}(d, z(.), \theta_1^{U}, \theta_2(.)) = 0 \\ f_{1A}^{L}(d, z(.), \theta_1^{L}, \theta_2(.)) = 0 \end{array}\right\} \text{ Active Constraints}$$

$$\left.\begin{array}{l} f_{1I}^{U}(d, z(.), \theta_1^{U}, \theta_2(.)) < 0 \\ f_{1I}^{L}(d, z(.), \theta_1^{L}, \theta_2(.)) < 0 \end{array}\right\} \text{ Inactive Constraints}$$

$$\left.\begin{array}{l} -1 + \dfrac{\partial f_{1A}^{U}}{\partial \theta_1}\hat{\lambda}_{1A}^{U} = 0, \; -1 + \dfrac{\partial f_{1A}^{L}}{\partial \theta_1}\hat{\lambda}_{1A}^{L} = 0 \\ \dfrac{\partial f_{1A}^{U}}{\partial \theta_2}\hat{\lambda}_{1A}^{U} = 0, \; \dfrac{\partial f_{1A}^{L}}{\partial \theta_2}\hat{\lambda}_{1A}^{L} = 0 \\ \\ \dfrac{\partial f_{1A}^{U}}{\partial z}\hat{\lambda}_{1A}^{U} = 0, \; \dfrac{\partial f_{1A}^{L}}{\partial z}\hat{\lambda}_{1A}^{L} = 0 \end{array}\right\} \text{ Stationary Conditions}$$

which correspond to a square system of equations satisfied by $\hat{\lambda}_{1A}^{U}, \hat{\lambda}_{1A}^{L}$.

$$\left.\begin{array}{l} \hat{\lambda}_{1A}^{U} > 0, \; f_{1A}^{U}(d, z(.), \theta_1^{U}, \theta_2(.)) = 0 \\ \hat{\lambda}_{1A}^{L} > 0, \; f_{1A}^{U}(d, z(.), \theta_1^{L}, \theta_2(.)) = 0 \end{array}\right\} \text{ Complementarity Conditions for Active Constraints}$$

$$\left.\begin{array}{l}\hat{\lambda}_{1I}^{U}=0,\ f_{1I}^{U}(d,z(.),\theta_1^{U},\theta_2(.))>0\\ \hat{\lambda}_{1I}^{L}=0,\ f_{1I}^{U}(d,z(.),\theta_1^{L},\theta_2(.))>0\end{array}\right\}\ \begin{array}{l}\text{Complementarity}\\ \text{Conditions}\\ \text{for Inactive Constraints}\end{array}$$

The incorporation of the above simplified KKT conditions within problem (2.10) proves the equivalence between (2.10) and (2.11).

A.2. Correction Factors

A.2.1. Derivation of the Correction factors

For the derivation of correction factors the KKT conditions for problem (2.11) will be compared with those of problems (B1), ($B2^{q_1}$) and (PQ). The Lagrangian of problem (2.11) is given by equation (2.4). Similarly, the Lagrangians of problems (B1), ($B2^{q_1}$) and (PQ) are given by the following equations:

$$L^2=(\theta_1^U-\theta_1^L)-\hat{\lambda}_1^U f_1^U(d,z(.),\theta_1^U,\theta_2(.))-\hat{\lambda}_1^L f_1^L(d,z(.),\theta_1^L,\theta_2(.))$$
$$L^{3q_1}=(\theta_2^{Uq_1}-\theta_2^{Lq_1})-\hat{\lambda}_2^{Uq_1} f_2^{Uq_1}(d,z(.),\theta_1^{q_1},\theta_2^{Uq_1})-\hat{\lambda}_2^{Lq_1} f_2^{Lq_1}(d,z(.),\theta_1^{q_1},\theta_2^{Lq_1})$$
$$L^{4q_1q_2}=P(d,z^{q_1q_2},\theta_1^{q_1},\theta_2^{q_1q_2})-\hat{\eta}^{q_1q_2} f(d,z^{q_1q_2},\theta_1^{q_1},\theta_2^{q_1q_2})$$

The KKT conditions corresponding to L^1 are shown below:

$$\frac{\partial L^1}{\partial\theta_1^U}=\frac{1}{2}\sum_{q_1=1}^{Q_1}w_1^{q_1}\frac{\theta_2^{Uq_1}-\theta_2^{Lq_1}}{2}\sum_{q_2=1}^{Q_2}w_2^{q_2}\ P(d,z^{q_1q_2},\theta_1^{q_1},\theta_2^{q_1q_2})\ J(\theta_1^{q_1},\theta_2^{q_1q_2})$$
$$-\lambda_1^U\frac{\partial f_1^U}{\partial\theta_1^U}\ -\ \sum_{q_1=1}^{Q1}\mu_1^{q_1}\{(-0.5)(1+v_1^{q_1})\}=0 \qquad \text{(A.1)}$$

$$\frac{\partial L^1}{\partial\theta_1^L}=-\frac{1}{2}\sum_{q_1=1}^{Q_1}w_1^{q_1}\frac{\theta_2^{Uq_1}-\theta_2^{Lq_1}}{2}\sum_{q_2=1}^{Q_2}w_2^{q_2}\ P(d,z^{q_1q_2},\theta_1^{q_1},\theta_2^{q_1q_2})\ J(\theta_1^{q_1},\theta_2^{q_1q_2})$$
$$-\lambda_1^L\frac{\partial f_1^L}{\partial\theta_1^L}\ -\ \sum_{q_1=1}^{Q1}\mu_1^{q_1}\{(-0.5)(1-v_1^{q_1})\}=0 \qquad \text{(A.2)}$$

$$\frac{\partial L^1}{\partial\theta_1^{q_1}}=\frac{\theta_1^U-\theta_1^L}{2}w_1^{q_1}\frac{\theta_2^{Uq_1}-\theta_2^{Lq_1}}{2}\sum_{q_2=1}^{Q_2}w_2^{q_2}\ \frac{\partial PJ}{\partial\theta_1^{q_1}}$$
$$-\lambda_2^{Lq_1}\frac{\partial f_2^{Lq_1}}{\partial\theta_1^{q_1}}\ -\ \lambda_2^{Uq_1}\frac{\partial f_2^{Uq_1}}{\partial\theta_1^{q_1}}$$
$$-\sum_{q_2=1}^{Q2}\eta^{q_1q_2}\frac{\partial f}{\partial\theta_1^{q_1}}\ -\ \mu_1^{q_1}=0 \qquad \text{(A.3)}$$

$$\frac{\partial L^1}{\partial z^{q_1q_2}}=\frac{\theta_1^U-\theta_1^L}{2}w_1^{q_1}\frac{\theta_2^{Uq_1}-\theta_2^{Lq_1}}{2}w_2^{q_2}\ \frac{\partial PJ}{\partial z^{q_1q_2}}\ -\ \eta^{q_1q_2}\frac{\partial f}{\partial z^{q_1q_2}}=0 \qquad \text{(A.4)}$$

$$\frac{\partial L^1}{\partial \theta_2^{Lq_1}} = -\frac{\theta_1^U - \theta_1^L}{2} w_1^{q_1} \sum_{q_2=1}^{Q_2} w_2^{q_2}\ P(d, z^{q_1 q_2}, \theta_1^{q_1}, \theta_2^{q_1 q_2})\ J(\theta_1^{q_1}, \theta_2^{q_1 q_2})$$
$$- \lambda_2^{Lq_1} \frac{\partial f_2^{Lq_1}}{\partial \theta_2^{Lq_1}} - \sum_{q_2=1}^{Q2} \mu_2^{q_1 q_2} \{(-0.5)(1 - v_2^{q_2})\} = 0 \quad \text{(A.5)}$$

$$\frac{\partial L^1}{\partial \theta_2^{Uq_1}} = \frac{\theta_1^U - \theta_1^L}{2} w_1^{q_1} \sum_{q_2=1}^{Q_2} w_2^{q_2}\ P(d, z^{q_1 q_2}, \theta_1^{q_1}, \theta_2^{q_1 q_2})\ J(\theta_1^{q_1}, \theta_2^{q_1 q_2})$$
$$- \lambda_2^{Uq_1} \frac{\partial f_2^{Uq_1}}{\partial \theta_2^{Uq_1}} - \sum_{q_2=1}^{Q2} \mu_2^{q_1 q_2} \{(-0.5)(1 + v_2^{q_2})\} = 0 \quad \text{(A.6)}$$

$$\frac{\partial L^1}{\partial \theta_2^{q_1 q_2}} = \frac{\theta_1^U - \theta_1^L}{2} w_1^{q_1} \frac{\theta_2^{Uq_1} - \theta_2^{Lq_1}}{2} w_2^{q_2} \frac{\partial PJ}{\partial \theta_2^{q_1 q_2}} - \eta^{q_1 q_2} \frac{\partial f}{\partial \theta_2^{q_1 q_2}} - \mu_2^{q_1 q_2} = 0 \quad \text{(A.7)}$$

Similarly, for L^2, L^{3q_1} and $L^{4q_1 q_2}$ the following KKT conditions are required:

$$\frac{\partial L^2}{\partial \theta_1^U} = 1 - \hat{\lambda}_1^U \frac{\partial f_1^U}{\partial \theta_1^U} = 0 \quad \text{(A.8)}$$

$$\frac{\partial L^2}{\partial \theta_1^L} = -1 - \hat{\lambda}_1^L \frac{\partial f_1^L}{\partial \theta_1^L} = 0 \quad \text{(A.9)}$$

$$\frac{\partial L^{3q_1}}{\partial \theta_2^{Lq_1}} = -1 - \hat{\lambda}_2^{Lq_1} \frac{\partial f_2^{Lq_1}}{\partial \theta_2^{Lq_1}} = 0 \quad \text{(A.10)}$$

$$\frac{\partial L^{3q_1}}{\partial \theta_2^{Uq_1}} = 1 - \hat{\lambda}_2^{Uq_1} \frac{\partial f_2^{Uq_1}}{\partial \theta_2^{Uq_1}} = 0 \quad \text{(A.11)}$$

$$\frac{\partial L^{4q_1 q_2}}{\partial z^{q_1 q_2}} = \frac{\partial P(d, z^{q_1 q_2}, \theta_1^{q_1}, \theta_2^{q_1 q_2})}{\partial z^{q_1 q_2}} - \hat{\eta}^{q_1 q_2} \frac{\partial f}{\partial z^{q_1 q_2}} = 0 \quad \text{(A.12)}$$

By comparing equations A.1 with A.8 and A.2 with A.9 the correction factors CF_1^U and CF_1^L are determined such as :

$$\lambda_1^U = CF_1^U \hat{\lambda}_1^U, \quad \lambda_1^L = CF_1^L \hat{\lambda}_1^L$$

$$CF_1^U = \tfrac{1}{2} \sum_{q_1=1}^{Q_1} w_1^{q_1} \frac{\theta_2^{Uq_1} - \theta_2^{Lq_1}}{2} \sum_{q_2=1}^{Q_2} w_2^{q_2}\ P(d, z^{q_1 q_2}, \theta_1^{q_1}, \theta_2^{q_1 q_2})\ J(\theta_1^{q_1}, \theta_2^{q_1 q_2})$$
$$- \sum_{q_1=1}^{Q1} \mu_1^{q_1} \{(-0.5)(1 + v_1^{q_1})\}$$

$$CF_1^L = \tfrac{1}{2} \sum_{q_1=1}^{Q_1} w_1^{q_1} \frac{\theta_2^{Uq_1} - \theta_2^{Lq_1}}{2} \sum_{q_2=1}^{Q_2} w_2^{q_2}\ P(d, z^{q_1 q_2}, \theta_1^{q_1}, \theta_2^{q_1 q_2})\ J(\theta_1^{q_1}, \theta_2^{q_1 q_2})$$
$$+ \sum_{q_1=1}^{Q1} \mu_1^{q_1} \{(-0.5)(1 - v_1^{q_1})\}$$

These equations involve the multipliers $\mu_1^{q_1}$ of the equations defining the quadrature points $\theta_1^{q_1}$ that are not available from the solution of (B1). However, they can be determined from the solution of equation A.3 for $\mu_1^{q_1}$:

$$\mu_1^{q_1} = \frac{\theta_1^U - \theta_1^L}{2} w_1^{q_1} \frac{\theta_2^{Uq_1} - \theta_2^{Lq_1}}{2} \sum_{q_2=1}^{Q_2} w_2^{q_2} \frac{\partial PJ}{\partial \theta_1^{q_1}} - \lambda_2^{Lq_1} \frac{\partial f_2^{Lq_1}}{\partial \theta_1^{q_1}} - \lambda_2^{Uq_1} \frac{\partial f_2^{Uq_1}}{\partial \theta_1^{q_1}} - \sum_{q_2=1}^{Q2} \eta^{q_1 q_2} \frac{\partial f}{\partial \theta_1^{q_1}}$$

Similarly, by comparing equations A.5 with A.10 and A.6 with A.11 the correction factors $CF_2^{Uq_1}$ and $CF_2^{Lq_1}$ can be determined such as:

$$\lambda_2^{Uq_1} = CF_2^{Uq_1} \hat{\lambda}_2^{Uq_1}, \ \lambda_2^{Lq_1} = CF_2^{Lq_1} \hat{\lambda}_2^{Lq_1}$$

$$CF_2^{Uq_1} = \tfrac{1}{2} \tfrac{\theta_1^U - \theta_1^L}{2} w_1^{q_1} \sum_{q_2=1}^{Q_2} w_2^{q_2} \ P(d, z^{q_1 q_2}, \theta_1^{q_1}, \theta_2^{q_1 q_2}) \ J(\theta_1^{q_1}, \theta_2^{q_1 q_2}) - \sum_{q_2=1}^{Q2} \mu_2^{q_1 q_2} \{(-0.5)(1 + v_2^{q_2})\}$$

$$CF_2^{Lq_1} = \tfrac{1}{2} \tfrac{\theta_1^U - \theta_1^L}{2} w_1^{q_1} \sum_{q_2=1}^{Q_2} w_2^{q_2} \ P(d, z^{q_1 q_2}, \theta_1^{q_1}, \theta_2^{q_1 q_2}) \ J(\theta_1^{q_1}, \theta_2^{q_1 q_2}) + \sum_{q_2=1}^{Q2} \mu_2^{q_1 q_2} \{(-0.5)(1 - v_2^{q_2})\}$$

The multipliers $\mu_2^{q_1 q_2}$ are obtained from the solution of equation A.7:

$$\mu_2^{q_1 q_2} = \frac{\theta_1^U - \theta_1^L}{2} w_1^{q_1} \frac{\theta_2^{Uq_1} - \theta_2^{Lq_1}}{2} w_2^{q_2} \frac{\partial PJ}{\partial \theta_2^{q_1 q_2}} - \eta^{q_1 q_2} \frac{\partial f}{\partial \theta_2^{q_1 q_2}}$$

Finally, by comparing equations A.4 with A.12 and considering:

$$\frac{\partial JP}{\partial z^{q_1 q_2}} = J(\theta_1^{q_1}, \theta_2^{q_1 q_2}) \frac{\partial P}{\partial z^{q_1 q_2}}$$

the correction factors $CF^{q_1 q_2}$ are determined such as:

$$\eta^{q_1 q_2} = CF^{q_1 q_2} \hat{\eta}^{q_1 q_2}$$

$$CF^{q_1 q_2} = \frac{\theta_1^U - \theta_1^L}{2} w_1^{q_1} \frac{\theta_2^{Uq_1} - \theta_2^{Lq_1}}{2} w_2^{q_2} \ J(\theta_1^{q_1}, \theta_2^{q_1 q_2})$$

A.2.2. Generalized Correction Factors

Feasibility Subproblems

$$\mu_i^{q_1..q_i} = \prod_{j=1}^{i} \{ \frac{\theta_j^u - \theta_j^l}{2} w_j \} \frac{\theta_{i+1}^u - \theta_{i+1}^l}{2}$$

$$\sum_{q_{i+1}} w_{i+1} \frac{\theta_{i+2}^u - \theta_{i+2}^l}{2} \{ \sum_{q_{i+2}} w_{i+2} \frac{\theta_{i+3}^u - \theta_{i+3}^l}{2} ... \{ \sum_{q_{N_\theta - 1}} w_{N_\theta - 1} \frac{\theta_{N_\theta}^u - \theta_{N_\theta}^l}{2}$$

$$\{ \sum_{q_{N_\theta}} w_{N_\theta} \sum_{S} w^s \frac{\partial (P \cdot J)}{\partial \theta_i} \} ... \}$$

$$- \sum_{k=i+1}^{N_\theta} \{ \sum_{Q=\{q_{i+2}..q_k\}} \lambda_k^u \frac{\partial f^u}{\partial \theta_i} + \lambda_k^l \frac{\partial f^l}{\partial \theta_i} \} - \sum_{Q=\{q_{i+1}..q_{N_\theta}\}} \sum_{S} \eta \frac{\partial f}{\partial \theta_i}$$

$$CF_i^{q_1..q_{i-1}} = \frac{1}{2} \prod_{j=1}^{i-1} \{ \frac{\theta_j^u - \theta_j^l}{2} w_j \} \frac{\theta_i^u - \theta_i^l}{2}$$

$$\sum_{q_i} w_i \frac{\theta_{i+1}^u - \theta_{i+1}^l}{2} \{ \sum_{q_{i+2}} w_{i+1} \frac{\theta_{i+2}^u - \theta_{i+2}^l}{2} ... \{ \sum_{q_{N_\theta - 1}} w_{N_\theta - 1} \frac{\theta_{N_\theta}^u - \theta_{N_\theta}^l}{2}$$

$$\{ \sum_{q_{N_\theta}} w_{N_\theta} \sum_{S} PJ \} ... \}$$

$$CF_i^u = CF_i - \sum_{q_i} \mu_i \{ -0.5(1 + \nu_i) \}$$
$$CF_i^l = CF_i + \sum_{q_i} \mu_i \{ -0.5(1 - \nu_i) \}$$

$$\lambda_i^u = CF_i^u \ \hat{\lambda}_i^u$$

$$\lambda_i^l = CF_i^l \ \hat{\lambda}_i^l$$

where $\hat{\lambda}_i$ are the Lagrange multipliers from the feasibility subproblems ($i = 1..N_\theta$), and λ_i are the corrected multipliers to use in the master problem.

Profit Optimization Subproblems

$$CF^{qs} = \prod_{j=1}^{N_\theta} \{ \frac{\theta_j^u - \theta_j^l}{2} w_j \} \, J$$

$$\eta^{qs} = CF^{qs} \, \hat{\eta}^{qs}$$

where $\hat{\eta}$ are the Lagrange multipliers from the economic function optimization subproblems, and η are the corrected multipliers for the master problem.

A.3. Sign of multipliers in problem (2.11)

The Lagrangian of (2.11) is of the following form:

$$L^1 = EP(d) - \sum_{q_1=1}^{Q1} \sum_{q_2=1}^{Q2} \eta^{q_1 q_2} f(d, z^{q_1 q_2}, \theta_1^{q_1}, \theta_2^{q_1 q_2})$$

$$\begin{aligned}
&- \lambda_{1A}^U f_{1A}^U(d, z(.), \theta_1^U, \theta_2(.)) \\
&- \lambda_{1A}^L f_{1A}^L(d, z(.), \theta_1^L, \theta_2(.)) \\
&- \lambda_{1I}^U f_{1I}^U(d, z(.), \theta_1^U, \theta_2(.)) \\
&- \lambda_{1I}^L f_{1I}^L(d, z(.), \theta_1^L, \theta_2(.)) \\
&- \sum_{q_1=1}^{Q1} \lambda_{2A}^{Uq_1} f_{2A}^{Uq_1}(d, z(.), \theta_1^{q_1}, \theta_2^{Uq_1}) \\
&- \sum_{q_1=1}^{Q1} \lambda_{2A}^{Lq_1} f_{2A}^{Lq_1}(d, z(.), \theta_1^{q_1}, \theta_2^{Lq_1})
\end{aligned}$$

$$\begin{aligned}
&- \sum_{q_1=1}^{Q1} \lambda_{2I}^{Uq_1} f_{2I}^{Uq_1}(d, z(.), \theta_1^{q_1}, \theta_2^{Uq_1}) \\
&- \sum_{q_1=1}^{Q1} \lambda_{2I}^{Lq_1} f_{2I}^{Lq_1}(d, z(.), \theta_1^{q_1}, \theta_2^{Lq_1}) \\
&- \sum_{q_1=1}^{Q1} \mu_1^{q_1} \{ \theta_1^{q_1} - 0.5[\theta_1^U (1 + v_1^{q_1}) + \theta_1^L (1 - v_1^{q_1})] \} \\
&- \sum_{q_1=1}^{Q1} \sum_{q_2=1}^{Q2} \mu_2^{q_1 q_2} \{ \theta_2^{q_1 q_2} - 0.5[\theta_2^{Uq_1} (1 + v_2^{q_2}) + \theta_2^{Lq_1} (1 - v_2^{q_2})] \}
\end{aligned}$$

$\lambda_{1I}^U = 0, \ \lambda_{1I}^L = 0$ since they correspond to inactive constraints of problem (B1) (see Appendix A.1). Similarly, $\lambda_{2I}^{Uq_1} = 0, \ \lambda_{2I}^{Lq_1} = 0$:

$$\lambda_{1I}^U = CF_1^U \hat{\lambda}_{1I}^U, \ \ \hat{\lambda}_{1I}^U = 0$$

$$\lambda_{1I}^L = CF_1^L \hat{\lambda}_{1I}^L, \ \ \hat{\lambda}_{1I}^L = 0$$

$$\lambda_{2I}^{Lq_1} = CF_2^{Lq_1}\hat{\lambda}_{2I}^{Lq_1}, \;\; \hat{\lambda}_{2I}^{Lq_1} = 0$$

$$\lambda_{2I}^{Lq_1} = CF_2^{Lq_1}\hat{\lambda}_{2I}^{Lq_1}, \;\; \hat{\lambda}_{2I}^{Lq_1} = 0$$

λ_{1A}^{U}, λ_{1A}^{L}, $\lambda_{2A}^{Lq_1}$, $\lambda_{2A}^{Lq_1}$ have unrestricted sign since they correspond to equalities. If we define $\lambda_1^U = [\lambda_{1A}^U, \lambda_{1I}^U]$, $\lambda_2^{Uq_1} = [\lambda_{2A}^{Uq_1}, \lambda_{2I}^{Uq_1}]$ the proof has been completed.

A.4. Uncertain prices

Property: Consider a profit function P(d,z,θ_s) of the following form:

$$P(d, z, \theta_s) = b^T\theta_s'' + P_0(d, z, \theta_s')$$

Then:

$$E_{\theta_s \in \mathbf{R}(d)}\{\max_z P(d, z, \theta_s)\} = \int_{\theta_s'} \max_z [P_0(d, z, \theta_s')] J(\theta_s') d\theta_s' + b^T E\{\theta_s''\} \int_{\theta_s'} J(\theta_s') d\theta_s'$$

where $\theta_s = (\theta_s' \bigcup \theta_s'')$.

Proof: The expectancy of the optimal economic function is evaluated through the following integral:

$$E_{\theta_s \in \mathbf{R}(d)}\{\max_z P(d, z, \theta_s)\} = \int_{\theta_s \in \mathbf{R}(d)} \max_z (P_0(d, z, \theta_s') + b^T\theta_s'') J(\theta_s) d\theta_s$$

The constant terms can be moved outside the maximization:

$$\int_{\theta_s} \max_z [P_0(d, z, \theta_s')] J(\theta_s) d\theta_s + \int_{\theta_s} b^T\theta_s'' J(\theta_s) d\theta_s$$

For statistically independent parameters, the integrals can be considered separately as follows:

$$\int_{\theta_s'} \int_{\theta_s''} \max_z [P_0(d, z, \theta_s')] J(\theta_s') J(\theta_s'') d\theta_s' \, d\theta_s'' + \int_{\theta_s'} \int_{\theta_s''} b^T\theta_s'' J(\theta_s') J(\theta_s'') d\theta_s' \, d\theta_s''$$

The first integral can be reformulated as:

$$\int_{\theta_s'} \max_z [P_0(d, z, \theta_s')] J(\theta_s') \{\int_{\theta_s''} J(\theta_s'') d\theta_s''\} \, d\theta_s'$$

and since the cost coefficient does not affect the feasible region, the inner integration is evaluated in the whole space of θ_s'' and is equal to 1.

The second integral, can also be simplified as:

$$\int_{\theta'_s} b^T \{ \int_{\theta''_s} \theta''_s J(\theta''_s) d\theta''_s \} J(\theta'_s) d(\theta'_s) = \int_{\theta'_s} b^T E\{\theta''_s\} J(\theta'_s) d\theta'_s$$

As a result:

$$\int_{\theta'_s} \max_z [P_0(d, z, \theta'_s)] J(\theta'_s) d\theta'_s + \int_{\theta'_s} b^T E\{\theta''_s\} J(\theta'_s) d\theta'_s$$
$$= \int_{\theta'_s} \max_z [P_0(d, z, \theta'_s)] J(\theta'_s) d\theta'_s + b^T E\{\theta''_s\} \int_{\theta'_s} J(\theta'_s) d\theta'_s$$

where $E\{\theta''_s\}$ is the expected value of this coefficient, reducing the degree of the integral and therefore the number of subproblems to be solved.

Appendix B

B.1. Capacity Expansion Consideration

The formulation of problem (3.1) can be extended to account for long-term demand variations by incorporating the possibility of capacity expansion possibility through the consideration of additional identical units operating out of phase which results in the following formulation (see also Wellons and Reklaitis, 1992):

$$\max_{V_j, N_j^1, N_j^2} \{ -\delta \sum_{j=1}^{M} N_j^1 \alpha_j V_j^{\beta_j} - \delta \exp(-rH^1) \sum_{j=1}^{M} (N_j^2 - N_j^1) \alpha_j V_j^{\beta_j}$$
$$+ \sum_{p=1}^{P} w^p \sum_{q_1=1}^{Q_1} w^{q_1} J^{q_1} \sum_{i=1}^{N} p_i Q_i^{1q_1} + \sum_{p=1}^{P} w^p \sum_{q_2=1}^{Q_2} w^{q_2} J^{q_2} \sum_{i=1}^{N} p_i Q_i^{2q_2}$$
$$- \gamma \sum_{p=1}^{P} w^p \sum_{q_1=1}^{Q_1} w^{q_1} J^{q_1} \sum_{i=1}^{N} (p_i \theta_i^{1q_1} - p_i Q_i^{1q_1}) - \gamma \sum_{p=1}^{P} w^p \sum_{q_2=1}^{Q_2} w^{q_2} J^{q_2} \sum_{i=1}^{N} (p_i \theta_i^{2q_2} - p_i Q_i^{2q_2})$$

subject to:
$$B_i \leq \frac{V_j}{S_{ij}^p} \; ; \; \forall i, j, p$$
$$T_{Li}^{1p} \geq \frac{t_{ij}^p}{N_j^1} \; ; \; \forall i, j, p$$
$$T_{Li}^{2p} \geq \frac{t_{ij}^p}{N_j^2} \; ; \; \forall i, j, p$$
$$\sum_{i=1}^{N} \frac{Q_i^{1q_1 p} T_{Li}^{1p}}{B_i} \leq H^1 \; ; \; \forall p$$
$$\sum_{i=1}^{N} \frac{Q_i^{2q_2 p} T_{Li}^{2p}}{B_i} \leq H^2 \; ; \; \forall p$$
$$Q_i^{1q_1 p} \leq \theta_i^{1q_1} \; ; \; \forall i, p, q_1$$
$$Q_i^{2q_2 p} \leq \theta_i^{2q_2} \; ; \; \forall i, p, q_2$$
$$V_j^{LO} \leq V_j \leq V_j^{UP}$$

In the above formulation the time horizon of plant operation is divided by the time where additional units $(N_j^2 - N_j^1)$ are used at each stage j to lower limiting cycle time and consequently to increase plant production. The objective function is augmented to incorporate the investment cost of capacity expansion where r is the interest rate used to calculate the present worth.

B.2. Evaluation of critical value of γ

Consider the design of multiproduct batch plant after the exponential transformations proposed by Kocis and Grossmann, 1988, problem (3.3) for the case of of two products i=1,2 produced in 2 stages where specific values of demand are considered:

$$\max_{v_j, Q_i} \{-\delta \sum_{j=1}^{2} \alpha_j \exp(\beta_j v_j) + \{\sum_{i=1}^{2} p_i Q_i\} - \gamma(\sum_{i=1}^{2} p_i \theta_i - \sum_{i=1}^{2} p_i Q_i)\}$$

$$\text{subject to:} \quad v_j \geq \ln(S_{ij}) + b_i \; ; \; i = 1,2, \; j = 1,2$$

$$\sum_{i=1}^{2} Q_i T_{Li} \exp(-b_i) \leq H$$

$$Q_i \leq \theta_i \; ; \; i = 1,2$$

$$\ln(V_j^{LO}) \leq v_j \leq \ln(V_j^{UP})$$

$$\theta_i \in T(\theta), \; \gamma \geq 0$$

The KKT optimality conditions of this problem are:

$$\alpha_1 \beta_1 \exp(\beta_1 v_1) - n_{11} - n_{21} = 0 \tag{B.1}$$

$$\alpha_2 \beta_2 \exp(\beta_2 v_2) - n_{12} - n_{22} = 0 \tag{B.2}$$

$$-\lambda Q_1 T_{L1} \exp(-b_1) + n_{11} + n_{12} = 0 \tag{B.3}$$

$$-\lambda Q_2 T_{L2} \exp(-b_2) + n_{21} + n_{22} = 0 \tag{B.4}$$

$$-(\gamma + 1) p_1 + \lambda T_{L1} \exp(-b_1) + \mu_1 = 0 \tag{B.5}$$

$$-(\gamma + 1) p_2 + \lambda T_{L2} \exp(-b_2) + \mu_2 = 0 \tag{B.6}$$

where λ is the lagrange multiplier for the horizon constraint; μ_1, μ_2 are the lagrange multipliers for the demand constraints; n_{11}, n_{12} and n_{21}, n_{22} are the lagrange multipliers for the constraints $v_j \geq \ln(S_{ij}) + b_i$ for product 1 and 2, respectively.

By adding together (B.1), (B.2), (B.3) and (B.4) we end up to the following expression for λ:

$$\lambda = \frac{\alpha_1 \beta_1 \exp(\beta_1 v_1) + \alpha_2 \beta_2 \exp(\beta_2 v_2)}{Q_1 T_{L1} \exp(-b_1) + Q_2 T_{L2} \exp(-b_2)} \tag{B.7}$$

Consider now the multiperiod formulation of the same problem:

$$\max_{v_j,Q_i}\{-\delta\sum_{j=1}^{2}\alpha_j\exp(\beta_j v_j)+\sum_{i=1}^{2}p_iQ_i\}$$

$$\begin{aligned}\text{subject to: }\ & v_j \geq \ln(S_{ij})+b_i\ ;\ i=1,2,\ j=1,2\\ & \sum_{i=1}^{2}Q_iT_{Li}\exp(-b_i)\leq H\\ & Q_i=\theta_i\ ;\ i=1,2\\ & \ln(V_j^{LO})\leq v_j\leq\ln(V_j^{UP})\\ & \theta_i\in T(\theta),\ \gamma\geq 0\end{aligned}$$

The KKT optimality conditions of this problem are:

$$\alpha_1\beta_1\exp(\beta_1v_1)-n'_{11}-n'_{21}=0 \tag{B.8}$$

$$\alpha_2\beta_2\exp(\beta_2v_2)-n'_{12}-n'_{22}=0 \tag{B.9}$$

$$-\lambda'Q_1T_{L1}\exp(-b_1)+n'_{11}+n'_{12}=0 \tag{B.10}$$

$$-\lambda'Q_2T_{L2}\exp(-b_2)+n'_{21}+n'_{22}=0 \tag{B.11}$$

$$-p_1+\lambda'T_{L1}\exp(-b_1)+\mu'_1=0 \tag{B.12}$$

$$-p_2+\lambda'T_{L2}\exp(-b_2)+\mu'_2=0 \tag{B.13}$$

where λ' is the lagrange multiplier for the horizon constraint; μ'_1,μ'_2 are the lagrange multipliers for the demand constraints; n'_{11},n'_{12} and n'_{21},n'_{22} are the lagrange multipliers for the constraints $v_j\geq\ln(S_{ij})+b_i$ for product 1 and 2, respectively.
By adding (B.8), (B.9), (B.10) and (B.11) we obtain the following expression for λ':

$$\lambda'=\frac{\alpha_1\beta_1\exp(\beta_1v_1)+\alpha_2\beta_2\exp(\beta_2v_2)}{Q_1T_{L1}\exp(-b_1)+Q_2T_{L2}\exp(-b_2)} \tag{B.14}$$

Comparing (B.7) with (B.14) we result in $\lambda'=\lambda$ for the critical value of γ (γ^c) since for this value of γ the solution of both formulations coincides. By comparing also (B.5) with (B.12) and (B.6) with (B.13) we obtain the critical value γ^c:

$$\gamma^c=\frac{-\mu'_1+\mu_1}{p_1}=\frac{-\mu'_2+\mu_2}{p_2}$$

B.3. Feasibility property for Multiproduct Batch plant operating in Single Product Campaign

B.3.1. V_j continuous

Problem formulation is as follows:

$$\max_{V_j,N_j,Q_i} \sum_i p_i Q_i - \delta \sum_j N_j a_j V_j^{\beta_j}$$

$$s.t. \quad \sum_i \frac{Q_i T_{Li}}{B_i} \leq H$$

$$T_{Li} \geq (\frac{t_{ij}}{N_j}) \; ; \; \forall i,j$$

$$B_i \leq \frac{V_j}{S_{ij}} \; ; \; \forall i,j$$

$$Q_i \leq \theta_i \; ; \; \forall i$$

Property- Any design (V_j, N_j) satisfying design constraints above for fixed product demands θ_i, i=1,..,N, is always feasible.

Proof- The feasibility test problem - with fixed V_j, N_j and θ_i - is:

$$\begin{aligned} &\min_{u,Q_i} u \\ s.t. \; &\sum_{i=1}^{N} \frac{Q_i}{B_i} T_{Li} - H \leq u \\ &Q_i - \theta_i \leq u \\ &-Q_i \leq u \end{aligned}$$

The KKT conditions of the above problem are:

$$\lambda \frac{T_{Li}}{B_i} + \mu_i^1 - \mu_i^2 = 0 \quad i = 1,..,N \tag{B.15}$$

$$\lambda + \sum_{i=1}^{N} \mu_i^1 + \sum_{i=1}^{N} \mu_i^2 = 1 \tag{B.16}$$

where λ is the Lagrange multiplier of the production constraint; μ_i^1, μ_i^2 are the Lagrange multipliers for the bounding constraints of production Q_i of product i.

Since there are N control variables Q_i the number of active constraints must be less than or equal to N+1. From the KKT conditions (B.15), (B.16) it can be easily

identified that the only potential active set consists of the production constraint and the lower bounds of production rates, which results in the following always negative feasibility function:

$$u = -\lambda H \leq 0 \; \forall \; \theta_i$$

This permanent feasibility implies that the feasible region of batch plant (in the space of uncertain parameters) coincides with the considered range of uncertain parameters independently of the design.

B.3.2. V_j discrete

In this case the problem formulation is as follows:

$$\max_{y_{jsn}, Q_i} \sum_i p_i Q_i - \delta \sum_j \sum_s \sum_n n a_j v_{js}^{\beta_j} y_{jsn}$$

$$s.t. \;\; n_i \geq \sum_s \sum_n \frac{Q_i S_{ij}}{v_{js}} y_{jsn} \; \forall i, j$$

$$T_i \geq \sum \sum (\frac{t_{ij}}{n}) n_i y_{jsn} \; \forall i, j$$

$$\sum_s \sum_n y_{jsn} = 1 \; \forall i, j$$

$$\sum_i T_i \leq H$$

$$Q_i \leq \theta_i \; \forall i$$

Property- Any design (y^*_{jsn}) satisfying design constraints above for fixed product demands θ_i, i=1,..,N, is always feasible.

Proof- The feasibility test problem - with fixed y^*_{jsn} and θ_i - is:

$$\min u$$

$$s.t. \quad \sum_s \sum_n \frac{Q_i S_{ij}}{v_{js}} y^*_{jsn} - n_i \leq u \; \forall i, j \tag{B.17}$$

$$\sum_s \sum_n (\frac{t_{ij}}{n}) n_i y^*_{jsn} - T_i \leq u \; \forall i, j \tag{B.18}$$

$$\sum_i T_i - H \leq u \tag{B.19}$$

$$Q_i - \theta_i \leq u \; \forall i \tag{B.20}$$

$$-Q_i \leq u \; \forall i \tag{B.21}$$

with the following KKT optimality conditions:

$$\sum_i \sum_j \lambda_{ij} + \sum_i \sum_j \mu_{ij} + \nu + \sum_i k_{i1} + \sum_i k_{i2} = 1 \tag{B.22}$$

$$\sum_j \sum_s \sum_n (\frac{S_{ij}}{v_{js}}) y^*_{jsn} \lambda_{ij} + k_{i1} - k_{i2} = 0 \;\; \forall i \tag{B.23}$$

$$-\sum_j \lambda_{ij} + \sum_j \sum_s \sum_n (\frac{S_{ij}}{v_{js}}) y^*_{jsn} \mu_{ij} = 0 \;\; \forall i \tag{B.24}$$

$$-\sum_j \mu_{ij} + \nu = 0 \;\; \forall i \tag{B.25}$$

where λ_{ij} are the Lagrange multiplier of the (B.17) constraints; μ_{ij}, are the Lagrange multipliers for the (B.18) constraints; ν is the Lagrange multiplier of the (B.19) constraint and k_{i1}, k_{i2} are the Lagrange multipliers for the bounding constraints of production Q_i of product i (B.20) and (B.21).

Since there are 3*N control variables $Q_i, n_i, T_i, i = 1, ..., N$ where N is the number of products, the number of active constraints must be less than or equal to 3*N+1. From the KKT conditions (B.25) it can be identified that (B.19) as well as (B.18) one $\forall i$ must be active. Following this result (B.24) suggests that also one (B.17) $\forall i$ must be active which in turn points out that from (B.23) that the lower bounding constraint for production of product i must be active. As constraint (B.20) is not included in the active set, it can be easily shown through some algebraic manipulations that we always get a negative feasibility function.

B.4. Steps of Global Optimization Algorithm

The global optimization algorithm of Figure 3.3 is implemented here for the example 2 of section 3.5. Consider as a starting point (V_1, V_2, V_3) = (3000,4500,4500).

Iteration 1

The solution of problem (P2) has an objective function of 146.7 units and provides a first upper bound on the global optimum. The Lagrange multipliers for the production constraints μ^q are all equal to zero resulting in zero Lagrange function gradient with respect to Q_i^q. Hence, it is only necessary to solve one RD problem with Q_i^q at either its

upper or lower bounds. The solution of this problem is (V_1, V_2, V_3) = (500,500,500), with a value of the objective function of -1394.5 units which is a first lower bound to the global optimum. The fixed value of y for the second iteration is (V_1, V_2, V_3) = (500,500,500).

Iteration 2

For (V_1, V_2, V_3) = (500,500,500) the solution of the primal problem yields a value of 297.3 units (no update of the upper bound). Since the qualifying constraints are $b_1 - b_1^L$, $b_2 - b_2^L$ which are greater or equal to zero for any (b_1, b_2), only one RD problem is also required at this iteration with Q_i^q at its upper bounds. The Lagrange function from the first iteration is also added in the current relaxed dual problem since the qualifying constraints for this Lagrange function are zero for any (b_1, b_2). The solution of the relaxed dual problem yields the design (V_1, V_2, V_3) = (883.7,1325.5,1767.4), with an objective value of -569.2 units which corresponds to a new lower bound. The fixed design for the next iteration is (V_1, V_2, V_3) = (883.7,1325.5,1767.4).

Iteration 3

The solution of the primal problem yields an expected profit of 20.2 units, which provides a new upper bound to the global optimum, and the corresponding Lagrange multipliers which are all nonzero. Four relaxed dual problems are then solved, for the combinations of bounds $(Q_1^{q_1}, Q_2^{q_1 q_2})$ equal to (0,0), $(\theta_1^{q_1}, 0)$, $(\theta_1^{q_1}, \theta_2^{q_1 q_2})$ and $(0, \theta_2^{q_1 q_2})$. Since the qualifying constraints of Lagrange functions from the first and second iterations are satisfied for every (b_1, b_2), they are both added in the relaxed dual problem. The solutions of the four relaxed problems are summarized in Table B.1. At the end of this iteration these four solutions are stored from which the design (V_1, V_2, V_3) = (500, 703.4, 937.8) with the smaller objective is selected for the next iteration.

Relaxed Dual	Combination of $(Q_1^{q_1}, Q_2^{q_1 q_2})$ bounds	Optimal Design (V_1, V_2, V_3)	Objective function
1	(0,0)	(1800,2700,3600)	-317.1
2	$(\theta_1^{q_1}, 0)$	(1298, 1948, 2597)	-85.4
3	$(\theta_1^{q_1}, \theta_2^{q_1 q_2})$	(500, 703.4, 937.8)	-323
4	$(0, \theta_2^{q_1 q_2})$	(1276.7, 1915.1, 957.5)	-53.8

Table B.1: Solutions of the Relaxed Dual Problems - Example 2

The algorithm requires 14 iterations to converge to the global optimum design

(V_1, V_2, V_3) = (1800, 2700, 3600) with an expected profit equal to 298.5 units (within a tolerance limit ϵ=0.0002). The computational results for the application of GOP from four different starting points with $\gamma = 0$ and considering a 5×5 quadrature grid are summarized in Table B.2.

Starting Design (V_1, V_2, V_3)	Number of Iterations	CPU s per iteration
(1000, 1000, 1000)	13	0.8
(3000, 4500, 4500)	14	0.8
(4500, 4500, 4500)	14	0.8
(500, 500, 500)	15	0.8

Table B.2: Results of GOP application - Example 2

Appendix C

C.1. Solution of Multi-Parametric LP problems

Consider the multi-parametric LP problem of the following form:

Problem (MLP)

$$\begin{aligned} \max_x \ & (c^0 + H\theta)^T x \\ s.t. \ & Ax = b^0 + F\theta \\ & x \geq 0 \\ & \theta \text{ vector parameter of length l} \end{aligned}$$

The following procedure is proposed by Gal and Nedoma, (1972) for the solution of problem (MLP).

Step 1: Solve the linear programming problem at the nominal point of the uncertain parameters (correspond to the expected values)

Step 2: From the information obtained by solving this problem (basis B) and the following equations, obtain the region where this basis remains optimal together with the expression of variables and objective as functions of θ.

$$\begin{aligned} b^0_{new} &= B^{-1} b^0_{old} \\ F_{new} &= B^{-1} F_{old} \\ c^0_{new} &= c^0_{old} B^{-1} \\ H_{new} &= H_{old} B^{-1} \end{aligned}$$

The region where B remains optimal is defined through the following equations that correspond to primal and dual feasibility, respectively:

$$b^0_{new} + F_{new}\theta \geq 0$$
$$c^0_{new} + H_{new}\theta \geq 0$$

Step 3: Find the neighbour regions, as follows:

3.1. Formulate the auxiliary problems (A1) and (A2) for all the rows i that satisfy the following constraints:
(i) $F_{i,j} \neq 0$ for at least one j, j=1,..,l
(ii) $a_{i,j} \leq 0$ for at least one j, j=1,..,n
and for all columns j that satisfy the constraints:
(i) $H_{i,j} \neq 0$ for at least one i, i=1,..,l
(ii) $a_{i,j} \geq 0$ for at least one i, i=1,..,m

$$-H\theta + \xi_1 = c^0_{new} \qquad (C.1)$$
$$-F\theta + \xi_2 = b^0_{new} \qquad (C.2)$$

where $\xi_1, \xi_2 \geq 0$ vectors with length $n' \leq n$ and $m' \leq m$, respectively. Determine succesively:

$$\begin{aligned} &\min \ \xi_i \\ &s.t. \ (C.1), \ (C.2) \end{aligned}$$

3.2. For these rows and columns with min $\xi_i = 0$ find pivot elements according to the dual or primal simplex rules respectively:
* for rows with min $\xi_i = 0$ the pivot elements are determined from the minimization of $\Delta c_j(\theta)/|a_{ij}|$, j=1,..,n (Dual Step)
* for columns with min $\xi_i = 0$ the pivot elements are determined from the minimization of$\Delta b_i(\theta)/a_{ij}$, i=1,..,m (Primal Step)

3.3. Without performing the appropriate dual or primal step determine the neighbour basis. If there is no new basis to be examined the procedure terminates, otherwise go to step 4.

Step 4: Choose one of the bases determined previously and pass to the corresponding neighbor by a dual or primal step. Return to step 2.

The above algorithm can be extended for the case when uncertainty is also involved in some elements of the matrix A, (i.e. the yields of some processes have to be considered to vary inside specified ranges). This is however, a much more computationally expensive task, which may result in a discontinuous optimal solution. The basic difference of this case is that the θ region, (K), for which the given problem has an optimal solution is not necessarily connected and that the objective $z_{max}(\theta)$ is not necessarily continuous over K.

Consider the following parametric LP problem with the elements a_{ij} of A depending on a vector of parameters θ.

$$\max z(\theta) = c^T x$$
$$s.t.\ \ A(\theta)x = b$$
$$\theta \epsilon T$$
$$x \geq 0$$

Steps 1 and 2 are the same in this case with the only difference that here the B^{-1} matrix depends also upon θ and its elements β_{ij} have to be determined through the following general formula (Bodewig's formula):

$$(B + pq^T)^{-1} = B^{-1} - \frac{B^{-1}pq^T B^{-1}}{1 + q^T B^{-1} p}$$

where p, q ϵ R^m are vectors.

After the expressions of $\beta_{ij}(\theta)$ have beeen determined the vectors $b(\theta)$, $\Delta c(\theta)$ can be found from:

$$b(\theta) = B^{-1}(\theta)b$$
$$\Delta c_j(\theta) = c_B^T B^{-1}(\theta) - c_j$$

The conditions :

$$b_i(\theta) \geq 0 \ \text{ for all i in basis B}$$
$$\Delta c_j(\theta) \geq 0 \ \text{ for all j not in basis B}$$

define the region [θ', θ''] where B remains optimal and correspond to primal and dual feasibility respectively.

The neighbour region is now to be determined. Setting θ'' into $b_i(\theta)$, $\Delta c_j(\theta)$ for at least one i $b_i(\theta) = 0$ or for at least one j $\Delta c_j(\theta) = 0$. Let's examine the first of the previous possibilities where one has to apply dual step to pass to a neighbour region. For this, at least one negative element must exist in ith row. If there is, then use this as a pivot element to pass to a neighbour region. If however, $\beta_{ij} \geq 0$ for all j then there is no optimal neighbour. In such a case the range of θ at which $\beta_{ij} \leq 0$ for at least one j has to be determined. The dual step then will lead to a new basis to be examined for the optimality. Analyzing the elements of this new tableau a critical element results with $b_i(\theta) \leq 0$ or with $\Delta c_j(\theta) \leq 0$ for some θ say $\theta \geq a$. If there is $b_i(\theta) \leq 0$ for $\theta \geq a$ and $\beta_{ij} \leq 0$ for $\theta \epsilon [d, e]$ and $[a, \infty) \bigcap [d, e] \neq \emptyset$, then pass to the next tableau in which either there exists

an interval for θ such that the solution is optimal or a similar analysis is performed until an optimal tableau is reached or there is no optimal solution for $\theta \geq \theta''$.

C.2. Evaluation of VPI function

The solution of the two multi-parametric linear problems (F1), (F2) results in analytical expressions of F_1, F_2 as a function of the vector of the uncertain parameters θ (for a fixed plan $\bar{x}_1$). These expressions, however, have different forms with respect to θ at different θ regions (reflecting the changes in basis). To model this, binary 0-1 variables, $\delta_{F_1,i}$ and $\delta_{F_2,j}$ are introduced, with which the VPI function VPI(θ) can be represented as follows:

$$VPI(\theta) = F_1(\theta) - F_2(\theta, \bar{x}_1) =$$

$$= \{\sum_i c_{F_1,i}\delta_{F_1,i} + \sum_i a_{F_1,i}\theta_{F_1,i}\} - \{\sum_j c_{F_2,j}\delta_{F_2,j} + \sum_j a_{F_2,j}\theta_{F_2,j}\}$$

$$s.t. \quad \sum_i \delta_{F_1,i} = \sum_j \delta_{F_2,j}$$

$$\sum_i \theta_{F_1,i} = \sum_j \theta_{F_2,j} = \theta$$

$$b^L_{F_1,i}\delta_{F_1,i} \leq \theta_{F_1,i} \leq b^U_{F_1,i}\delta_{F_1,i}$$

$$b^L_{F_2,j}\delta_{F_2,j} \leq \theta_{F_2,j} \leq b^U_{F_2,j}\delta_{F_2,j}$$

$$i = 1,..,n_{F_1}, \quad j = 1,..n_{F_2}$$

where n_{F_1}, n_{F_2} are the number of θ regions where F_1 and F_2 have different expressions, respectively.

For example, if F_1 and F_2 are piece-wise linear functions, having the following expressions:

$$F1(\theta) = \begin{cases} c_{F_1,1} + a_{F_1,1}\theta \;\; b^L_{F_1,1} \leq \theta \leq b^U_{F_1,1} \\ \\ c_{F_1,2} + a_{F_1,2}\theta \;\; b^L_{F_1,2} \leq \theta \leq b^U_{F_1,2} \end{cases}$$

$$F2(\theta, \bar{x_1}) = \begin{cases} c_{F_2,1} + a_{F_2,1}\theta \;\; b^L_{F_2,1} \leq \theta \leq b^U_{F_2,1} \\ \\ c_{F_2,2} + a_{F_2,2}\theta \;\; b^L_{F_2,2} \leq \theta \leq b^U_{F_2,2} \end{cases}$$

the VPI(θ) function has the following form:

$$VPI(\theta) = \{c_{F_1,1}\delta_{F_1,1} + a_{F_1,1}\theta_{F_1,1} + c_{F_1,2}\delta_{F_1,2} + a_{F_1,2}\theta_{F_1,2}\} - \{c_{F_2,1}\delta_{F_2,1} + a_{F_2,1}\theta_{F_2,1} + c_{F_2,2}\delta_{F_2,2} + a_{F_2,2}\theta_{F_2,2}\}$$

$$\begin{aligned} s.t.\ \ & \delta_{F_1,1} + \delta_{F_1,2} = \delta_{F_2,1} + \delta_{F_2,2} \\ & \theta_{F_1,1} + \theta_{F_1,2} = \theta_{F_2,1} + \theta_{F_2,2} = \theta \\ & b^L_{F_1,1}\delta_{F_1,1} \le \theta_{F_1,1} \le b^U_{F_1,1}\delta_{F_1,1} \\ & b^L_{F_1,2}\delta_{F_1,2} \le \theta_{F_1,2} \le b^U_{F_1,2}\delta_{F_1,2} \\ & b^L_{F_2,1}\delta_{F_2,1} \le \theta_{F_2,1} \le b^U_{F_2,1}\delta_{F_2,1} \\ & b^L_{F_2,2}\delta_{F_2,2} \le \theta_{F_2,2} \le b^U_{F_2,2}\delta_{F_2,2} \end{aligned}$$

It should be noted that the advantage of deriving exact expressions for the VPI function $VPI(\theta)$ over the entire parameter range θ is that the assignment of a single conservative risk estimate for a specific plan via the maximum VPI can be avoided. It becomes also clear that the incorporation of different norms is indeed possible.

If the price and demand of the same material or the price of a product and the availability of a raw material used for its production are considered simultaneously as independent uncertain parameters, then bilinear terms are introduced in the regret function. In order to preserve linearity, the following monotonicity analysis scheme can be employed.

Consider that the VPI function, derived from the difference $F_1(\theta) - F_2(\theta, x_1)$ for a specific plan x_1, is of the following form, where $\theta 1$ is the uncertain parameter that appear only in the objective function coefficients:

$$VPI(\theta, \theta 1) = \begin{cases} VPI_1(\theta, \theta 1) & \theta 1^L_1 \le \theta 1 \le \theta 1^U_1 \\ \\ VPI_2(\theta, \theta 1) & \theta 1^L_2 \le \theta 1 \le \theta 1^U_2 \end{cases}$$

Since $\theta 1$ lies within the range $\theta 1^L_1 \le \theta 1 \le \theta 1^U_1$, the maximum value of regret, with respect to $\theta 1$, can be found by examining the derivative of VPI with respect to $\theta 1$ as follows:

$$VPI^U_1(\theta, \theta 1^U_1) \quad \text{if} \quad \frac{\partial VPI_1}{\partial \theta_1} > 0$$

and

$$VPI^L_1(\theta, \theta 1^L_1) \quad \text{if} \quad \frac{\partial VPI_1}{\partial \theta_1} < 0$$

Similarly for the range $\theta 1^L_2 \le \theta 1 \le \theta 1^U_2$. As a result, linear expressions of the maximum

value of VPI as a function of the rest of uncertain parameters can still be obtained:

$$\max_{\theta 1} VPI(\theta, \theta 1) = \begin{cases} VPI_1^U \text{ or } VPI_1^L \text{ depending on the sign of } \dfrac{\partial VPI_1}{\partial \theta_1}, \quad \theta 1_1^L \leq \theta 1 \leq \theta 1_1^U \\ \\ VPI_2^U \text{ or } VPI_2^L \text{ depending on the sign of } \dfrac{\partial VPI_2}{\partial \theta_1}, \quad \theta 1_2^L \leq \theta 1 \leq \theta 1_2^U \end{cases}$$

LOYOLA UNIV.