INTEGRATION OF HEAT AND WATER NETWORKS IN SCHEDULING OF CHEMICAL PLANTS

SUDHA CHAUHAN

DEPARTMENT OF CHEMICAL ENGINEERING

INDIAN INSTITUTE OF TECHNOLOGY DELHI

OCTOBER 2022

INTEGRATION OF HEAT AND WATER NETWORKS IN SCHEDULING OF CHEMICAL PLANTS

by

Sudha Chauhan

Department of Chemical Engineering

Submitted

in fulfillment of the requirements for the degree of Doctor of Philosophy

to the

Indian Institute of Technology Delhi

October 2022

I would like to dedicate this thesis to my loving family

CERTIFICATE

We are satisfied that the thesis presented by **Ms. Sudha Chauhan** on "***Integration of Heat and Water Networks in Scheduling of Chemical Plants***" is worthy of consideration for the award of the degree of Doctor of Philosophy and is a record of the original bonafide research work carried out under our guidance and supervision and that the results contained in it have not been submitted in part or full to any other university or institute for award of any degree/diploma. We certify that she has pursued the prescribed course of research.

Prof. Munawar A. Shaik
Associate Professor
Department of Chemical Engineering, Indian Institute of Technology, Delhi, India
(Currently working at Department of Chemical Engineering, UAE University, Al Ain, UAE)


27/10/2022

Prof. Manojkumar C. Ramteke
Associate Professor
Department of Chemical Engineering, Indian Institute of Technology, Delhi, India

ACKNOWLEDGEMENTS

I would like to express my gratitude to my advisor, Prof. Munawar A. Shaik for his suggestions, constant support, and encouragement throughout this research work. He kept on motivated me towards the research by sharing ideas to get a deep insight into the subject. I also gratefully acknowledge essential contributions he made to my professional development, especially writing and presentation skills.

I am also obliged to my acting/co-supervisor Prof. Manojkumar C. Ramteke for providing me valuable technical suggestions to improve the quality of my work as well as for providing me all the essential facilities related to my research. I would also like to thank my SRC members Prof. Shalini Gupta, Prof. Hariprasad Kodamana and Prof. Jitendra K. Madan for their valuable comments and suggestions that helped a lot in improving the quality of the presentation and research as well.

I greatly acknowledge the financial support from the Council of Scientific and Industrial Research (CSIR), India and ONGC, Govt. of India for funding some part of my research.

I would also like to give my sincere thanks to the faculty and staff of the Department of Chemical Engineering, who always helped me during this research work. I am very thankful to my labmates Dr. Rohit Omar, Dr. Edo B. Jiru, Dr. Vaibhav Kumar and Ms. Shipra Batra for their excellent technical discussions and feedbacks. I am also thankful to my friends, Surita, Debashish and Feleke for their concern, love and support.

I am very grateful to my parents for their moral support over the course of this research journey. I owe entire of my academic achievements to my parents, who have tremendously encouraged me throughout my academic pursuance as well as whole life. I am also thankful to my in-laws for their love and kind support. I want to convey a token of love to my younger sister Shraddha who made this journey a bit easier with her presence. Here, I want to express my special gratitude towards my dear husband Dr. Gaurav Mishra who consistently kept my moral high by motivating and cheering me up during the odd times of this work and life as well.

At last, but certainly not the least, I express my whole hearted regards to almighty God, without whom my work at this level would have not been possible.

(Sudha Chauhan)

Abstract

In the present scenario, batch plants are being used widely in the chemical industry due to their flexibility which allows the production of different products by sharing the same equipment or vessel. Batch processes are suitable for the production of small volume and high value added products, such as specialty chemicals, food and pharmaceutical industry. As the demand for such products is quite seasonal and low in volume, a batch process is preferred in comparison to a continuous process. In comparison to continuous processes, the nature of batch processes is more complex due to their multiproduct production behavior. The other reason of the complexity is that the material transfer between two operations within the same process has to be coordinated in time and quantity as well.

Now-a-days, due to stringent environmental regulations and increasing cost of effluent treatment and energy, there is more emphasis on water and energy savings. The motivation behind this research work is to present a methodology for simultaneous optimization based on exploring water reuse and heat integration opportunities in the production scheduling of batch plants. To meet this goal, multiple models are proposed for water allocation network (WAN) and heat exchanger network (HEN) synthesis which are combined with the batch production scheduling model.

In the first part, simultaneous optimization of batch scheduling and water allocation network is considered using a unit-specific event-based continuous time representation, and a state-task-network process representation. A three-index unit-specific event based model has been adapted from the scheduling literature, and new constraints are proposed to deal with additional features: handling multiple states having different processing time durations for the same task in a processing unit, using three-index timing variable for the finish time. Additionally, the scheduling model introduces constraints to handle storage violation for production and consumption of the same state in the same unit. In WAN, water reuse opportunities have been incorporated by using central water storage tank and regenerator. The work also features comparison of sequential and simultaneous approaches while optimizing the production schedule and freshwater consumption. Four case studies are solved from the literature for single and multiple contaminants to evaluate the performance of the proposed model, which gives better savings in terms of freshwater consumption. Further, two-objective optimization is presented where revenue is maximized and total water cost is minimized simultaneously.

In the second part, the HEN model based on direct heat integration is combined with flexible batch scheduling instead of using fixed schedules which are employed in the sequential approach. In the formulation of HEN model, heat consuming and heat producing tasks are aligned over a common time interval for effective transfer of energy between the processing tasks. To handle different types of problems, three different models are developed for HEN with different features. Four case studies from the literature are solved to test the proposed models, resulting in better objective values. The work is extended to two-objective optimization where product revenue is maximized and external utility cost is minimized simultaneously.

In the third part, a combined model is proposed that simultaneously optimizes production scheduling, WAN, and HEN models in a single framework, with additional features including post processing unit-wait policy in washing units. It provides additional temporary storage capacity for used water in the processing units after completion of the washing operation, along with offering additional flexibility in the alignment of tasks in other washing units. The combined model leads to a mixed integer nonlinear programming (MINLP) formulation, which is tested using two examples from the literature, giving better results in terms of freshwater consumption and external utility requirements.

***Keywords*:** Batch Plants, Production Scheduling, Optimization, Mathematical Programming, Water Resue, Water Allocation Network Synthesis, Heat Integration, Heat Exchanger Network Synthesis.

सार

वर्तमान परिदृश्य में बैच के पौधों का उपयोग उनके लचीलेपन के कारण रासायनिक उद्योग में व्यापक रूप से किया जा रहा है जो एक ही उपकरण या पोत को साझा करके विभिन्न उत्पादों के उत्पादन की अनुमति देता है। बैच प्रक्रियाएं छोटी मात्रा और उच्च मूल्य वर्धित उत्पादों, जैसे कि विशेषता रसायन, खाद्य और दवा उद्योग के उत्पादन के लिए उपयुक्त हैं। चूंकि ऐसे उत्पादों की मांग काफी मौसमी और मात्रा में कम होती है, इसलिए निरंतर प्रक्रिया की तुलना में एक बैच प्रक्रिया को तरजीह दी जाती है। निरंतर प्रक्रियाओं की तुलना में, बैच प्रक्रियाओं की प्रकृति उनके बहुउत्पाद उत्पादन व्यवहार के कारण अधिक जटिल है। जटिलता का दूसरा कारण यह है कि एक ही प्रक्रिया के भीतर दो परिचालनों के बीच सामग्री हस्तांतरण को समय और मात्रा में भी समन्वित करना होता है।

आजकल पर्यावरण के कड़े नियमों और अपशिष्ट उपचार और ऊर्जा की बढ़ती लागत के कारण जल और ऊर्जा की बचत पर अधिक जोर दिया जा रहा है। इस शोध कार्य के पीछे प्रेरणा बैच संयंत्रों के उत्पादन शेड्यूलिंग में पानी के पुनः उपयोग और गर्मी एकीकरण के अवसरों की खोज के आधार पर एक साथ अनुकूलन के लिए एक पद्धति प्रस्तुत करना है। इस लक्ष्य को पूरा करने के लिए, जल आवंटन नेटवर्क (डब्ल्यूएएन) और हीट एक्सचेंजर नेटवर्क (एचईएन) संश्लेषण के लिए कई मॉडल प्रस्तावित हैं जो बैच उत्पादन शेड्यूलिंग मॉडल के साथ संयुक्त हैं।

पहले भाग में, बैच शेड्यूलिंग और जल आवंटन नेटवर्क का एक साथ अनुकूलन एक इकाई-विशिष्ट घटना-आधारित निरंतर समय प्रतिनिधित्व, और एक राज्य-कार्य-नेटवर्क प्रक्रिया प्रतिनिधित्व का उपयोग करके माना जाता है। शेड्यूलिंग साहित्य से तीन-सूचकांक इकाई-विशिष्ट घटना आधारित मॉडल को अनुकूलित किया गया है, और अतिरिक्त फीचर्स से निपटने के लिए नई अड़चनें प्रस्तावित हैं: एक प्रसंस्करण इकाई में एक ही कार्य के लिए विभिन्न प्रसंस्करण समय अवधि वाले कई राज्यों को संभालना, फिनिश टाइम के लिए थ्री-इंडेक्स टाइमिंग वेरिएबल का उपयोग करना। इसके अतिरिक्त, शेड्यूलिंग मॉडल एक ही इकाई में एक ही राज्य के उत्पादन और खपत के लिए भंडारण उल्लंघन को संभालने के लिए बाधाओं का परिचय देता है। वान में, केंद्रीय जल भंडारण टैंक और पुनर्जनन का उपयोग करके जल पुनः उपयोग के अवसरों को शामिल किया गया है। इस कार्य में उत्पादन अनुसूची और मीठे पानी की खपत को अनुकूलित करते हुए अनुक्रमिक और एक साथ दृष्टिकोणों की तुलना भी शामिल है। प्रस्तावित मॉडल के प्रदर्शन का मूल्यांकन करने के लिए एकल और एकाधिक दूषित पदार्थों के लिए साहित्य से चार केस स्टडी हल की जाती हैं, जो मीठे पानी की खपत के मामले में बेहतर बचत देती हैं। इसके अलावा, दो-उद्देश्य अनुकूलन प्रस्तुत किया जाता है जहां राजस्व को अधिकतम किया जाता है और कुल जल लागत को एक साथ कम किया जाता है।

दूसरे भाग में, प्रत्यक्ष गर्मी एकीकरण पर आधारित एचईएन मॉडल को निश्चित शेड्यूल का उपयोग करने के बजाय लचीला बैच शेड्यूलिंग के साथ जोड़ा जाता है जो अनुक्रमिक दृष्टिकोण में नियोजित होते हैं। एचईएन मॉडल के निर्माण में, प्रसंस्करण कार्यों के बीच ऊर्जा के प्रभावी हस्तांतरण के लिए गर्मी की खपत और गर्मी उत्पादन कार्यों को एक सामान्य समय अंतराल पर संरेखित किया जाता है। विभिन्न प्रकार की समस्याओं को संभालने के लिए, तीन अलग-अलग मॉडल विभिन्न विशेषताओं के साथ एचईएन के लिए विकसित किए जाते हैं। प्रस्तावित मॉडलों का परीक्षण करने के लिए साहित्य से चार केस अध्ययन हल किए जाते हैं, जिसके परिणामस्वरूप बेहतर उद्देश्य मूल्य होते हैं। कार्य को दो-उद्देश्य अनुकूलन तक बढ़ाया जाता है जहां उत्पाद राजस्व को अधिकतम किया जाता है और बाहरी उपयोगिता लागत को एक साथ कम किया जाता है।

तीसरे भाग में, एक संयुक्त मॉडल प्रस्तावित है जो एक साथ एकल ढांचे में उत्पादन शेड्यूलिंग, डब्ल्यूएएन और एचईएन मॉडल का अनुकूलन करता है, जिसमें वाशिंग इकाइयों में पोस्ट प्रोसेसिंग यूनिट-प्रतीक्षा नीति सहित अतिरिक्त विशेषताएं शामिल हैं। यह वाशिंग ऑपरेशन के पूरा होने के बाद प्रसंस्करण इकाइयों में उपयोग किए गए पानी के लिए अतिरिक्त अस्थायी भंडारण क्षमता प्रदान करता है, साथ ही अन्य वाशिंग इकाइयों में कार्यों के संरेखण में अतिरिक्त लचीलापन प्रदान करता है। संयुक्त मॉडल एक मिश्रित पूर्णांक नॉनलाइनर प्रोग्रामिंग सूत्रीकरण की ओर जाता है, जिसे साहित्य से दो उदाहरणों का उपयोग करके परीक्षण किया जाता है, जिससे मीठे पानी की खपत और बाहरी उपयोगिता आवश्यकताओं के मामले में बेहतर परिणाम मिलते हैं।

कीवर्डः बैच संयंत्र, उत्पादन निर्धारण, अनुकूलन, गणितीय प्रोग्रामिंग, जल रेस्यू, जल आवंटन नेटवर्क संश्लेषण, गर्मी एकीकरण, हीट एक्सचेंजर नेटवर्क संश्लेषण।

Table of Contents

Certificate *i*

Acknowledgements *iii*

Abstract *v*

सार *vii*

List of Figures *xiii*

List of Tables *xv*

Abbreviations *xvii*

Nomenclature *xix*

Chapter 1

Introduction……………………………………………………………………………..1

1.1. Classification of process scheduling models…………………………………….....1

1.1.1. Time representation………………………………………………………...1

1.1.2. Process representation…………………………………………………………3

1.2. Water Allocation Networks (WANs)………………………………………………..3

1.2.1. Direct water re-use……………………………………………………..…4

1.2.2. Indirect water re-use……………………………………………………….....4

1.2.3. Sequential methodology……………………………………………………..5

1.2.4. Simultaneous methodology..5

1.3. Heat Exchanger Networks (HENs)…………………………………………………5

1.3.1. Direct heat-integration………………………………………………………6

1.3.2. Indirect heat-integration……………………………………………………..7

1.4. Combination of water and energy integration…………………………………………7

1.5. Motivation for proposed research……………………………………………………...8

1.6. Thesis outline…………………………………………………………………………10

Chapter 2

Literature review…………………………………………………………………………11

2.1. Scheduling of batch plants…………………………………………………………11

2.2. Wastewater minimization in batch plants scheduling……………………………...13

2.2.1. Sequential methodology and direct/indirect water re-use………………………...13

2.2.2. Simultaneous methodology and indirect water re-use……………………………13

2.2.3. Simultaneous methodology and direct water re-use……………………………...14

2.3. Energy integration in batch plants scheduling……………………………………..15

2.3.1. Sequential methodology and direct/indirect heat integration……………………..15
2.3.2. Simultaneous methodology and direct heat integration…………………………..15
2.3.3. Simultaneous methodology and indirect heat integration………………………...16
2.4. Integration of water and heat in batch process scheduling……………………………...17
2.4.1. Sequential methodology…………………………………………………………..17
2.4.2. Simultaneous methodology…………………………………………………………17
2.5. Research gaps…………………………………………………………………………18
2.5.1. Discrepancies in the literature model for scheduling and WAN……………………18
2.5.2. Different time duration of the same task in different modes (standalone/heat-integrated)…………………………………………………………………………18
2.5.3. Limitation of sequential technique………………………………………………..19
2.5.4. Simultaneous integration of heat and water networks in scheduling of batch plant ……………………………………………………………………………………19
2.6. Research objectives…………………………………………………………………...19
2.6.1. To develop a combined model for batch scheduling and WAN based on unit-specific event based time representation……………………………………………………..19
2.6.2. To develop a unit-specific event based model for batch scheduling combined with heat exchanger networks……………………………………………………………………..19
2.6.3. To develop a combined model for batch scheduling, water allocation and heat Exchanger networks…………………………………………………………..20
Chapter 3
Simultaneous Scheduling and Synthesis of Water Allocation Networks………………..21
3.1. Problem Statement……………………………………………………………………21
3.2. Mathematical formulation………………………………………………………… 22
3.2.1. Production scheduling model……………………………………………………..22
3.2.1.1. Handling multiple states having different processing time durations for the same task in a processing unit………………………………………………………...22
3.2.1.2. Duration constraints…………………………………………………………23
3.2.1.3. Sequencing constraints………………………………………………………23
3.2.1.4. Tightening constraint………………………………………………………...24
3.2.1.5. Storage constraints…………………………………………………………...24
3.2.2. Water Allocation Network (WAN) model………………………………………..24
3.2.2.1. Mass balance of water around washing unit…………………………………...24
3.2.2.2. Water mass balance around the central water storage tank……………………26

3.2.2.3. Water mass balance around regeneration unit……………………………….27
3.2.2.4. Sequencing constrains for water reuse…………………………………………28
3.2.2.5. Sequencing constraints for storage tank………………………………………..28
3.2.2.6. Sequencing constraints associated with regeneration unit……………………..28
3.2.2.7. Scheduling constraints for washing…………………………………………….29
3.2.2.8. Modifications in the scheduling model………………………………………...30
3.2.2.9. Objective function…………………………………………………………...32
3.3. Important contributions of the proposed work……………………………………….32
3.4. Computational Results…………………………………………………………….33
3.4.1. Case study 1………………………………………………………………...33
3.4.2. Case study 2………………………………………………………………...39
3.4.2.1. Limitations of the literature Gantt chart from Majozi and Gouws (2009)…….42
3.4.3. Case study 3………………………………………………………………...42
3.4.3.1. Limitations of the literature Gantt chart from Adekola and Majozi (2011)…...44
3.4.4. Case study 4………………………………………………………………...45
3.4.4.1. Limitations of literature Gantt chart from Adekola and Majozi (2011)……….47
3.5. Two-objective optimization for the case studies……………………………………….48
3.6. Conclusion…………………………………………………………………………...50
Chapter 4
Direct Heat Integration in Batch Plant Scheduling……………………………………53
4.1. Problem statement……………………………………………………………………53
4.2. Mathematical formulation…………………………………………………………….54
4.2.1. Heat Exchanger Network (HEN) model M1………………………………..54
4.2.2. Heat Exchanger Network (HEN) model M2………………………………..57
4.2.3. Heat Exchanger Network (HEN) model M3………………………………..60
4.3. Important contributions of the proposed work…………………………………………62
4.4. Computational Results……………………………………………………………….62
4.4.1. Case study 1………………………………………………………………....63
4.4.2. Case study 2………………………………………………………………....65
4.4.3. Case study 3…………………………………………………………………68
4.4.4. Case study 4…………………………………………………………………71
4.5. Two-objective optimization for the case studies……………………………..……74
4.6. Conclusion ……………………………………………………………………...75

Chapter 5

Integration of heat and water networks in batch process scheduling…………………..77

5.1. Problem statement……………………………………………………………………77

5.2. Mathematical formulation……………………………………………………………78

5.2.1. Sequencing constraints for washing…………………………………………...78

5.2.2. Sequencing constraints for scheduling………………………………………...79

5.2.3. Objective function……………………………………………………………..79

5.3. Important contributions of the proposed work………………………………...……..80

5.4. Computational results………………………………………………………………...80

5.4.1. Case study 1……………………………………………………………………80

5.4.2. Case study 2……………………………………………………………………83

5.5. Conclusion……………………………………………………………………………87

Chapter 6

Summary and Scope for Future Work…………………………………………………….89

6.1. Summary of research contributions…………………………………………………..89

6.1.1. Simultaneous scheduling and synthesis of water allocation networks (WAN) in batch plants……………………………………………………………………….............89

6.1.2. Simultaneous scheduling and heat integration in batch plants…………….……..90

6.1.3. Integration of heat and water networks in batch process scheduling……………..90

6.2. Scope for future work………………………………………………………………….90

Appendix A…………………………………………………………………………………...93

References……………………………………………………………………………………95

List of Publications…………………………………………………………………………..99

Author's Bio-data…………………………………………………………………………...101

List of Figures

Fig. 1.1 (a) Discrete and (b) continuous time representation……………………………………2
Fig. 1.2 Different time representations……………………………………………………………2
Fig. 1.3 Different process representation…………………………………………………………..3
Fig. 1.4 Water usage possibilities in a washing unit……………………………………………….5
Fig. 1.5 Basic structure for energy integration……………………………………………………..6
Fig. 1.6 (a) Direct and (b) Indirect heat integration………………………………………………..7
Fig. 1.7 Interconnections between the process subsystems and the environment……………..7
Fig. 1.8 Percentage of energy consumption in different sectors ……………………………….....9
Fig. 1.9 Percentage of water consumption in different sectors………………………………….9
Fig. 3.1 Superstructure for water mass balance in a given unit *j*……………………………….25
Fig. 3.2 Superstructure for water mass balance in central water storage tank……………….26
Fig. 3.3 Washing sequence with no unit wait policy for washing units……………………..29
Fig. 3.4 STN representation for case study 1……………………………..........................33
Fig. 3.5 Production schedule obtained for the sequential approach…………………………35
Fig. 3.6 Gantt chart for the sequential approach without using water storage tank for case study...36
Fig. 3.7 Gantt chart for the sequential approach using water storage tank for case study 1…36
Fig. 3.8 Gantt chart for the simultaneous approach without a water storage tank for case study 1...37
Fig. 3.9 Gantt chart for the simultaneous approach with water storage tank for case study 1……………………………………………………………………………………37
Fig. 3.10 Gantt chart for the simultaneous approach for case study 2………………………41
Fig. 3.11 Reported Gantt chart from Majozi and Gouws (2009)……………………………41
Fig. 3.12 Gantt chart obtained for the simultaneous approach for case study 3 with water storage tank…………………………………………………………………………..43
Fig. 3.13 Gantt chart obtained for the simultaneous approach for case study 3 with water storage tank and regenerator ………………………………………………………44
Fig. 3.14 Reported Gantt chart from Adekola and Majozi (2011)…………………………...45
Fig. 3.15 Gantt chart for the simultaneous approach for case study 4 with water storage tank and regenerator…………………………………………………………………47
Fig. 3.16 Reported Gantt chart for case study 4 from Adekola and Majozi (2011)…………48

Fig. 3.17 Pareto plots (a), (b) and (c) for the case studies 1, 2 and 3, for the two-objective optimization……………………………………………………………………………….50
Fig. 4.1 Direct energy integration when start time of heating and cooling tasks are the same at an event……………………………………………………………………………………58
Fig. 4.2 Direct energy integration when start time of heating and cooling tasks are different at an event……………………………………………………………………………………61
Fig. 4.3 STN for case study 1 ……………………………………………………………….63
Fig. 4.4 Optimum production schedule for case study 1 in standalone mode…………..…...64
Fig. 4.5 Optimum production schedule for case study 1 in heat integrated mode…………..64
Fig. 4.6 STN for case study 2………………………………………………………………..66
Fig. 4.7 Optimum production schedule for case study 2 in standalone mode……………….67
Fig. 4.8 Optimum production schedule for case study 2 in heat integrated mode…………..68
Fig. 4.9 STN representation for the case study 3……………………………………………69
Fig. 4.10 Optimum production schedule for case study 3 using HEN model M2…………..70
Fig. 4.11 Optimum production schedule for case study 3 using HEN model M3…………..70
Fig. 4.12 STN representation for case study 4………………………………………………72
Fig. 4.13 Optimum production schedule for case study 4 using HEN model M3…………..73
Fig. 4.14 Pareto plots (a), (b) and (c) for the case studies 1, 2 and 3, for two-objective optimization ………………………………………………………………………………75
Fig. 5.1 Washing sequence with unit-wait policy for washing units………………………...78
Fig. 5.2 STN representation for case study 1………………………………………………...81
Fig. 5.3 Gantt chart of the combined model for example 1 …………………………………82
Fig. 5.4 STN representation for case study 2………………………………………………...83
Fig. 5.5 Gantt chart of the combined model for case study 2………………………………..85
Fig. 5.6 Reported Gantt chart from Seid and Majozi (2014) for case study 2……………….86

List of Tables

Table 3.1. Input data for production scheduling for case study 1……………………...........34
Table 3.2. Storage limits and the selling price of various states for case study 1…………...34
Table 3.3. Input data for washing of the reactor units for case study 1……………………...34
Table 3.4. Results obtained for the sequential approach for case study 1…………………...38
Table 3.5. Results obtained for the simultaneous approach for case study 1………………..38
Table 3.6. Input data for the production scheduling of case study 2………………………...39
Table 3.7. Storage limits and the selling price of various states for case study 2…………...39
Table 3.8. Input data for washing of reactor units for case study 2…………………………40
Table 3.9. Mass loads of various contaminants for case study 2……………………………40
Table 3.10. Washing duration of various reactor units for case study 2……………………40
Table 3.11. Comparison of results from the literature for case study 2…………………….41
Table 3.12. Contaminant removal ratio for case study 3…………………………………....42
Table 3.13. Comparison of results for case study 3………………………………………....44
Table 3.14. Production data for case study 4……………………………………………….46
Table 3.15. Wastewater minimization data for case study 4…………………………….....46
Table 3.16. Maximum allowed inlet contaminant concentration for case study 4…………46
Table 3.17. Contaminant removal ratio for case study 4…………………………………....46
Table 4.1. Data for case study 1……………………………………………………………63
Table 4.2. Selling price and utility cost data for case study 1……………………………....63
Table 4.3. Comparison of results for case study 1…………………………………………65
Table 4.4. Production scheduling data for case study 2……………………………………66
Table 4.5. Stoichiometric data for case study 2…………………………………………….66
Table 4.6. Cost related data for case study 2………………………………………………...67
Table 4.7. Comparison of results for case study 2………………………………………….68
Table 4.8. Production scheduling data for case study 3…………………………………….69
Table 4.9. Energy data for case study 3…………………………………………………….69
Table 4.10. Comparison of results for case study 3………………………………………....71
Table 4.11. Production scheduling data for case study 4…………………………………...72
Table 4.12. Energy data for case study 4…………………………………………………...72
Table 4.13. Comparison of proposed work with the literature for case study 4 in heat integration mode……………………………………………………………………………73
Table 5.1. Scheduling data for case study 1………………………………………………...81

Table 5.2. Energy and cleaning requirements for case study 1……………………………...81
Table 5.3. Comparison of results for case study 1…………………………………………..83
Table 5.4. Production scheduling data for case study 2……………………………………..84
Table 5.5. Energy data for case study 2……………………………………………………...84
Table 5.6. Washing data for case study 2……………………………………………………84
Table 5.7. Comparison of results for case study 2…………………………………………...86

Abbreviations

CPU	Computational Processing Unit
DFIS	Dedicated Finite Intermediate Storage
FIS	Finite Intermediate Storage
FW	Fresh Water
HEN	Heat Exchanger Network
MILP	Mixed Integer Linear Programming
MINLP	Mixed Integer Non-Linear Programming
RTN	Resource-task-network
RW	Reused Water
SSN	State-sequence-network
STN	State-task-network
WAN	Water Allocation Network

Nomenclature

<u>Scheduling (Chapters 3, 4, 5)</u>

Indices

i, i'	tasks
j, j'	units
n, n'	events
+/4s	states

Sets

I	tasks
I_j	tasks that can be performed in unit *j*
J_i	units which are suitable for performing task *i*
I_s^p	tasks that produce state *s*
I_s^c	tasks that consume state *s*
I^{PC}	tasks that produce and consumes same state
J	units
N	total number of event points
S	states
S^R	states that are raw materials
S^I	states that are intermediates
S^P	states that are products
S^{dfis}	intermediates states with dedicated finite intermediate storage
S^{PC}	states that are being produced and consumed in the same unit

Parameters

B_i^{min}	minimum batch size of task *i*
B_i^{max}	maximum batch size of task *i*
ST_s^0	initial amount available for state *s*
ST_s^{max}	maximum storage capacity for state
ρ_{is}	fraction of state s produced ($\rho_{is} > 0$) or consumed ($\rho_{is} < 0$) by task *i*
α_{is}	fixed term of processing time of task *i* for state *s*
α_{is}^l	largest fixed term of processing time of task *i* for state *s*
β_{is}	variable term of the processing time of task *i* for state *s*
H	short-term scheduling horizon
P_s	price of state *s*
Δn	limit on the maximum number of events over which a task is allowed to continue
M+-	large positive number in big-M constraints
D_s	demand of final product state *s*

Binary Variables

w(i,n,n')	binary variable for task *i* that starts at event *n* and ends at event *n'*

Positive Variables

$T_s(i,n)$	start time of task *i* at event *n*

$T_f(i,n)$	finish time of task *i* at event *n*

$T_f(i,s,n)$	finish time of task *i* for state *s* at event *n*

b(i,n,n')	batch size of task *i* that starts at event *n* and ends at event *n*'

$ST_0(s)$	initial amount of state *s* required form external resources

ST(s,n)	excess amount of state *s* that needs to be stores at event *n*

MP	maximum profit

MS	makespan

Water Allocation Network (Chapters 3, 5)

Indices

I_R	task that require washing

c	contaminants

stt	storage tanks

Sets

C	contaminants species

Stt	storage tanks

Parameters

CF	cost of fresh water

CE	cost of effluent water treatment

$M_{i,c}^{load}$	mass load of contaminant *c* added from task *i* to the water stream

Mw_i^U	maximum inlet water mass to task *i*

$C_{i,c}^{in,U}$	maximum inlet concentration of contaminant *c* for task *i*

$C_{i,c}^{out,U}$	maximum outlet concentration of contaminant *c* for task *i*

α_i^w	time required for washing after task *i*

Qw_s^0	initial amount of water in storage tank

Qw_s^U	maximum storage capacity of the tank

$Cs_c^{out,0}$	initial concentration of contaminant *c* in the storage vessel

RR_c	contaminant removal ratio

freg	regenerator flow rate

Binary Variables

$yw(i,n)$	binary variable signifies the occurrence of washing task *i* at event *n*

$yw_r(i,i',n)$	binary variable shows the transfer of water from task *i* to task *i'* at event *n*

$ys_{in}(i,n)$ binary variable shows the transfer of water to the storage tank from task *i* at event *n*

$ys_{out}(i,n)$ binary variable shows the transfer of water from storage tank to task *i* at event *n*

$yreg_{in}(stt,n)$ binary variable shows the transfer of water from storage tank to regenerator at event *n*

$yreg_{out}(i,n)$ binary variable shows the transfer of water from the regenerator to task *i* at event *n*

Positive Variables

$mw_{in}(i,n)$ mass of water consumed for washing unit for task *i* at the end of event *n*

$mw_{out}(i,n)$ mass of water exiting after washing unit for task *i* at the end of event *n*

$mw_f(i,n)$ mass of fresh water used for washing unit for task *i* at the end of event *n*

$mw_e(i,n)$ mass of effluent water produced after washing the unit for task *i* at the end of event *n*

$mw_r(i,i',n)$ mass of water recycled from task *i* to task *i'* at event *n*

$ms_{in}(i,n)$ mass of water to storage from task *i* at event *n*

$ms_{out}(i,n)$ mass of water coming from storage to task *i* at event *n*

$mreg_{in}(stt,n)$ mass of water coming to regenerator from storage at event *n*

$mreg_{out}(i,n)$ mass of water coming out from regenerator to task *i* at event *n*

$m_{dirt}(c,n)$ mass of contaminant *c* removed from water by regenerator at event *n*

$c_{in}(i,c,n)$ inlet concentration of contaminant *c*, entering task *i* at event *n*

$c_{out}(i,c,n)$ outlet concentration of contaminant *c*, exiting task *i* at event *n*

$cs_{in}(c,n)$ inlet concentration of contaminant *c*, entering storage at event *n*

$cs_{out}(c,n)$ outlet concentration of contaminant *c*, exiting from storage at event *n*

$creg_{out}(c,n)$ outlet concentration of contaminant *c*, exiting from regenerator at event *n*

$tw_{in}(i,n)$ inlet time of water used for task *i*, at event *n*

$tw_{out}(i,n)$ outlet time of water used for task *i*, at event *n*

$tw_r(i,i',n)$ water recycle time from task *i* to task *i'*, at event *n*

$treg_{in}(stt,n)$ inlet time of water in regenerator from storage tank at event *n*

$treg_{out}(i,n)$ outlet time of water from regenerator to task *i* at event *n*

Heat Exchanger Network (Chapter 4, 5)

Indices

u utilities

Sets

I_u tasks that consume utility *u*

I_C tasks that use cold utility

I_H tasks that use hot utility

U Utilities

Parameters

α_i fixed processing time of task *i*

β_i linear coefficient of the variable term of the processing time of heating task *i*

$\beta_{i'}$ linear coefficient of the variable term of the processing time of cooling task *i'*

α_{H1i} fixed processing time of heating task *i* in standalone mode

α_{H2i} fixed processing time of heating task *i* in heat integrated mode

$\alpha_{C1i'}$ fixed processing time of cooling task *i'* in standalone mode

$\alpha_{C2i'}$ fixed processing time of cooling task *i'* in heat integrated mode

γ_{H1i} coefficient of constant term for hot utility for task *i* in standalone mode

γ_{H2i} coefficient of constant term for hot utility for task *i* in heat integrated mode

$\gamma_{C1i'}$ coefficient of constant term for cold utility for task *i'* in standalone mode

$\gamma_{C2i'}$ coefficient of constant term for cold utility for task *i'* in heat integrated mode

δ_{H1i} coefficient of variable term for hot utility for task *i* in standalone mode

δ_{H2i} coefficient of variable term for hot utility for task *i* in heat integrated mode

$\delta_{C1i'}$ coefficient of variable term for cold utility for task *i'* in standalone mode

$\delta_{C2i'}$ coefficient of variable term for cold utility for task *i'* in heat integrated mode

P_u price of utility *u*

T_i^{in} incoming temperature of feed for heating task *i*

T_i^{out} outgoing temperature of feed for heating task *i*

$T_{i'}^{in}$ incoming temperature of feed for cooling task *i'*

$T_{i'}^{out}$ outgoing temperature of feed for cooling task *i'*

Cp_i heat capacity for heating task *i*

$Cp_{i'}$ heat capacity for cooling task *i'*

Q_i^{max} maximum allowed heat available for exchange for heating task *i*

$Q_{i'}^{max}$ maximum allowed heat available for exchange for cooling task *i'*

Binary Variables

x(i,i',n) binary variable for allocation of heat integration between task *i* and *i'* at event *n*

Positive Variables

$T_{ss}(i,n)$ start time of heat integration of heating task *i* at event *n*

$T_{ff}(i,n)$ finish time of heat integration of heating task *i* at event *n*

$T_{ss}(i',n)$ start time of heat integration of cooling task *i'* at an event *n*

$T_{ff}(i',n)$ finish time of heat integration of cooling task *i'* at an event *n*

dur(i,n) duration of heating task *i* at an event *n*

dur(i',n) duration of cooling task *i'* at an event *n*

Ut_u	total utility
q(i,i',n)	heat exchanged between task *i* and *i'* at event *n*
HL(i,n)	heating load required for a task *i* at event *n*
CL(i',n)	cooling load required for a task *i'* at event *n*
HL'(i,n)	average heat load per hour for a task *i* at event *n*
CL(i',n)	average cooling load per hour for a task *i'* at event *n*
HL''(i,n)	heating load exchanged during heat integration for a task *i* at event *n*
CL''(i',n)	cooling load exchanged during heat integration for a task *i'* at event *n*
HLsa(i,n)	amount of external hot utility in standalone mode for a task *i* at event *n*
HLhi(i,n)	amount of external hot utility in heat integrated mode for a task *i* at event *n*
CLsa(i',n)	amount of external cold utility in standalone mode for a task *i'* at event *n*
CLhi(i',n)	amount of external cold utility in heat integrated mode for a task *i'* at event *n*
st(i,n)	amount of steam supplied externally for a task *i* at event *n*
cw(i',n)	amount of cooling water supplied externally for a task *i'* at event *n*
$r_1(i,n,n')$	linearization terms
$r_2(i,i',n)$	linearization terms
$r_3(i',n,n')$	linearization terms
$r_4(i,i',n)$	linearization terms