

T.R.
GEBZE TECHNICAL UNIVERSITY
GRADUATE SCHOOL OF NATURAL AND APPLIED SCIENCES

MIXED-INTEGER NONLINEAR PROGRAMMING APPLICATIONS
IN CHEMICAL ENGINEERING

EMRULLAH ERTÜRK
A THESIS SUBMITTED FOR THE DEGREE OF
MASTER OF SCIENCE
DEPARTMENT OF CHEMICAL ENGINEERING

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GEBZE
2023

T.C.
GEBZE TEKNİK ÜNİVERSİTESİ
FEN BİLİMLERİ ENSTİTÜSÜ

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GEBZE
2023

GTÜ Fen Bilimleri Enstitüsü Yönetim Kurulu'nun 21/06/2023 tarih ve 2023/36 sayılı kararıyla oluşturulan jüri tarafından 10/07/2023 tarihinde tez savunma sınavı yapılan Emrullah Ertürk'ün tez çalışması Kimya Mühendisliği Anabilim Dalında YÜKSEK LİSANS tezi olarak kabul edilmiştir.

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..... / / tarih ve / sayılı kararı.

SUMMARY

This thesis focuses on applications of mixed integer nonlinear programming (MINLP), an important class of optimization problems commonly encountered in chemical engineering, which involves both continuous variables such as temperature and pressure and integer variables such as number of trays, number of stages, etc. The effectiveness and practical implementation of MINLP techniques on various chemical engineering problems are explored in different sections. A complex reaction network reduction problem is presented in the first application. Removing the reaction terms in the model reduced the computational load while maintaining the dynamic model's prediction of process variables with acceptable error. Another application covered in this work is process design using superstructure optimization. Unlike existing studies that mainly rely on commercial software, this thesis demonstrates the design of a Dimethyl Ether process using a free/open-source process simulation environment. Finally, the thesis considers the topological optimization of processes described by partial differential equations (PDE) using integer programming methods. A brief explanation of topological optimization and its relationship to the PDE constrained optimization process is provided to enhance understanding. Simultaneous design and optimization of heat and flow systems results are presented. This thesis consolidates various techniques into a single study that includes practical examples of different methods such as rigorous optimization using differential algebraic equations and black box optimization using a process simulation environment. Therefore, it adds to the existing knowledge in the field of chemical engineering and shows practical applications of MINLP optimization in complex processes.

Key Words: Mixed Integer Nonlinear Programming (MINLP), Reaction Network Reduction, Superstructure Optimization, Topology Optimization.

ÖZET

Bu tez çalışması, kimya mühendisliğinde yaygın olarak karşılaşılan, hem sıcaklık ve basınç gibi sürekli değişkenleri hem de tepsisi sayısı, kademe sayısı gibi tamsayıli değişkenleri barındıran, optimizasyon problemlerinin önemli bir sınıfı karma tamsayıli doğrusal olmayan programlama (MINLP) uygulamalarına odaklanmaktadır. Çeşitli MINLP tekniklerinin kimya mühendisliği problemleri üzerindeki etkinliği ve pratik uygulamaları farklı bölümlerde incelenmiştir. İlk uygulamada karmaşık bir reaksiyon ağ küçültme problemi sunulmuştur. Modeldeki reaksiyon terimlerinin atılması, dinamik modelin proses değişkenlerini kabul edilebilir hatalarla tahmin etmesini sağlarken hesaplama yükünü azaltmıştır. Bu çalışmada ele alınan bir diğer uygulama ise süper yapı optimizasyonu kullanılarak proses tasarımıdır. Çoğunlukla ticari yazılımlara dayanan mevcut çalışmaların aksine, bu tez ücretsiz/açık kaynaklı bir proses simülasyon ortamı kullanarak bir Dimetil Eter prosesi tasarımı gösterilmektedir. Son olarak, kısmi diferansiyel denklemler (PDE) ile tanımlanan süreçlerin tam sayılı programlama yöntemleri kullanılarak topolojik optimizasyonu ele alınmıştır. Topolojik optimizasyonun kısa bir açıklaması ve PDE kısıtlı optimizasyon süreci ile ilişkisi, anlayışı geliştirmek için verilmiştir. Bu doğrultuda ısı ve akış sistemlerinin eşzamanlı tasarım ve optimizasyon sonuçları sunulmuştur. Bu tez, diferansiyel cebirsel denklemler kullanarak titiz optimizasyon ve bir süreç simülasyon ortamı kullanarak kara kutu optimizasyonu gibi farklı yöntemlerin pratik örneklerini içeren tek bir çalışmada çeşitli teknikleri birleştirmektedir. Böylece kimya mühendisliği alanındaki bilgi birikimine katkıda bulunmakta ve karmaşık süreçlerde MINLP optimizasyonunun pratik uygulamalarını göstermektedir.

Anahtar Kelimeler: Karma Tamsayıli Doğrusal Olmayan Programlama (MINLP), Reaksiyon Ağı İndirgeme, Süper Yapı Optimizasyonu, Topoloji Optimizasyonu.

ACKNOWLEDGEMENTS

I would like to begin by expressing my heartfelt appreciation to my supervisor, Dr. Hasan ŞILDIR, for their invaluable guidance, constructive feedback, and unwavering intellectual support throughout my academic journey. Their mentorship played a pivotal role in fostering my pursuit of new knowledge and instilling a passion for scientific inquiry.

Lastly, I extend my deepest gratitude to my family, specifically my mother Havva ERTÜRK and my brother Ali ERTÜRK, for their unwavering support, boundless love, and constant encouragement. Their presence and belief in my abilities have been instrumental in my accomplishments.



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LIST of ABBREVIATIONS and ACRONYMS

<u>Abbreviations</u>	<u>Explanations</u>
<u>and Acronyms</u>	
ρ	: Density
C_p	: The specific heat capacity
k	: The thermal conductivity of solids
h	: The heat transfer coefficient
K	: Kelvin
T	: Temperature
P	: Pressure
M	: Molar
A_s	: The heat transfer area
K_{eq}	: Equilibrium constant
NaCl	: Sodium chloride
H ₂ O	: Hydrogen oxide
THF	: Tetrahydrofuran
HMF	: 5-hydroxymethylfurfural
FA	: Formic acid
LA	: Levulinic acid
DME	: Dimethyl ether
BONMIN	: Basic Open-source Nonlinear Mixed Integer programming
CDT	: Canonical Duality Theory
DICOPT	: Discrete and Continuous Optimizer
GA	: Genetic Algorithm
IC	: Initial concentration
MILP	: Mixed Integer Linear Programming
MINLP	: Mixed-Integer Nonlinear Programming
MIQP	: Mixed Integer Quadratic Programming
NAND	: Nested Analysis and Design
NLP	: Nonlinear programming
OA	: Outer Approximation
PDE	: Partial Differential Equation

PSE	: Process Systems Engineering
RM	: Reduced model
SAD	: Simultaneous Analysis and Design
SCIP	: Solving Constraint Integer Programs
SHOT	: Supporting Hyperplane Optimization Toolkit
SVD	: Singular Value Decomposition
TO	: Topology Optimization



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1. INTRODUCTION

The rapid growth of the world's population has increased environmental concerns, leading regulators to impose various measures to limit the footprint of human activities. The chemical industry is one of the sectors affected by these new regulations and must either improve efficiency or find production alternatives [1]. Many researchers have been exploring alternative methods that are more eco-friendly, but most of them are not feasible in terms of cost and scalability. Therefore, there is a need to optimize existing chemical processes to improve efficiency and sustainability.

As computational capabilities have improved over time, the scope of chemical process optimization studies has expanded to include all steps from raw material sourcing to product delivery. Process systems engineering (PSE) is a multidisciplinary field that applies advanced mathematical and computational methods to design, control, and optimize complex chemical processes and systems [2]. Mixed-integer nonlinear programming (MINLP) is a class of optimization problems that involve both continuous and discrete (integer or binary) decision variables and nonlinear objective functions and/or constraints [3]. MINLP problems arise frequently in PSE applications such as process synthesis, design, scheduling, planning, and control. For example, an MINLP problem can be used to determine the optimal structure and operating conditions of a chemical plant that minimize the total annualized cost while satisfying product demand and specifications. MINLP problems are generally very difficult to solve due to their combinatorial nature and nonconvexity. Therefore, specialized algorithms and solvers are required to find high-quality solutions in a reasonable amount of time.

The primary objective of this thesis is to investigate different applications of MINLP problems through case studies. The first study focuses on reaction network reduction. Followed by superstructure optimization was investigated by integrating a process simulator and a genetic algorithm, a heuristic algorithm based on evolutionary mechanisms observed in nature. In the last study, the topology optimization of heat and flow systems with a mixed-integer formulation was presented. It is worth noting that it is impossible to cover all the applications of MINLP in this thesis due to the wide range of applications.

Chapter 2 presents a method for reducing the complexity of reaction network models by using MINLP. The method involves introducing binary variables to indicate

whether rate constants are included or excluded in the model, along with continuous variables to minimize the error between the model predictions and the data. The binary variables are enforced by linking constraints. The method considers the effects of different initial and operating conditions on the model reduction. The performance of various solvers, both commercial and free, is compared in terms of computation time and results. The method is applied to a reaction network model derived from an experimental study in the literature.

One way to simultaneously design and optimize processes is to integrate process flowsheet simulators and optimization algorithms, which can be formulated as a MINLP problem. In Chapter 3, the study uses DWSIM, a free and open-source simulator, as a black-box function for evaluation of genetic algorithms in MATLAB. The proposed approach is applied to a dimethyl ether process, which involves optimization of process conditions and selection of feedstock type, reactor, and separation unit.

The topological optimization of complex processes remains a challenging open problem in the field of partial differential equation constrained optimization. Existing nested and sequential approaches commonly employed in this area often face difficulties due to multi-step solution requirements. Chapter 4 addresses this issue by proposing a novel mixed integer programming formulation that has received limited research attention. By simultaneously considering both topology and process variables, which exhibit strong interdependencies in many engineering systems, a more advanced system design can be achieved. The proposed methodology is applied to heat and flow optimization problems, demonstrating its potential for simultaneous design and optimization of complex processes. However, it should be noted that the size of the problems that can be tackled is currently limited by the capabilities of existing optimization algorithms.

The last chapter includes the implications and limitations of the current state of the art, summarizing the main findings and contributions of the previous chapters.

2. REACTION NETWORK REDUCTION WITH MIXED INTEGER NONLINEAR PROGRAMMING

2.1. Introduction

Chemical production processes are expressed with differential and algebraic equations. These types of equations can be classified as first-principle, empirical, or hybrid models in terms of the physical reality they contain. First-principal models theoretically provide reliable predictions over a wide operational window, as they clearly include the effects that govern the process at the fundamental level. On the other hand, the complexity of the theoretical knowledge and experimental data required to construct these sets of equations is the biggest obstacle to obtaining models using this method. In addition, it is often computationally challenging to determine the parameters they contain and to solve the equations. Alternatively, empirical models based on data obtained from experimental observations, based on actual events, and directly based on data, evaluate the process like a black box and establish relationships between inputs and outputs. In particular, advanced sensor and computing capabilities have enabled many applications in this field. However, this approach cannot show the expected performance under external operating conditions because it is too dependent on the obtained data and does not contain physical reality at a basic level. In addition, in empirical models where a large number of parameters are defined, significant estimation errors can be obtained in both the learning and test regions. Hybrid models, in which the benefits of both first-principal models and empirical models are integrated, can offer approaches that are more reliable and more practical to develop.

In addition to the state variables describing the reaction processes, the multiplicity of parameters expressing the physical interactions makes it difficult to obtain accurate and reliable models. The large number of parameters defined in the equations causes the model not to be constructed or to be more complex than necessary [4]. In addition to computational cost challenges, overfitting can lead to large changes in predictions even with small changes in parameters and input variables. These results may also include outputs that are not theoretically possible.

One of the important areas whose inference is critical is reaction network models. The complex nature of reaction network models has led research studies to

develop smaller models with similar predictive performance. Due to the nature of these models, they contain more than one parameter set, and their non-convex structure creates mathematical difficulties [5]. For this reason, the extraction of models with fewer parameters and predicting the process behavior in general is of great importance in obtaining more robust predictions.

There are different approaches to the extraction, simplification, and reduction of reaction process models. In model simplification, improvement is applied with mathematical arrangements without discarding parameters and variables. By making scaling arrangements on the equations, the variables are unitless, and mathematically simpler model equations are obtained [6]. In the model decay method, sub-model groups are formed that can be analyzed in parts. In this approach, the number of equations that need to be calculated at once is reduced without changing the model equations. In the grouping method, a reduced model (RM) is obtained by expressing a high-dimensional variable vector with a representative vector with smaller dimensions [7]. The time-scale utilization method examines the dynamic system at different time intervals and aims to determine the fast-slow response terms. By using this distinction, it can be assumed that the fast response variables reach a steady state. In the same way, the slow-response terms can be accepted as constant, and model reduction can be achieved. By using singular value decomposition (SVD) analysis, which examines the effects of parameters on the system response, complex models can also be reduced by discarding parameters that have little effect. The parameters that are planned to be discarded are determined according to the sensitivity targets of the model. Another downscaling method is downsizing with an optimization approach. In the optimization problem, it is aimed to minimize the difference between the experimental measurements and the values produced by the model by assigning bivalent variables to the model parameters and variables that are desired to be minimized [8]. Machine learning and artificial neural networks can create mathematical models that predict changes in chemical processes. Very complex reaction networks can be expressed with smaller equation sets with this method [9,10].

In this study, model reduction was done by using mixed-integer nonlinear programming. In the MINLP problem, in addition to the usual rate constants, binary variables describing their presence or absence are defined. These binary variables are included in the MINLP equations as linking constraints, making it possible to have nonzero values of only the calculated rate constants. Details on the MINLP formula

are given in the next section. The theoretical approach was applied to an experimentally obtained complex chemical network. The prediction performance of the reduced model obtained as a result of the method at different temperatures and initial conditions and the resulting model structures are presented in the case study section. The last part contains the conclusion.

2.2. Method

Dynamic models, which are widely employed in reaction modeling, are mathematically expressed in sets of differential and algebraic equations. A common equation:

$$\frac{d\mathbf{x}(t, \boldsymbol{\theta})}{dt} = \mathbf{f}(t, \mathbf{x}(t, \boldsymbol{\theta}), \boldsymbol{\theta}) \quad (2.1a)$$

$$\mathbf{y}(\mathbf{x}, \boldsymbol{\theta}) = \mathbf{g}(\mathbf{x}(t, \boldsymbol{\theta}), \boldsymbol{\theta}) \quad (2.1b)$$

$$\mathbf{x}(t_0) = \mathbf{x}_0 \quad (2.1c)$$

which $\mathbf{x} \in R^{N_x}$ is state variable vector and generally represents concentrations of chemical compounds in reaction system. Chemical reaction rates are given with $\mathbf{f}: R^{1 \times N_x \times N_\theta} \rightarrow R^{N_x}$ and $\boldsymbol{\theta}$ is the parameter vector consist of N_θ elements. $\mathbf{g}: R^{N_x \times N_\theta} \rightarrow R^{N_y}$ functions are algebraic equations expressing the observable and measurable state variables of the system. The initial time and conditions are given with t_0 and $\mathbf{x}(t_0) = \mathbf{x}_0$, respectively.

Nonlinear programming (NLP) optimization problems in conventional data modeling approaches attempt to minimize the discrepancy between model prediction and measurements by using model parameters as decision variables. These strategies attempt to identify parameters appropriate for the existing network structure rather than a change in the network structure since all decision variables and their lower/upper bounds are continuous variables. Conversely, binary variables are also needed to describe the presence or absence of terms in the model, resulting in a MINLP problem:

$$\min_{\mathbf{c}, \mathbf{y}} r(\mathbf{c}, \mathbf{y}) \quad (2.2a)$$

$$s. t.$$

$$\mathbf{h}(\mathbf{c}, \mathbf{y}) = 0 \quad (2.2b)$$

$$\mathbf{g}(\mathbf{c}, \mathbf{y}) \leq 0 \quad (2.2c)$$

$$\mathbf{c} \in \mathcal{C} \subseteq \mathbb{R}^N \quad (2.2d)$$

$$\mathbf{y} \in \mathcal{Z} \quad (2.2e)$$

r given in problem (2.2) is the objective function and in general, process outputs such as cost, profit, product quantity, estimation error are optimized; $\mathbf{c}$ and $\mathbf{y}$ are the continuous and integer variable vectors, respectively. The equality constraint is represented by the $\mathbf{h}$ function, which is specified for mass and energy balances. The inequality constraint, denoted by $\mathbf{g}$, is used for criteria that must be satisfied, such as environmental limits or the degree of desired purity [11].

In chemical engineering, MINLP problems are used for equipment and process design, production planning, and a variety of other applications [3]. While the variable vector $\mathbf{c}$ is utilized to represent the parameters in the model reduction study, the integer vector $\mathbf{y}$ is constructed with binary variables that represent the existence or absence of reactions in the network. By specifying the linking constraint, these binary variables are used to determine which reactions should be present in the model.

The MINLP problem used for model reduction is shown in Equation (2.3):

$$\min_{\mathbf{k}, \mathbf{b}} \sum \| \mathbf{x} - \hat{\mathbf{x}} \| \quad (2.3a)$$

$$s. t. \quad (2.3b)$$

$$\frac{d\hat{\mathbf{x}}}{dt} = f(\mathbf{x}, \mathbf{k}, t) \quad (2.3c)$$

$$\hat{\mathbf{x}}(t_0) = \mathbf{x}_0 \quad (2.3d)$$

$$k_i - k_i b_i = 0, i = 1, \dots, 12 \quad (2.3e)$$

$$\sum_{i=1}^{12} b_i = \mu \quad (2.3f)$$

$$0 \leq k_i \leq 1, i = 1, \dots, 12 \quad (2.3g)$$

$$\mathbf{b} \in \{0, 1\} \quad (2.3h)$$

which $\hat{\mathbf{x}}$ is the reduced model prediction; $\mathbf{x}$ represents the measurement values, the difference of the reduced model with the measured data is defined in the objective function. $\mathbf{k}$ is the reaction rate constant vector, and the equation $\hat{\mathbf{x}}(t_0) = \mathbf{x}_0$ defines the initial conditions for the state variables in the reduced network. $\mathbf{b}$ refers to the binary variables defined for all reactions and is not directly included in the model. The linking constraint is added to the problem to ensure the relevant rate constant is zero when the reaction is not defined. In this way, a computational advantage is achieved for the solver operating in a narrow solution space. μ contains the total number of rate constants desired in the reduced model.

In this study, the model taken from the literature was reduced. We do not have experimental data, so the required measurement data is generated synthetically by using the original reaction network. A flowchart of the detailed components of data generation can be found in Appendix B1. For various temperatures and initial concentrations, reduced versions of the complex reaction network models were calculated using the MINLP problem given in Equation (2.3). In addition, the performance of different solver programs used in MINLP problem solving was evaluated. MINLP problems are solved using DICOPT [12] and BONMIN [13] in the PYOMO mathematical programming environment [14]. Appendix B2 contains the information flow chart of the proposed MINLP problem solution procedure.

2.3. Case Study

2.3.1. Reference Model Used for Reduced Model (RM) Calculations

The 5-hydroxymethylfurfural (HMF) synthesis reaction network model was used as the basic model in this study. In the related study, the synthesis of HMF, which can be used as a potential precursor chemical, from glucose, which is a renewable resource, was investigated in a NaCl-H₂O/THF biphasic medium. The reaction rate constants in a comprehensive reaction network containing many parameters have been determined experimentally for different temperatures. The related reaction network is shown in Figure 2.1 [15]:

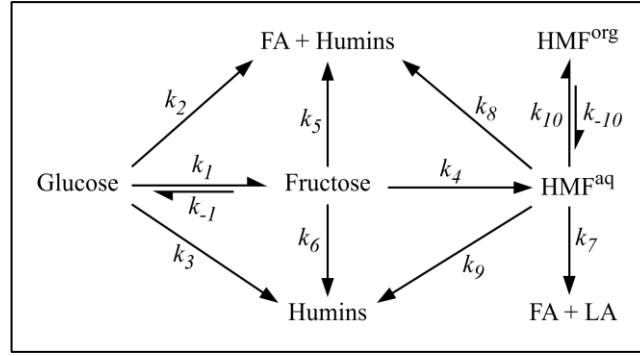


Figure 2.1: AlCl₃ catalyzed HMF synthesis reaction network from glucose in NaCl-H₂O/THF medium.

In this network, fructose is formed from glucose by an isomerization reaction, and HMF is obtained after dehydration. k_1 and k_{-1} are rate constants for the reversible isomerization reaction. k_4 is the rate constant of the dehydration reaction. With the degradation of glucose, side reactions also occur. The formation reaction rate constants of by-products such as formic acid (FA) and humins are k_2 and k_3 , respectively. Fructose degrades to FA with k_5 reaction rate and to humin products with k_6 . k_{10} and k_{-10} are the mass transfer rate of HMF between media in the reaction that takes place in a two-phase medium. Levulinic acid (LA) and FA synthesis reaction rate with rehydration of HMF is k_7 . The reactions included in the proposed network in the related study are given in Equation (2.4) [15].





Tang et al. (2017) carried out their experiments for the proposed reaction network model at four different temperatures: 403K, 413K, 423K, and 433K. These temperatures were also used in the calculation of rate constants other than k_{10} and k_{-10} . Additionally, it has been reported that $k_{10}, k_{-10} \gg k_i, i = -1, \dots, 9$ and $\frac{k_{10}}{k_{-10}} \approx K_{eq} = 3.51$. For this reason, it was calculated as $k_{10} = 3.51 \times k_{-10}$ and $k_{-10} = k_4 \times 10$, and these rate constants are given in Table 2.1.

Using the proposed network and determined rate constants, the differential equations of the model are given in Equation (2.5):

$$\frac{dx_1}{dt} = k_{-1}x_2 - (k_1 + k_2 + k_3)x_1 \quad (2.5a)$$

$$\frac{dx_2}{dt} = k_1x_1 - (k_{-1} + k_4 + k_5 + k_6)x_2 \quad (2.5b)$$

$$\frac{dx_3}{dt} = k_4x_2 + k_{-10}x_4 - (k_7 + k_8 + k_9 + k_{10})x_3 \quad (2.5c)$$

$$\frac{dx_4}{dt} = k_4x_3 - k_{-10}x_4 \quad (2.5d)$$

$$\frac{dx_5}{dt} = k_2x_1 + k_5x_2 + (k_7 + k_8)x_3 \quad (2.5e)$$

$$\frac{dx_6}{dt} = k_7x_3 \quad (2.5f)$$

In Equation (2.5), x_1 : Glucose, x_2 : Fructose, x_3 : HMF^{aq} , x_4 : HMF^{org} , x_5 : FA, and x_6 : LA. Humins are a polymer group that was not expressed numerically in the study.

To create and verify dynamic models, the concentration values of the components must be measured with respect to time. Equation (2.4) was taken as a reference in this study, and the synthetic data obtained by solving this equation was used instead of experimental measurement. Arbitrary points were selected from the simulation solution values and used as synthetically created measurement data in the optimization problem.

Table 2.1: Proposed rate constants.

Rate Constant ($\times 10^{-5} \text{ min}^{-1}$)	Temperature (K)			
	403	413	423	433
k_{-1}	16.000	23.000	35.000	65.000
k_1	23.000	52.000	89.000	172.000
k_2	14.000	29.000	49.000	92.000
k_3	0.009	0.030	2.000	3.000
k_4	34.000	101.000	202.000	465.000
k_5	25.000	39.000	71.000	112.000
k_6	14.000	25.000	29.000	56.000
k_7	0.300	0.700	1.000	2.000
k_8	3.000	6.000	10.000	17.000
k_9	0.001	0.010	0.400	2.000
k_{10}	1193.400	3545.100	7090.000	16321.500
k_{-10}	340.000	1010.000	2020.000	4650.000

Tang et al. (2017) investigated the scenario where there was only 0.25M glucose initially in their study. Reported rate constants and the concentration profile at 413K are given in Figure 2.2.

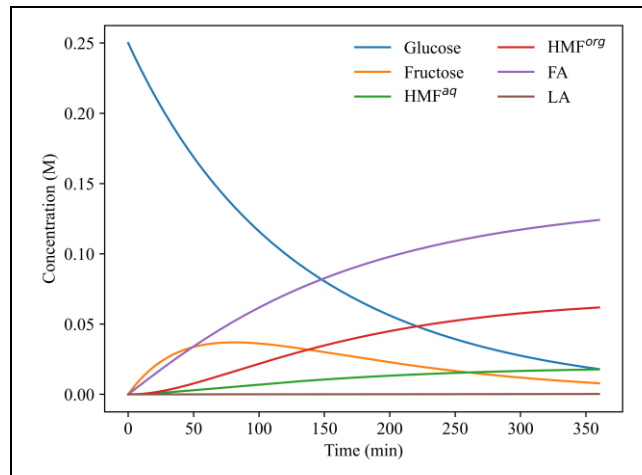


Figure 2.2: Solution of Equation (2.4) at 413K temperature parameter set.

A large amount of data is required to correctly derive Equation (2.4) due to its complex and highly interactive nature. In addition, the experimental conditions in

which these data were collected have a significant impact on shaping the network structure. Theoretically, especially in nonlinear models, parameter sensitivity can behave locally. In other words, operating regions can cause parameters to have different sensitivity effects. Therefore, it is possible to detect terms that contribute little statistically to data collected in regions or conditions of low sensitivity. For this reason, the effect of temperature and initial conditions, which reflect different operating conditions, on mesh extraction was investigated. In addition, the optimization problem in question is computationally complex, and the effects of different solvers are investigated.

2.3.2. Reduced Models at Different Temperatures

In endothermic reactions, the amount of reacting substance per unit time increases in direct proportion to the temperature [16]. Tang et al. (2017) observed that raising the temperature increased HMF production from glucose. The process reaches a steady state in less time due to the higher conversion rate.

The MINLP solution recommended the same reaction constants in the RM at 403, 413, and 423 K. This indicates that the same reaction model may properly explain the process at different temperatures and that the reaction mechanism does not vary significantly. For the higher temperature (433K), the reduced model (RM8R) with 8 reactions was requested, and it was discovered that RM8R comprised all of the reactions in RM5R. The network structure of the RM5R and RM8R is depicted in Figure 2.3. Reactions that are not included in the MINLP solution are highlighted in red.

In order to examine the performance of the reaction network models obtained by the MINLP problem method to predict the synthetic data obtained with the model, including all reactions, Equation (2.5) is solved with the new calculated parameters and the same initial concentration. Synthetic data (SD) for 403K are shown in Figure 2.4 with asterisks; the reduced model (RM) concentration profile is shown as a curve.

Table 2.2: Reduced Model (RM) parameters at different temperatures.

Reaction Rate Constant ($\times 10^{-5} \text{ min}^{-1}$)	Temperature (K)			
	403	413	423	433
k_{-1}	0.00	0.00	0.00	0.00
k_1	13.89	30.04	47.68	129.07
k_2	18.28	38.64	68.31	113.08
k_3	2.07	7.44	16.80	18.53
k_4	40.73	103.36	189.69	538.96
k_5	0.00	0.00	0.00	0.00
k_6	0.00	0.00	0.00	0.00
k_7	0.00	0.00	0.00	1.87
k_8	0.00	0.00	0.00	34.93
k_9	0.00	0.00	0.00	0.00
k_{10}	165.69	192.86	303.35	1000.00
k_{-10}	0.00	0.00	0.00	264.77

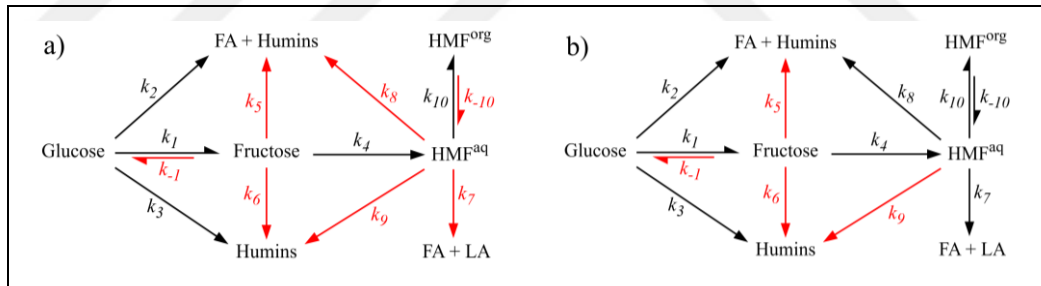


Figure 2.3: RM networks a) RM5R network generated for 403K, 413K and 423K b) RM8R network generated for 433K.

In Figure 2.5, the concentration profile of the RM8R network for 433K is plotted. Figures 2.4 and 2.5 show that the drastically reduced models predict SV with an acceptable error.

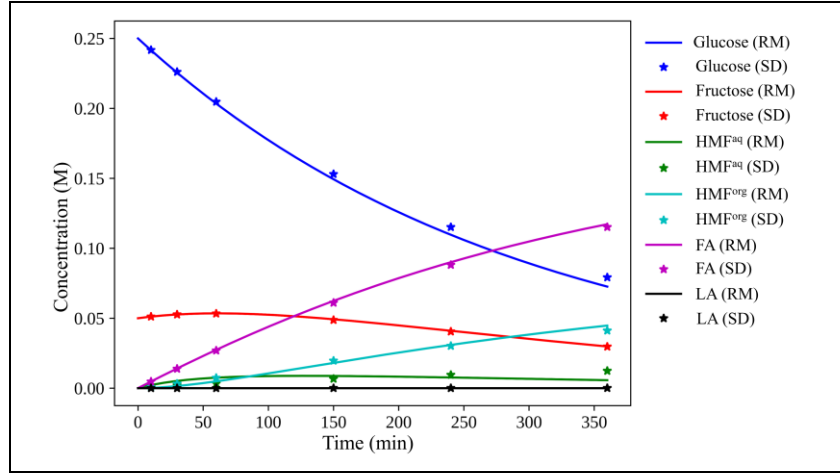


Figure 2.4: Synthetic data prediction performance of RM5R reduced with MINLP at 403K.

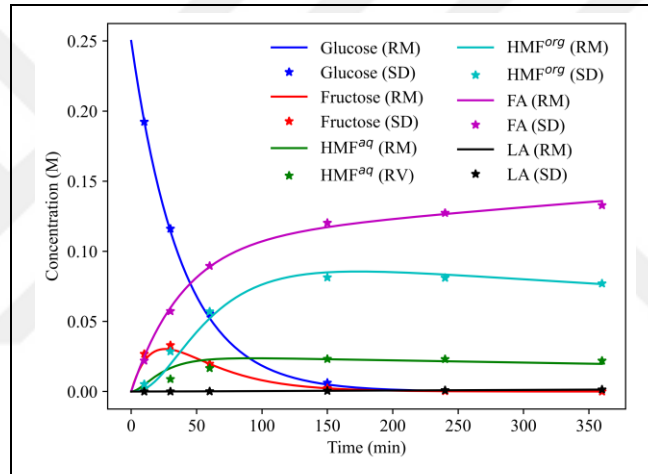


Figure 2.5: Synthetic data prediction performance of RM8R reduced with MINLP problem at 433K.

2.3.3. Effect of Initial Conditions to Reduced Model

Different initial concentrations change the dynamic profiles of the compounds. Therefore, parameters and variables affect the solution with varying sensitivity. In addition, reaction rate constants and concentrations have different effects on the obtained profiles. Algorithms and software used in MINLP problem solving are sensitive to the effect of parameters and variables on the system's response. Therefore, the components that are not initially present in the reaction medium have less effect on the system. In model reduction calculations, deleting the reaction rate constants, which have little effect, allows the model to make inferences with relatively less error.

Therefore, rigorous solvers start with model reduction by not including these variables [17].

Table 2.3: Initial concentrations (IC) used for generation of synthetic data.

Components	Initial concentrations (IC) (M)			
	IC ₁	IC ₂	IC ₃	IC ₄
Glucose	0.25	0.25	0.25	0.25
Fructose	0.00	0.05	0.00	0.05
HMF ^{aq}	0.00	0.00	0.00	0.00
HMF ^{org}	0.00	0.00	0.05	0.05
FA	0.00	0.00	0.00	0.00
LA	0.00	0.00	0.00	0.00

The initial concentration values used in this study are given in Table 2.3. As stated above, Tang et al. (2017) used IC₁ values in their study. In IC₂, fructose was added in addition to glucose. Fructose is the most important intermediate in the synthesis of HMF, so a model reduction study was carried out under the conditions of HMF and fructose in the reaction medium. The reason for keeping the preferred concentrations low is to preserve glucose as the primary raw material. It was aimed to investigate the effect of the system formed in the case of HMF in IC₃ on the model reduction. More chemical species have been identified in IC₄.

Minimized models were created by solving the MINLP problem at 403 K and applying four initial conditions to Equation (2.5). For IC₁ and IC₂, the RM5R network contains a set of k_1 , k_2 , k_3 , k_4 , and k_{10} reaction rate constants. RM7R network model obtained with k_1 , k_2 , k_4 , k_5 , k_8 , k_9 , and k_{10} reaction rate constants for IC₃. Similarly, IC₄ yielded the RM5R network consists of k_1 , k_4 , k_5 , k_6 , and k_{10} reaction rate constants. Table 2.4 lists the relevant reaction rate constant values.

Reduced network models for IC₁, IC₂, IC₃, and IC₄ are shown in Figure 2.6a, 2.6b, 2.6c, and 2.6d, respectively. Reactions that are in the initial reaction network but eliminated in the reduced network models are shown in red.

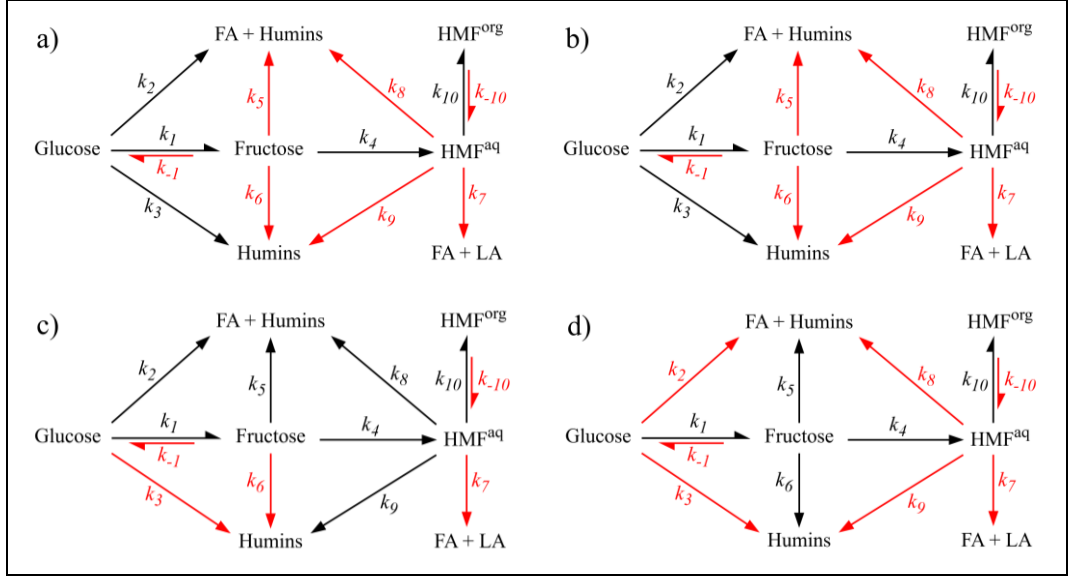


Figure 2.6: a) RM5R network reduced for IC₁ and 403K, b) RM5R network reduced for IC₂ and 403K, c) RM7R network reduced for IC₃ and 403K, d) RM5R network reduced for IC₄ and 403K.

Table 2.4: RM rate constants at different initial concentrations (IC) and 403K.

Reaction Rate Constants ($\times 10^{-5} \text{ min}^{-1}$)	Initial Concentrations			
	IC ₁	IC ₂	IC ₃	IC ₄
k_{-1}	0.00	0.00	0.00	0.00
k_1	13.89	6.73	20.87	32.38
k_2	18.28	21.26	13.67	0.00
k_3	2.07	4.38	0.00	0.00
k_4	40.73	33.26	62.95	33.94
k_5	0.00	0.00	17.27	75.50
k_6	0.00	0.00	0.00	14.80
k_7	0.00	0.00	0.00	0.00
k_8	0.00	0.00	28.72	0.00
k_9	0.00	0.00	40.79	0.00
k_{10}	165.69	168.02	27.86	48.52
k_{-10}	0.00	0.00	0.00	0.00

2.3.4. Reduced Model Prediction Performance at Different Conditions

The MINLP method allows for determining the number of reactions in model reduction. The same data used in the evaluation of RMs in the previous chapters was also used in their derivation. Therefore, the ability of RMs to describe data that is not used in model generation is a critical benchmark for their behavior under different process conditions. In other words, RMs can be used for different conditions. Considering this need, the RM8R network was created by reducing the model for 403K and IC₁ conditions. Instead of producing new models for different ICs, the performance of the model with the varying IC was investigated without changing the temperature. The concentration profile of the obtained RM8R network for IC₂ is given in Figure 2.7.

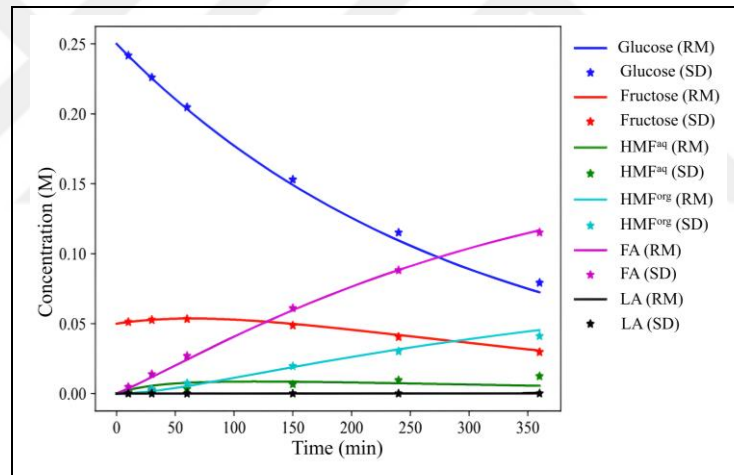


Figure 2.7: IC₂ prediction plot of RM8R network obtained for IC₁ at 403K.

Tang et al. (2017) observed that 433K shows higher rate constants. As a result, responses occur more quickly and approach the steady state. The RM8R network was constructed in 433K by using IC₁. Figure 2.8 illustrates the performance of the obtained RM8R network in IC₄ and 433K. The reduced network models derived from the MINLP problem can be employed at varying concentrations.

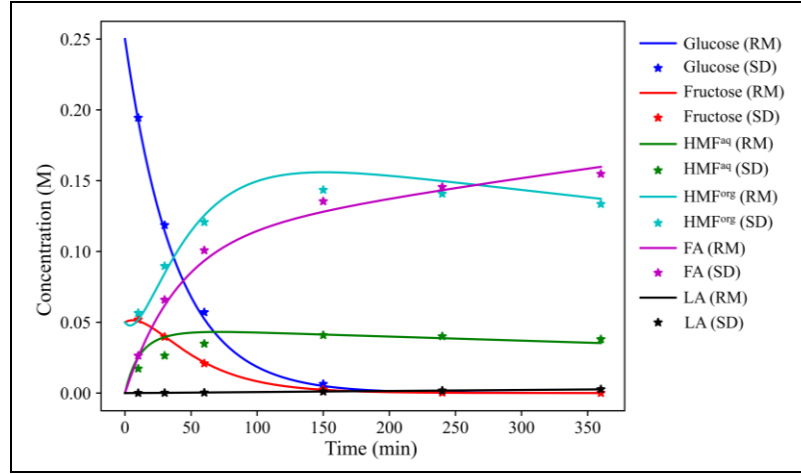


Figure 2.8: IC₄ prediction plot of RM8R network obtained for IC₁ at 433K.

2.3.5. Effect of MINLP Solver to Reduced Model

Optimization problems, which are divided into different classes as mathematical formulations, are solved by advanced and specialized programs. For example, linear and nonlinear problems are solved by different solver software. For this reason, it is necessary to use the correct solver program and to set up the problem in accordance with this program.

In this study, DICOPT and BONMIN solver programs were used. DICOPT is a paid MINLP solver program that uses the external approximation (OA) algorithm proposed by Duran and Grossmann in 1986 [18]. BONMIN is a free and open-source solution program that can solve problems with multiple algorithms. In its default settings, it solves using the simple branch and bound (BB) method, the emergence of which dates back to 1960 [19]. To compare the solver programs, the solutions were created with the default parameters, and the solution times were recorded. The PYOMO package is used to solve the optimization problem in two levels. The described case is transcribed according to the formulation format of the solvent used in the first phase. The problem is solved in the second phase by the solver. The number of variables, parameters, and constraints in the issue extends both processes.

The MINLP problem was developed for 413K and IC₁ and solved using DICOPT and BONMIN in the Linux Mint 20.04 64-Bit operating system. The Python programming language's built-in time function was used to measure time. The computations were run four times to get the solution times, and the average of the times was taken. Table 2.5 displays the averages of the recorded timings in seconds.

Table 2.5: Solver run times for model reduction calculations for IC₁ at 413K.

Solution Time (s)	The number of rate constants in the RM		
	12	8	5
DICOPT	0.9	4.1	2.9
BONMIN	27.4	100.1	3.0

The PYOMO library formulates the problem in 0.21 seconds. DICOPT reached a faster result in the solution of the optimization problem with many parameters in the analysis performed at the default settings. The reduced models and reaction rate constants remained unchanged while repeating the computations. This suggests that the provided solutions are stable. Apart from the usual methods, BONMIN's outer approximation (OA) algorithm has been examined, but no solution has been found. This is an indication that the options used in the solver algorithms should be correctly determined.

2.4. Conclusions

Mathematical models form the basis of computational analysis studies in engineering. The complexity of the equations they contain leads to computational problems in design and control work. In this study, the model reduction method, which is one of the alternative model creation methods that can overcome the problems brought by complex models and at the same time predict the dynamic behavior of the process in the best way, was applied to an exemplary reaction network model by using an innovative MINLP problem formulation.

Although the application's reaction network model is somewhat sophisticated, the same method is applicable to biological systems with considerably more complex models. The MINLP problem method is flexible and adaptable to various model networks, which provides advantages in industrial applications. Commercial or free solver programs are also available for the problem.

Different numbers of reactions can be obtained with the models obtained as a result of the MINLP problem solution. It is observed that these models, which are smaller compared to the reference model, can predict the behavior of the system at an acceptable error level. The constraints used in the MINLP problem formulation help shape the model to be obtained. It has been shown that the reduced models obtained

with different temperatures and initial concentrations can provide highly accurate predictions even at different initial concentrations.



3. SUPERSTRUCTURE OPTIMIZATION OF DIMETHYL ETHER PROCESS

3.1. Introduction

Chemical processes include complex and integrated pathways combined by several unit operations in which conversion occurs from feedstocks to valuable products. Such a conversion, in general, can be obtained through high number of alternative paths, which hinders the process architecture and operating condition selection under economic considerations and tightly ensured process constraints. Thus, a superstructure optimization problem formulation addressing simultaneously the aforementioned issues has become an important research area over the past decades.

A mixed-integer nonlinear problem is formulated, in general, to obtain a smaller architecture from a larger superstructure that is predefined and includes all alternative units, flows and many other considerations. The resulting MINLP formulation includes integer variables to account for sequences of events, alternative candidates, and the existence of units, whereas the continuous variables represent states. The MINLP problem is flexible and can include various user-defined considerations from economic and environmental aspects [3].

Significant developments in theory and computation have provided substantial capabilities to solve various complex optimization problems over the past decades [20]. With many alternatives and modifications, MINLP solvers can be classified roughly into two major groups as rigorous, and heuristic based on solution approach. Rigorous solvers utilize all mathematical tools to exploit optimality through the explicit formulation of all superstructure elements and might ensure global optimality for many cases. As an alternative, black-box or evolutionary algorithms benefit from the patterns from successive function evaluations, rather than focusing on derivative-based iterations, to provide optimality. Evolutionary algorithms, although suffering from significant computational load and local optimality issues, might deliver practical and satisfactory solutions to complex MINLPs once the associated plant models are challenging to derive and requires a priori knowledge due to numerous unknown driving forces and their nonlinearly interacting nature [21]. In contrast, despite significant computational developments and theoretical advancements, rigorous

solvers have scalability problems for large superstructures. In addition, integration of those to process flowsheet simulators which have widespread industrial use is a challenging task, hindering rigorous solver implementations. A significant fraction of superstructure optimization studies focusses on commercial software [22]. On the other hand, some free alternatives, including DWSIM, might provide similar performance to commercial ones [23]. Teerapat and Amata used a DWSIM simulation environment to validate an optimized DME process [24].

This study focuses on the simultaneous design and optimization of a comprehensive dimethyl ether (DME) process under several scenarios including different feedstock and unit operation prices using a free process flowsheet simulator, DWSIM, which is automated through Python. The superstructure involves different feedstocks which are processed through different reactors and separation units to be determined by the optimization problem in addition to some operating conditions. A genetic algorithm is used for the evolutionary solution of MINLP problem, which accounts for the existence of the units and plant operating conditions. The case studies show different process configurations are required for profitability based on feedstock and product prices.

3.2. Superstructure of DME Production Process

Dimethyl ether is one of the prominent candidates for relatively clean and sustainable alternatives to fossil fuels. The increased demand for DME can be met from synthesis gas or methanol from biological waste [25].

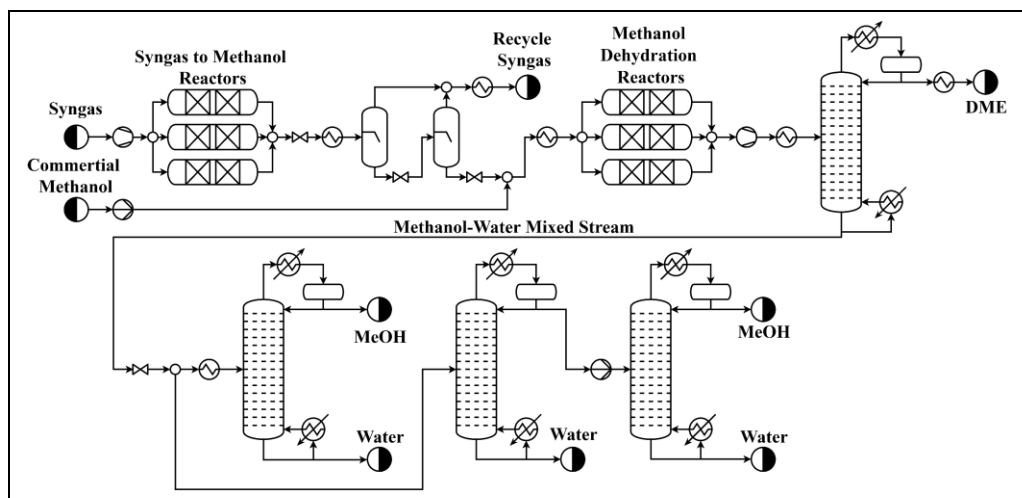


Figure 3.1: Superstructure of DME production process.

The proposed superstructure in this study is presented in Figure 3.1. DME production might be obtained with dehydration of methanol and from various feedstocks, primarily from syngas, as an emerging trend to favor carbon management and biomass utilization. The conditions specified in the kinetic study of Nestler *et al.* (2020) were used for modelling methanol synthesis at three different catalyst density yields high to low conversion [26]. Sequential flash units separate syngas from methanol with minimal loss at different pressures. Next, DME is produced with preheated methanol in catalytic dehydration reactor with three conversion preferences. Pressurized and cooled reactor effluent consists of mainly water, methanol and DME, which is obtained using 30 bar distillation column at high purity. Next, unreacted methanol and side product water recovered with two different distillation column arrangements. Side products are marketable/recyclable as well.

3.3. MINLP Formulation and Solution Method

Superstructure of DME process optimized with MINLP problem formulated as:

$$\min_{m,y,T,P} \quad IC + (OC - S \cdot (1 - f)) \cdot t_f \quad (3.1a)$$

$$s. t.$$

$$y_1 + y_2 = 1 \quad (3.1b)$$

$$y_3 + y_4 + y_5 = 1 \quad (3.1c)$$

$$y_6 + y_7 + y_8 = 1 \quad (3.1d)$$

$$y_9 + y_{10} = 1 \quad (3.1e)$$

$$m_6 = y_6 \cdot (m_1 y_1 + m_{F2} y_2) \quad (3.1f)$$

$$m_7 = y_7 \cdot (m_1 y_1 + m_{F2} y_2) \quad (3.1g)$$

$$m_8 = y_8 \cdot (m_1 y_1 + m_{F2} y_2) \quad (3.1h)$$

$$m_9 = y_9 \cdot m_{T101,B} \quad (3.1i)$$

$$m_{10} = y_{10} \cdot m_{T101,B} \quad (3.1j)$$

$$y_2 \cdot y_3 \cdot 6 \leq m_3 \leq y_2 \cdot y_3 \cdot 10.5 \quad (3.1k)$$

$$y_2 \cdot y_4 \cdot 6 \leq m_4 \leq y_2 \cdot y_4 \cdot 12.5 \quad (3.1l)$$

$$y_2 \cdot y_5 \cdot 6 \leq m_5 \leq y_2 \cdot y_5 \cdot 15.5 \quad (3.1m)$$

$$y_1 \cdot m_{1,min} \leq m_1 \leq y_1 \cdot m_{1,max} \quad (3.1n)$$

$$y_1 \cdot m_{2,min} \leq m_2 \leq y_2 \cdot m_{2,max} \quad (3.1o)$$

$$301 \leq T_1 \leq 308 \quad (3.1q)$$

$$360 \leq T_2 \leq 380 \quad (3.1r)$$

$$46 \leq P_1 \leq 50 \quad (3.1s)$$

$$y_j \in \{0, 1\} \quad j = 1 \dots 10 \quad (3.1t)$$

where t_f is the project lifetime which is 20 years for this case; f is the tax rate; y_1 and y_2 are binary variables for commercial methanol and syngas feedstock selection, respectively; y_3 , y_4 , and y_5 represent the selection of syngas to methanol reactor with corresponding mass flow rates m_3 , m_4 and m_5 ; y_6 , y_7 , and y_8 methanol dehydration reactor selection variables; m_{F2} is the flash unit effluent; $m_{T101,B}$ is the bottom product of DME distillation column; y_9 and y_{10} are one column and sequential two-column distillation route selection binaries, respectively; S is the income from the products. Equality constraints which include binary variables solely ensure selection of a single path among many. Commercial methanol and syngas stream mass flow rates are represented with m_1 and m_2 . High to low DME reactor inlet stream mass flow rates are m_6 , m_7 and m_8 , respectively. m_9 is 30-stage column and m_{10} is sequential two 15-stage columns mass flow rates. $m_{F102,B}$ is second flash unit bottom product stream that contains mainly produced methanol, mass flow rate. All produced or purchased methanol fed to DME reactor and this feed stream, $m_{R2,in}$, expressed with fifth equality constraint. $m_{T101,B}$ is bottom product mass flow rate of DME recovery column which fed to selected separation route. T_1 , P_1 are temperature and pressure of flash unit, and T_2 DME recovery column feed stream temperature, respectively. Inequality constraints limit syngas feed mass flow for prevent exceeding equipment sizes which assumed fixed for practical calculation of capital cost investments. The capital cost investment, IC , the operating cost, OC , is calculated from:

$$IC = F_{LANG} \cdot \left(\sum_i C_{BM,i} \cdot y_i + \sum_j C_{BM,fixed,j} \right) \quad (3.2)$$

$$OC = m_1 \cdot y_1 \cdot C_{MeOH} + m_2 \cdot y_2 \cdot C_{Syngas} + \sum_j Q_j C_{utility,j} \quad (3.3)$$

where F_{LANG} is the correction for the liquid phase operations; $C_{BM,i}$ is the bare module cost of i^{th} equipment which is related to the y_i ; $C_{BM,j}$ is the bare module cost of j^{th} equipment which exist in the structure independent of the optimization problem; C_{MeOH} and C_{Syngas} are methanol and syngas prices, respectively; Q_j and $C_{utility,j}$ is the quantity and the unit cost of j^{th} utility. Equipment purchases and operational cost calculations performed using Turton, (2018) and updated to current prices using CEPCI [27]. The distillation column fixed cost provided from ChemSep [28]. Process equipment sizing considers the dimensions that could meet the highest production capacity. For this reason, even if there is a high investment cost in low-capacity production preferences, meeting the upper limit production capacity is ensured.

A genetic algorithm (GA), introduced by Holland, is a heuristic search and optimization technique that mimics the process of evolution by iteratively generating and refining a population of potential solutions to the optimization problem [29]. The MINLP problem in Equation (3.1) is solved using GA which treats the process flow sheet simulation as a black-box function which is evaluated in DWSIM. Python has a key role in the implementation of the MINLP problem as it provides the communication between DWSIM and MATLAB's GA. A detailed implementation of the GA as well as sample code for generic optimization problems can be found in [30]. A simplified information flow diagram is shown in Figure 3.2. Detailed information flow diagram is given in Appendix B3.

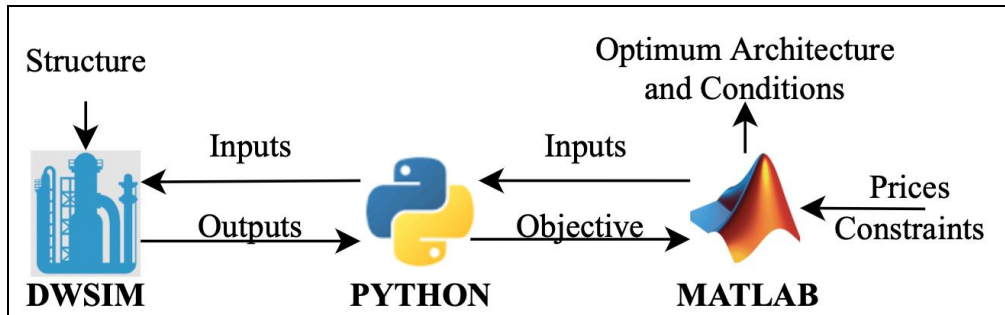


Figure 3.2: Superstructure optimization information flow diagram.

3.4. Results

MINLP problem in Equation (3.1) has been solved using MATLAB R2021a and DWSIM v6 on i5 9400 CPU 8 GB RAM Windows 10 x64 PC. In our case, the commercial methanol feedstock route results in an unprofitable process due to high purchase costs. The non-zero results of the solution are presented in Table 3.1.

In our case, syngas is selected as the primary raw material thanks to its low cost despite subsequent unit operations and associated operating costs. The resulting architecture proposes the highest conversion reactor for methanol production to favor the DME production and methanol which can be sold as a side product in our MINLP formulation.

Table 3.1: Non-zero process variables and economic measures of optimal results of Equation (3.1).

Plant variables									Economic Measures [M\$]		
m_2 [kg/s]	m_4 [kg/s]	m_{10} [kg/s]	$m_{R2,in}$ [kg/s]	$m_{F102,B}$ [kg/s]	$m_{T101,B}$ [kg/s]	T_1 [K]	T_2 [K]	P_1 [bar]	IC	OC	S
10.5	6.4	3.2	6.4	6.4	3.2	301	380	50	92	16	86

Temperature and pressure of flash unit maximize methanol yield while removing unreacted syngas. Produced methanol fed to medium conversion dehydration reactor to balance the DME conversion and related IC and OC. Sequential two 15-stage columns ensure the removal of high latent heat components while benefiting from the installation of large and single distillation column operations with high costs. The temperature of the feed stream as well as the temperature of the reboiler and condenser affect the efficiency of the separation process. However, feed stream temperature manipulation allows us to tune DME recovery column performance and operational costs. Overall process operation is performed at a maximum raw material rate within the defined operating window.

3.5. Conclusions

Optimum process design and synthesis under economic and environmental consideration is one of the contemporary challenges of the process systems engineering field. The idea of combining the advantages of process flowsheet simulators to obtain predictions without undergoing a significant modelling approach is useful once it is used in the black-box optimization algorithms which do not need first principal expressions explicitly. Commercial process simulators have been widely used in previous studies. Although these software packages provide complete environments, the license fees can be high. In contrast, alternative free simulators can provide competitive results at no additional cost. In addition, open-source simulators can be used in different systems to improve operational integration. The combination of an open-source DWSIM simulation environment with a black-box optimization solver allows us to simultaneously synthesize the process and optimize the conditions that consider feedstock selection, unit operation, catalyst selection, and related operating regimes. Such a sophisticated integration of a large number of process equipment alternatives and feedstocks results in a nonconvex and significantly nonlinear mixed-integer nonlinear optimization problem. The heuristic nature of genetic algorithms and all other derivative-free optimization approaches suffers from local optimality. Although they can provide a global optimum with an infinite time budget, this is not possible in practical applications. As a result, the global optimality of the proposed structure is beyond the scope.

A major decision variable on the plant profitability is determined by the feedstock, which is economically syngas over a wide price spectrum under current economic specifications. Furthermore, the proposed process flow diagram is comprehensive as it enables the selection of different-size unit operations to address the capacity, installation, and operating costs to deliver a realistic evaluation to some extent. Note that, the actual process is more complex than Figure 3.1 and requires a more advanced MINLP formulation which also takes uncertainties of plant variables and time-varying prices into consideration in addition to other economic considerations such as inflation and other realistic details including depreciation, land prices, and many other issues. A more detailed process synthesis and the including the impact of the price uncertainties which are characterized by logistic issues and market demands is beyond the scope. Thus, the simulations are performed for a particular and

acceptable price value under marketable feed and product compositions. The architecture is flexible to address those considerations and the impact of those variables on the ultimate plant design and operations conditions can also be calculated using the proposed scheme.



4. SIMULTANEOUS TOPOLOGY DESIGN AND OPTIMIZATION OF PDE CONSTRAINED PROCESSES BASED ON MIXED INTEGER FORMULATIONS

4.1. Introduction

Many engineering processes are described by partial differential equations (PDEs) to incorporate the intricate dynamics of transport phenomena, enabling a more sophisticated design for more efficient operational and control capabilities. Challenging optimization tasks for processes described by PDEs are broadly categorized into two categories: Nested Analysis and Design (NAND) and Simultaneous Analysis and Design (SAD) [31]. The NAND approach is often regarded as a block-box methodology based on the sequential realization of computational tasks after pseudo-decomposition of coupled equations into decentralized decision-making steps, still treating the state variables as implicit functions of the design variables, although indirectly. Thus, the state variables are basically exact solutions of the PDEs in each optimization iteration, which might yield suboptimal decisions based on a heuristic methodology during the solution. SAD methods, in contrast, satisfy process-related constraints and many other considerations simultaneously through a rigorous optimization framework. The simultaneous nature of the approach, despite increased computational load, introduces theoretical foundations to exploit all available benefits both in terms of process design and its management in real time, which would be harvested once rigorous solvers are used after some advanced mathematical reformulations.

Topology optimization (TO) is a research field dedicated to the development of algorithms for wiser architectures to obtain better processing performance based on case-dependent requirements. NAND methods, employing cumbersome trial-and-error procedures, might require a near-optimal initial guess to make use of the available degree of freedom under physical constraints [32]. However, a more innovative solution to expand the boundaries of traditional design paradigms and deliver superior performance in various engineering applications is an important concern and requires

a significant number of mathematical formulations and tools. Potential benefits from the field have gained significant attention over time and resulted in various studies employing different assumptions at micro and macro scales for TO problems. Borrvall and Petersson calculated an optimum flow profile in a 2-dimensional channel to minimize energy dissipation, considering Stokes flow of an incompressible fluid under low Reynolds numbers [33]. Gersborg-Hansen *et al.* and Olesen *et al.* considered a wider range of Reynolds numbers, incorporating fluid inertial effects and nonlinearities [34,35]. Evgrafov studied TO for slightly compressible fluids by relaxing the incompressibility constraint [36]. The impact from porous media within solid regions has been explored by Evgrafov, Guest *et al.*, and Wiker *et al.* [37–39]. Pingen and Maute considered non-Newtonian fluids in TO, while Challis and Guest used a discrete optimization problem with the level set method to solve Stokes flow [40,41]. Yoon applied TO to turbulent flows using the Spalart-Allmaras model, and more recently, Dilgen *et al.* demonstrated that optimized designs outperformed those created under a frozen turbulence assumption [42,43]. Sá *et al.* expanded the topology optimization model to include turbulent flows in rotating fluid domains using the Spalart-Allmaras model [44]. Beckers pioneered the use of formal mathematical programming with binary variables calculated by a sequential approximate programming and a Lagrangian dual method optimizer [45]. Later on, Sivapuram and Picelli addressed problems with binary design variables using sequential linear approximation and constraint relaxation [46]. Liang and Cheng proposed a method based on canonical duality theory (CDT) to solve the integer problem in binary TO [47]. In addition to fluid related problems TO has found significant implementations in other engineering disciplines, including the heat transfer problems, through including related driving fundamental equations and more sophisticated formulations, when needed. Choi introduced several novel preconditioners for small regularization parameters and demonstrated PDE-constrained solutions for static and dynamic systems for heat transfer problems [48]. Wolfmayr successfully achieved optimal heating of a swimming pool by dynamically optimizing the temperature profile of the air beneath a glass dome [49]. Furthermore, Gnegel *et al.* presented linear PDE-constrained optimization applications using the CPLEX rigorous solver for modeling the spread of wildfires and the mitigation of water contamination problems through a discretize-then-optimize approach [50].

To the best of the authors' knowledge, a simultaneous approach addressing architectural design and process related constraints has not found significant attention in the literature. With a complex set of process related expressions and advanced optimization tasks, global optimality of the solution and computational issues are important challenges unless those equations are tailored and solved using rigorous solvers with acceptable accuracy. In this study, we address these challenges by reformulating PDE-constrained MINLPs into MILPs to ensure global optimality by eliminating non-convex terms and handling computational aspects, still considering possible nonlinearities through piecewise approximations, if needed.

The remainder of this paper is structured as follows. In Section 4.2, we outline the proposed methodology and describe the computational environment used in our study. Section 4.3 presents the derived numerical optimization formulations for heat system design and topology optimization of channel flow. Moving forward, Section 4.4 provides detailed computational results from various case studies, accompanied by a discussion on the effects of different modeling components. In Section 4.5, we summarize our conclusions and offer insights into potential future research directions.

4.2. Simultaneous Topology Design and Optimization

The methodology employed in this study involves leveraging various computational methods and advanced mathematical formulations for the simultaneous design and optimization of PDE constrained processes through rigorous formulations. Such a comprehensive task is also associated with superstructure optimization tasks, in theory, where the existence of a particular variable from a larger domain, in which all available combinations are present, is calculated after the solution of a MINLP problem. Mixed-integer nature mostly appears due to existence issues and often leads to computationally challenging and NP-hard problems, hindering the solution unless formulations are tailored well to handle non-convex terms, when desired. In order to obtain a satisfactory solution under a manageable computational load, piecewise linear approximations and assumptions are introduced. The reformulated problems are subsequently solved using state-of-the-art solvers known for their ability to handle the ultimate mixed-integer linear programming (MILP) and mixed-integer quadratic programming (MIQP) problems. In particular, state-of-the-art solvers such as Gurobi [51] and CPLEX [52] are used to efficiently and effectively solve the optimization

challenges posed by the reformulated PDE-constrained problems. These solvers have established themselves as powerful tools in the field, enabling the solution of complex optimization tasks with a high degree of accuracy and computational efficiency. In addition to that, the one-dimensional heat problem is solved using several solvers, including a local solver, SHOT [53], and a global solver, SCIP [54]. All computations are performed using the Python/PYOMO environment [14]. The implementation of the proposed approach is demonstrated through heat transfer and fluid problems.

4.3. Heat Transfer Problem

The transient heat equation with heat generation is defined as follows:

$$\rho C_p \frac{\partial T}{\partial t} = k \left[\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right] + Q_{gen} \quad (4.1)$$

where ρ is density (g/cm^3); C_p and k are the specific heat capacity ($J/g.K$) and the thermal conductivity of solid ($W/cm.K$), respectively; Q_{gen} is the heat generation term (W); x, y and z are the spatial coordinates (cm); T is the temperature ($^{\circ}C$). Small changes in temperature do not affect the properties of metals, such as density, heat capacity, and thermal conductivity, so these properties are assumed to be constant.

The convective heat transfer equation with constant heat transfer rate expressed as:

$$Q_{conv} = hA_s(T - T_{\infty}) \quad (4.2)$$

where Q_{conv} is the heat dissipated by convection (W); h is the heat transfer coefficient ($W/cm^2.K$); A_s is the heat transfer area (cm^2); T_{∞} is the surrounding temperature ($^{\circ}C$). Integration of Equation (4.1) and (4.2) for the one-dimensional system yields typical unsteady-state heat transfer equation with conduction, convective energy loss and generation with heat generation is defined by:

$$\rho C_p \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial x^2} + Q_{gen} - h(T - T_{\infty}) \quad (4.3)$$

With many implementations in engineering, Q_{gen} is an externally added heating source at certain locations to favor a particular temperature profile under dynamic regime.

Thus, the location and the energy rate provided by these become an important decision variable as other terms in the equation are considered environmental contributions with no explicit manipulation capability.

Following simultaneous optimization problem is solved for the calculation of the location of the energy sources and their rates:

$$\min_{T, Q, b} \sum_{i=1}^N w_T T_{s,i} (T_{i,t_f} - T_{set})^2 + w_Q Q_{Total} \quad (4.4a)$$

s. t.

$$\rho C_p \frac{\partial T_i}{\partial t} = k \frac{\partial^2 T_i}{\partial x^2} + Q_{gen,i} - h(T_i - T_{\infty}) \quad i = 1, \dots, N \quad (4.4b)$$

$$Q^{LB} b_i \leq Q_{gen,i} \leq Q^{UB} b_i \quad i = 1, \dots, N \quad (4.4c)$$

$$\sum_{i=1}^N b_i \leq Q_{num} \quad (4.4d)$$

$$\sum_{i=1}^N Q_{gen,i} = Q_{Total} \quad (4.4e)$$

$$Q_{gen,i} \geq 0 \quad i = 1, \dots, N \quad (4.4f)$$

$$T^{LB} \leq T_{i,t_f} \leq T^{UB} \quad i = 1, \dots, N \quad (4.4g)$$

$$b \in \{0,1\} \quad (4.4h)$$

$$T_s \in \{0,1\} \quad (4.4i)$$

where b_i is a binary variable representing the existence of an energy source at discretization point i ; T_{set} is the desired temperature; $T_{s,i}$ is a binary pre-specified parameter value for i^{th} discretization point to account for the deviations form T_{set} ; w_T and w_Q are weights for temperature and total energy rate, respectively; Q^{LB} and Q^{UB} are lower and upper bounds for energy rate, respectively; Q_{num} is the desired number of energy sources; Q_{Total} is the total energy rate available for the process; T^{LB} and T^{UB} are lower and upper bounds for temperature, respectively; t_f is the final time. With simultaneous calculation of the binary variables and energy rates, the optimization problem delivers the optimal configuration for energy source placement, thereby enabling precise temperature control and achieving the desired thermal performance while also calculating the energy rate of each energy source. By linking constraints,

those rates are constrained to non-zero values only once the corresponding binary variable is one. Those constraints also tighten the search space for the optimization tasks, introducing more efficiency and reducing the computational load. In addition, the total number of energy sources and total available energy are also introduced as constraints. Note that the proposed formation is flexible, and any process requirement can be included to yield an optimum topology once those requirements enable a feasible solution.

A 50-cm-long aluminum rod was used for the transient one-dimensional case studies, and the parameters used for system description are given in Table 4.1.

Table 4.1: Constant parameters of the transient heat system used in Case 1 & 2.

$\rho \left[\frac{g}{cm^3} \right]$	$C_p \left[\frac{J}{g \cdot K} \right]$	$k \left[\frac{W}{cm \cdot K} \right]$	$h \left[\frac{W}{cm^2 \cdot K} \right]$	$T_{\infty} [^{\circ}C]$
2.7	0.897	2.37	0.01	22

Equation (4.4) is solved using three different considerations to show how those change the structural properties of the ultimate process in addition to operation condition values. Some of the results are provided in Table 4.2.

Table 4.2: Energy source locations and their rates.

	Case 1		Case 2		Case 3
Location [cm]	T_{set} [$^{\circ}C$]	Q_{gen} [W]	T_{set} [$^{\circ}C$]	Q_{gen} [W]	Q_{gen} [W]
5.0				0.8	
7.5					1.03
10.0	40	0.73	40		1.03
15.0					1.03
25.0	45	1.28	45	0.8	
32.5				0.8	
35.0					1.03
37.5				0.8	
40.0	50	1.84	50	0.8	
42.5					1.03

Case 1 includes a time-invariant temperature set point for the described locations. This case does not impose any specific constraints on individual energy sources, besides box constraints, and the resulting configuration contains three energy

sources located exactly at the set point defined locations, with different energy rates. The corresponding temperature profiles and energy sources are presented in Figure 4.1a.

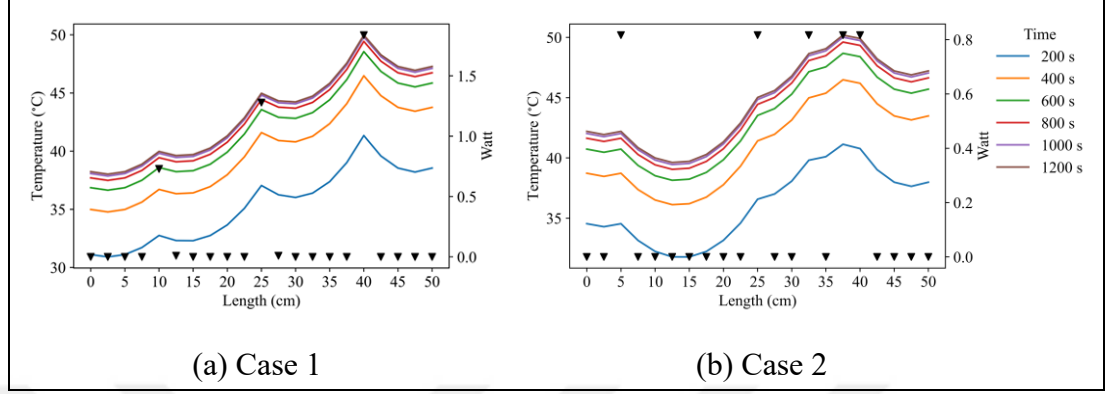


Figure 4.1: Temperature profiles and energy sources.

Case 2 imposes further restrictions on the energy rates by fixing all of them to a particular value within the box constraints. Such a case is commonly encountered in industrial processes where some energy sources (i.e., electricity rods) have a discrete operating regime capability with limited options. The resulting architecture could achieve the desired set points using five energy sources. The energy rates and the locations are presented in Table 4.2 and Figure 4.1b. Note that, Case 1 delivers a 6.1% energy saving relatively. This illustrates the effectiveness of the proposed methodology in optimizing heater placement and power distribution to achieve improved energy efficiency in the system.

Equation (4.5) is further modified to consider the impact of the time-dependent set point handling capability and transformed into:

$$\min_{T, Q, b} \sum_{i=1}^4 w_T (T_{25,i} - T_{set,i})^2 + w_Q Q_{Total} \quad (4.5a)$$

s. t.

$$\rho C_p \frac{\partial T_i}{\partial t} = k \frac{\partial^2 T_i}{\partial x^2} + Q_{gen,i} - h(T_i - T_{\infty}) \quad i = 1, \dots, N \quad (4.5b)$$

$$Q^{LB} b_i \leq Q_{gen,i} \leq Q^{UB} b_i \quad i = 1, \dots, N \quad (4.5c)$$

$$\sum_{i=1}^N b_i \leq Q_{num} \quad (4.5d)$$

$$\sum_{i=1}^N Q_{gen,i} = Q_{Total} \quad (4.5e)$$

$$Q_{gen,i} \geq 0 \quad i = 1, \dots, N \quad (4.5f)$$

$$T^{LB} \leq T_{i,t_f} \leq T^{UB} \quad i = 1, \dots, N \quad (4.5g)$$

$$\mathbf{b} \in \{0,1\} \quad (4.5h)$$

where $T_{set,i}$ is the setpoint temperature of the center location at a particular time, and temperatures of 40, 45, 50, and 55 °C were employed for time points of 300, 600, 900, and 1200 s, respectively.

Such a requirement delivers a different configuration for the energy source locations, which are shown in Table 4.2, and in turn delivers a temperature profile in Figure 4.2.

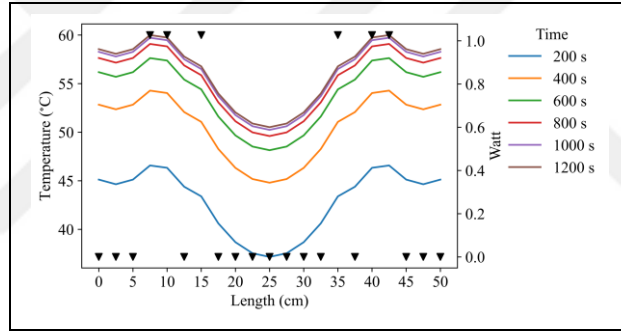


Figure 4.2: Temperature profiles and energy sources for Case 3.

4.4. Channel Topology Optimization for 2-D Stokes Flow

The governing equations of the steady state simplified incompressible Stokes flow are given by:

$$0 = -\nabla p + \mu \nabla^2 \mathbf{v} \quad (4.6a)$$

$$0 = (\nabla \cdot \mathbf{v}) \quad (4.6b)$$

where μ is the viscosity of fluid; p is the pressure; and $\mathbf{v}$ is the velocity. Equation (4.6) has found significant amount of application in the process engineering where many steams are combined and flow patterns are formed using different elbow and pipe

designs to ensure an acceptable pressure drop throughout the flow regime, reducing the pumping cost and lengthening the equipment durability in addition to a smoother flow regime. A typical mixed integer optimization formulation for the task is given by:

$$\min_{u,v,b} \sum_{i=1}^N \sum_{j=1}^M \left\{ \left(\frac{\partial p_{i,j}}{\partial x_{i,j}} \right)^2 + \left(\frac{\partial p_{i,j}}{\partial y_{i,j}} \right)^2 \right\} \quad (4.7a)$$

s. t.

$$0 = -\frac{1}{\rho} \frac{\partial p_{i,j}}{\partial x_{i,j}} + \frac{\mu}{\rho} \left(\frac{\partial^2 u_{i,j}}{\partial x_{i,j}^2} + \frac{\partial^2 u_{i,j}}{\partial y_{i,j}^2} \right) \quad \forall i,j \in \Omega_d \quad (4.7b)$$

$$0 = -\frac{1}{\rho} \frac{\partial p_{i,j}}{\partial y_{i,j}} + \frac{\mu}{\rho} \left(\frac{\partial^2 v_{i,j}}{\partial x_{i,j}^2} + \frac{\partial^2 v_{i,j}}{\partial y_{i,j}^2} \right) \quad \forall i,j \in \Omega_d \quad (4.7c)$$

$$\frac{\partial u_{i,j}}{\partial x_{i,j}} + \frac{\partial v_{i,j}}{\partial y_{i,j}} = 0 \quad \forall i,j \in \Omega_d \quad (4.7d)$$

$$\sum_{i=1}^N \sum_{j=1}^M b_{i,j} \leq \Theta \quad (4.7e)$$

$$\left. \frac{\partial p}{\partial x} \right|_{i,j} = \left. \frac{\partial p}{\partial y} \right|_{i,j} = 0 \quad \forall i,j \in \Gamma_{wall} \quad (4.7f)$$

$$u_{i,j}, v_{i,j}, b_{i,j} = 0 \quad \forall i,j \in \Gamma_{wall} \quad (4.7g)$$

$$b_{i,j} = 1 \quad \forall i,j \in (\Gamma_{in} \cup \Gamma_{out}) \quad (4.7h)$$

$$u_{i,j}, v_{i,j} \geq 0 \quad \forall i,j \in (\Gamma_{in} \cup \Gamma_{out}) \quad (4.7i)$$

$$u^{LB} b_{i,j} \leq u_{i,j} \leq u^{UB} b_{i,j} \quad \forall i,j \in \Omega_d \quad (4.7j)$$

$$v^{LB} b_{i,j} \leq v_{i,j} \leq v^{UB} b_{i,j} \quad \forall i,j \in \Omega_d \quad (4.7k)$$

where Ω_d is the domain set, defined by $N \times M$ discretization points on which the fluid motion is theoretically allowed and governing equations hold; b is a matrix with proper dimensions to represent the existence of any non-zero state variable through binary variables and ensures zero velocities through linking constraints, benefiting from upper and lower bounds of velocities, for computational efficiency tasks to eliminate the multiplication of binary variable and the corresponding velocity in the governing equations, contributing to theoretical advancements in mixed-integer linear solutions; θ is a pre-defined tuning parameter to manipulate the extent of discretization points

where no fluid motion is observed; Γ_{in} and Γ_{out} are discretization point sets to define flow inputs and outputs, respectively; Γ_{wall} is the set where no fluid motion is possible and corresponding binary variable is also zero. Figure 4.3 shows these sets for a tubular flow case where fluid is fed from the left as an example:

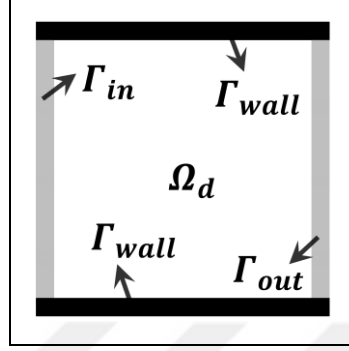


Figure 4.3: A domain set example for tubular flow.

The objective function in Equation (4.7) includes the impact of the pressure change on discretization points and minimized through the simultaneous consideration of velocities in addition to b which in turn defines topology. Note that, the formulation is flexible to any flow-related requirement including maximum velocities, velocity and pressure gradients, and many other variables, if needed. A further advancement is introduced on the quadratic penalty in the objective function using piecewise linear approximations and given by:

$$\min_{\lambda, \beta} \frac{\partial p}{\partial x} \quad (4.8a)$$

$$s. t.$$

$$\alpha_1 \lambda_1 + \dots + \alpha_{20} \lambda_{20} = \frac{\partial p}{\partial x} \quad (4.8b)$$

$$\delta_1 \lambda_1 + \dots + \delta_{20} \lambda_{20} = \left(\frac{\partial p}{\partial x} \right)^2 \quad (4.8c)$$

$$\sum_{i=1}^{20} \lambda_i = 1 \quad (4.8d)$$

$$\lambda_1 \leq \beta_1 \quad (4.8e)$$

$$\lambda_i \leq \beta_{i-1} + \beta_i, i = 2, \dots, 19 \quad (4.8f)$$

$$\lambda_{20} \leq \beta_{19} \quad (4.8g)$$

$$\beta \in \{0,1\} \quad (4.8h)$$

where α and δ are breakpoints for the approximation; λ and β is a binary variable vector for the formulation. Thus, Eq. 4.7 can be solved using mixed-integer linear solvers once Equation (4.8) is integrated after it is implemented considering all spatial dimensions.

4.4.1. Tubular Flow

A tubular flow scenario with a narrow exit is desired by solving Equation (4.7) after piecewise approximations and introducing the additional constraints to ensure a symmetric flow profile:

$$b_{i,j} = b_{i,n-j} \quad \forall i, j \in \Omega_d \quad (4.9)$$

The resulting flow profile is shown in Figure 4.4a which also demonstrates the pressure profile as background color spectrum with an increasing pattern as whiteness intensity increases.

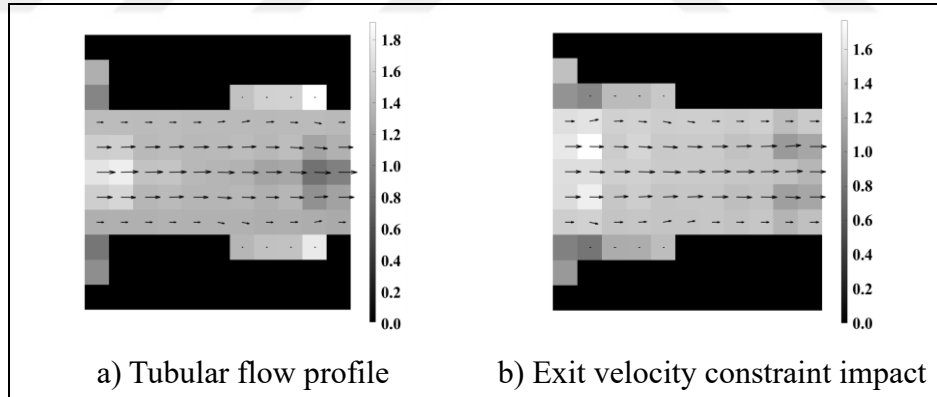


Figure 4.4: Tubular flow profile calculation results.

Additionally, Figure 4.4b is calculated through adding a maximum exit flow rate velocity constraint. Such a constraint changes the location of the expansion and contraction region in Figure 4.4a towards the inlet, lowering the center exit velocity by a more saturated flow profile, rather than concentrating the whole material flow around the center, which causes velocity increase.

4.4.2. Curved Pipe Design

In contrast to Equation (4.9), which delivers a symmetric topology profile with respect to x axis, symmetry constraints to ensure diagonal symmetry is obtained through using:

$$b_{i,j} = b_{n-i,n-j} \quad \forall i, j \in \Omega_d \quad (4.10)$$

The occurrence of expanding and contracting channel structures is eliminated with the introduction of the channel width constraint, and is given by:

$$5 \leq \sum_{j=2}^{M-1} b_{i,j} \leq 7, i = 1, \dots, N \quad (4.11)$$

The restriction of channel width promotes the development of a plain structure and reduce the computational burden. Equation (4.11) allows the formation of a topology of 5 to 7 discrete points in width by considering the input width and involving the formation of curvature.

Figure 4.5b shows the impact of Equation (4.11) on the domain set provided in Figure 4.5a.

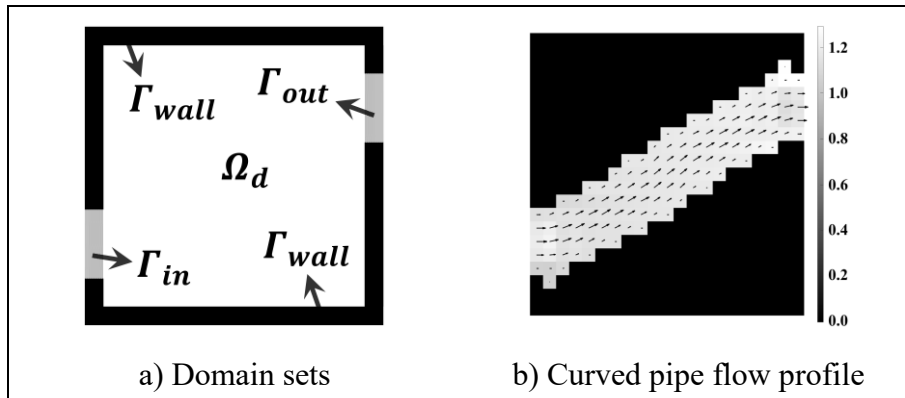


Figure 4.5: Curved pipe design domain and calculation results.

Figure 4.5b depicts the optimal topology achieved through a higher number of discrete points, in contrast to Figure 4.5b, for a more accurate solution to consider high curvature due to desired task.

4.4.3. Design of Flow Joint

Through the modification of the tubular flow problem, a flow joint topology optimization is formulated, wherein two feed streams are combined before leaving the mixing zone through a single exit as shown in Figure 4.6.

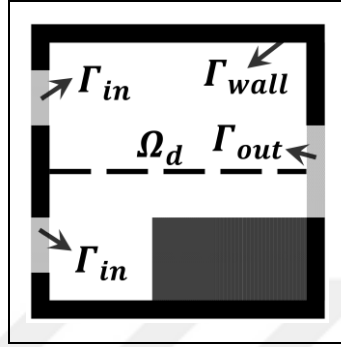


Figure 4.6: Two input and one output flow joint problem domain.

An initial topology guess, preferably close to the optimal design, combined with a flow profile guess has a significant impact on the computational load. That knowledge is usually built upon historical data or generic process knowledge enhanced by governing equations. The proposed explicit formulation and rigorous solution method also benefit from this once those are defined by additional constraints. In this case, the Y-shaped flow enables the merging of two flows while accounting for energy loss resulting from pressure variations. Figure 4.7a is calculated with no additional constraint on the shaded in Figure 4.6, which is a region where no significant flow profile is anticipated due to the locations of feed and exit, resulting a 6-hour computation delivering 1.16% optimality gap.

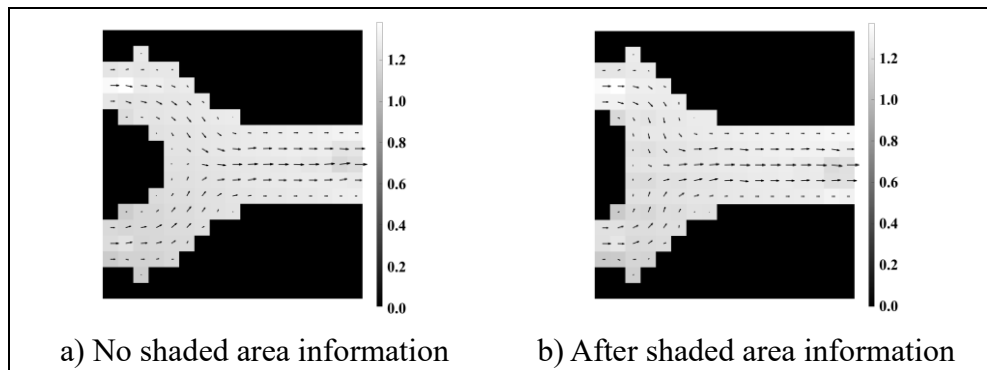


Figure 4.7: Optimized joint flow topologies with different domain sets.

Similar task is performed by defining the shaded area as additional constraints in 30 seconds with 0.01% optimality gap. The resulting topology and flow profile is given in Figure 4.7b.

4.4.4. Conclusions

The decentralized decision-making process in the design and operating of complex processes hinders the exploiting all theoretical benefits and potential improvements. Such a downside is commonly desired due to pseudo-decomposition of process variables and decoupling of some governing equations, which in turn enable a local but computationally and mathematically more manageable sets of equations. Both the complexity of the equations combined with the nonlinear interactions among process variables and topology introduces the theoretical and practical challenges once a simultaneous approach is desired to avoid successive and iterative processes. Those nested methods usually employ a fixed topology during the optimization which are mostly limited to functions of continuous variables from the governing equations or other tasks. Thus, those iterations are highly exposed to local solutions and sensitive to initial topology guess. In addition, topology and other constraints need to be decomposed to different layers in the hierarchy, introducing additional theoretical discrepancies among those and might result in infeasible solutions, which could be handled more easily using simultaneous approach which treats all variables in the same and unified optimization problem.

This study presents a mixed integer formulation for simultaneous topology design and optimization, which has attracted little attention in the literature so far and would introduce significant theoretical and practical advancements in recent engineering problems. Proposed formulation benefits from high number of binary variables to constrain the continuous variables in the governing equations to zero, representing the location or existence of a particular impact. Logic constraints are also introduced to tighten the search space for the optimization problem. Nonlinear terms in the optimization problem are approximated through piecewise approximations which introduce additional binary variables. Such an approach is intuitively and theoretically more desirable since all process requirements are formulated explicitly and solved to global optimality when rigorous solvers are used after reformulations and decompositions on the optimization problem. With an increased computational load,

such approach benefits from high parallelization capability due to strong achievements in the mixed integer linear algorithms and sophisticated solvers. Thus, a more complex topology and process requirements can also be solved, if needed.

The methodology is implemented on a heat transfer and fluid problem. In the first case, simultaneous design and dynamic optimization of the process calculates the location and power of heaters, introducing a significant decrease in energy consumption, highlighting the potential benefits of the approach. Second problem focuses on the stokes flow whose flow pattern is formed to minimize the pressure drop. In summary, the proposed formulation offers promising improvements for simultaneous topology optimization and dynamic optimization tasks. By combining advanced formulation techniques with robust solvers, we aim to increase the efficiency and effectiveness of the optimization process, leading to improved designs and informed decision-making in various engineering applications. Our current focus is the development of more advanced mathematical reformulations to deal with more complex problems.

5. CONCLUSION

Due to increasingly stringent regulations, the design and operation of engineering systems are becoming more complex. Mixed integer nonlinear programming is frequently encountered in the synthesis, optimization, and control of chemical engineering systems. Many modern rigorous and heuristic solvers have been developed for these problem solutions, which remain challenging because of the combinatorial nature of the problems. Rigorous algorithms employ explicit mathematical expressions to find the optimal solution, whereas heuristic algorithms rely on algorithms inspired by various sources and iterative function evaluations to find the optimal solution. These advancements in the solution algorithms have significantly increased the scale of problems that can be tackled, but there remain limitations to their application. Despite the progress made, there is still room for improvement to enable us to solve a broader range of problems.

Engineering computational analysis studies rely heavily on mathematical models, which can pose significant computational challenges due to their complex equations. To address these issues, this study employs the model reduction method, an alternative approach that predicts process dynamics while simplifying complex models. An innovative MINLP problem formulation is used to apply this method to an exemplary reaction network model. While the reaction network model is intricate, the same approach is applicable to biological systems with much more complex models. Moreover, the MINLP problem formulation is adaptable and flexible, providing an advantage in industrial applications. Commercial or free solver programs are also available to solve the problem.

The models generated by the MINLP problem solution produce varying numbers of reactions. However, these models are smaller than the reference model, yet they can predict the system's behavior with an acceptable margin of error. Additionally, the constraints used in the MINLP problem formulation shape the resulting model. The study further demonstrates that reduced models obtained at different temperatures and initial concentrations can provide highly accurate predictions, even at varying initial concentrations.

Designing and synthesizing optimal processes that account for both economic and environmental factors is a pressing challenge in process systems engineering. A promising approach is to combine the benefits of process flowsheet simulators with

black-box optimization algorithms, which do not require explicit first-principles expressions. The integration of the open-source DWSIM simulation environment with a black-box optimization solver allows for simultaneous process synthesis and optimization of conditions, unlike many studies that focus on commercially available software packages and a limited range of process options. However, this integration results in a highly complex and nonlinear mixed-integer optimization problem, which cannot guarantee global optimality.

The feedstock is a crucial decision variable that significantly impacts plant profitability and is economically syngas over a broad price range under current economic specifications. The proposed process flow diagram enables the selection of different-sized unit operations to address capacity, installation, and operating costs, providing a realistic evaluation to some extent. However, the actual process is more intricate than Figure 3.1 and requires a more advanced MINLP formulation that considers plant variable uncertainties, time-varying prices, inflation, depreciation, land prices, and other realistic details. While the proposed scheme is flexible enough to address these considerations, a more detailed process synthesis that incorporates the impact of price uncertainties characterized by logistic issues and market demands is beyond the scope of this study. Therefore, simulations are performed for a specific price value and marketable feed and product compositions. Nonetheless, the proposed architecture provides a foundation for exploring the impact of these variables on plant design and operation conditions.

The presented mixed integer formulation for solving PDE-constrained optimization problems allow simultaneous treatment of topology and process variables, which are highly interacting in many engineering systems. The methodology is implemented in the design of transient heat and 2-dimensional Stokes flow systems. Simultaneous dynamic optimization of the position and power of heaters yields a significant decrease in energy consumption, highlighting the potential benefits of our approach. Common benchmark flow topology problem results indicated that high-quality topologies were limited by solver capabilities. Overall, our proposed formulation offers promising improvements for PDE-constrained topology optimization problems. By combining advanced formulation techniques with robust solvers, we aim to increase the efficiency and effectiveness of the optimization process, leading to improved designs and informed decision-making in various engineering applications. In conclusion, our study contributes to the field of PDE-

constrained optimization by presenting a novel mixed integer formulation that addresses the challenging task of topological optimization.

Optimization problems are prevalent in various fields such as engineering, economics, and computer science. However, the progress in the improvement of algorithms for solving these problems has slowed down in recent years. To overcome this challenge, future work should focus on improving the problem modeling approach and formulation. One promising approach is the use of mathematical linearization and relaxation methods to tackle mixed-integer nonlinear programming problems. These methods can help overcome the difficulties in finding exact solutions for such problems, and they have been successful in several practical applications. Moreover, empirical modeling approaches such as artificial neural networks have gained attention in recent years due to their ability to represent nonlinear behavior in a flexible manner. A hybrid structure combining these models with first-principles relationships can be a promising approach for solving complex optimization problems. Overall, focusing on the problem modeling approach and formulation can lead to significant improvements in solving complex optimization problems, and combining different approaches can further enhance the performance of these methods.

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BIOGRAPHY

Emrullah ERTÜRK successfully earned his bachelor's degrees in both Bioengineering and Chemical Engineering from Yıldız Technical University in 2019 and 2020, respectively. In 2021, he commenced his graduate studies at Gebze Technical University in Chemical Engineering department. From January 2021 to 2023, he served as a research assistant within the Department of Chemical Engineering at Gebze Technical University. Subsequently, in February 2023, he transitioned to the same position at the Izmir Institute of Technology, where he continues his research endeavors.



APPENDICES

Appendix A1: Publications

Erturk E., Aydin E., Sildir H., (2021), “Tam Sayılı ve Sürekli Optimizasyon Problemi ile Reaksiyon Ağ Modellerinin Küçültülmesi” Konya Journal of Engineering Sciences, Vol. 9, 142–156.

Appendix A2: Book Chapters

Erturk E., Aydın E., Sarrafi S., Deliismail O., Zahidova A., Sildir H., (2022), “Superstructure Optimization of Dimethyl Ether Process” In: “Computer Aided Chemical Engineering”, Elsevier, pp. 661–666.

Appendix A3: Proceedings & Presentations

Sildir H., Erturk E., Sarrafi S., (2022), “Simultaneous Design and Optimization of Complex Processes Constrained by Partial Differential Equations using Mixed Integer Formulations”, The 19th EUROPT Workshop on Advances in Continuous Optimization, Lisbon, Portugal.

Erturk E., Aydin E., Deliismail O., Zahidova A., Sarrafi S., Sildir H., (2022), “Superstructure Optimization of Dimethyl Ether Process”, European Symposium on Computer-Aided Process Engineering-32, Toulouse, France.

Erturk E., Aydin. E., Sildir H., (2021), “Tam Sayılı ve Sürekli Optimizasyon Problemi ile Reaksiyon Ağ Modellerinin Küçültülmesi”, Ulusal Kimya Mühendisliği Kongresi, Online.

Appendix B1: Sample Data Generation

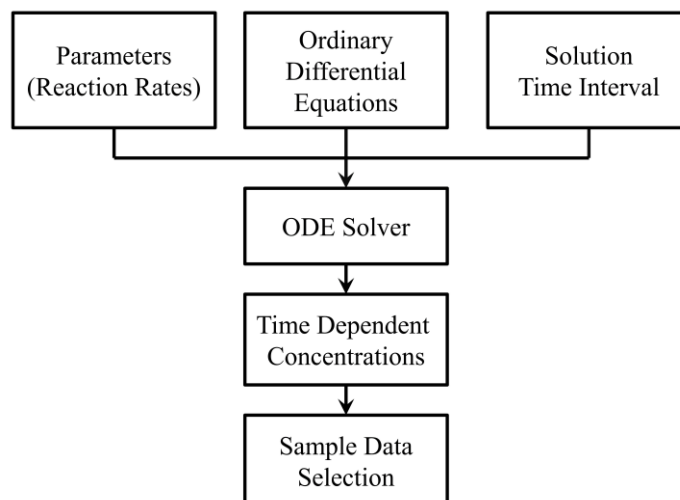


Figure B1.1: Data generation procedure elements and information flow diagram.

Appendix B2: Implementation of Reaction Network Reduction in PYOMO

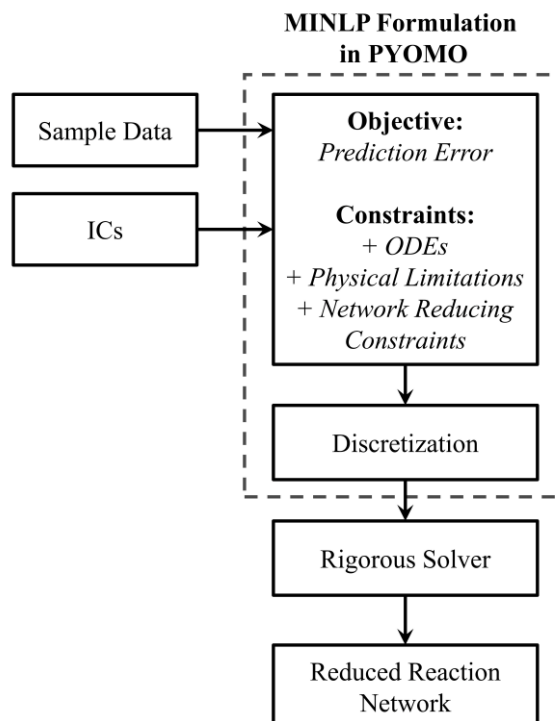


Figure B2.1: Components of reaction network reduction implementation with PYOMO.

Appendix B3: Detailed Computation Framework

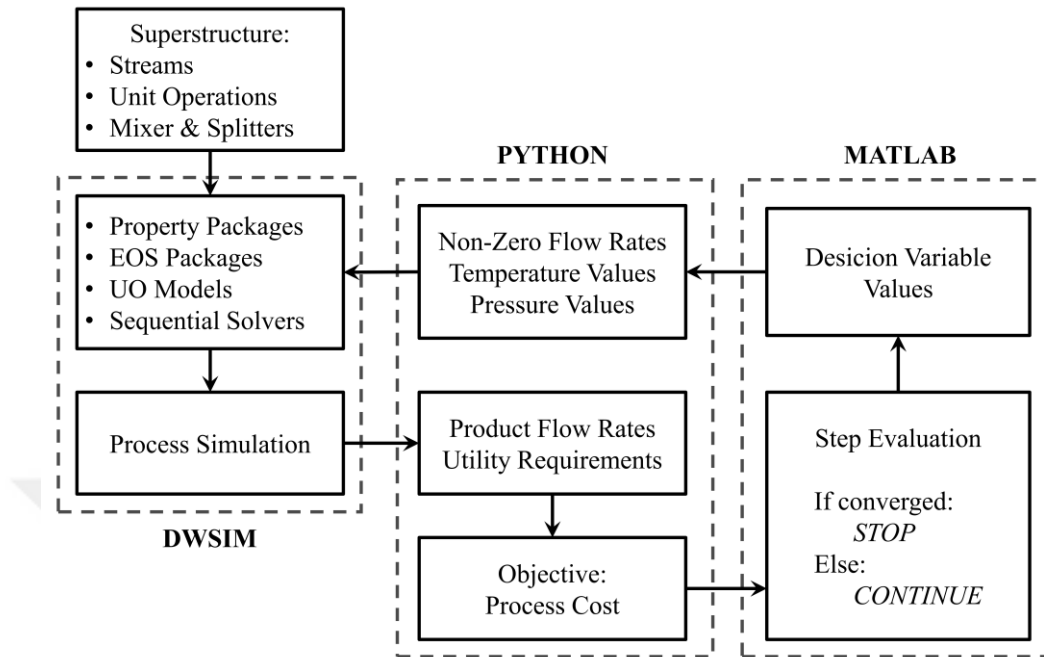


Figure B3.1: Information flow diagram of superstructure optimization of dimethyl ether process by integrating DWSIM with MATLAB GA.