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# Synthesis of Optimum Chemical Reactor Network Using Combination of Superstructure Model and Fuzzy Approach Method

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**Abstract**

Given the mechanism of reaction kinetics and the reaction rate equations, this paper presents a systematic approach to determine the optimum chemical reactor network to achieve the desired objective function. A general superstructure configuration is used to select the optimum combination of plug flow reactor (PFR) and continuous stirred tank reactor (CSTR) to get maximum yield of desired product (maximum concentration), minimum volume of the reactor, minimum operating temperature, or maximum selectivity and conversion. PFR is approximated as a series of CSTRs. The superstructure approach allows for series and parallel reactor network as it contains all possible sequences. This model can be formulated as nonlinear programming (NLP) problems, which can be solved using GAMS. Final decisions representing reactor types, sequence, and volume can be made using continuous parameters. Results obtained from GAMS are further optimized using fuzzy approach. Two literature examples are presented and solved to demonstrate the effectiveness of the approach.

***Keywords:*** *CSTR; PFR; Reactor network; Superstructure; General algebraic modeling system, Nonlinear programming.*

## 1. Introduction

Chemical reactor network synthesis plays a vital role in the design and optimization of chemical processes, offering significant opportunities to enhance efficiency, minimize costs, and achieve desired product specifications. The design of an optimal reactor network involves selecting suitable reactor types, determining their configurations, and optimizing operating conditions to maximize desired outcomes. Over the years, researchers have developed various methods and techniques to tackle the complexities associated with chemical reactor network synthesis. This paper aims to provide a new systematic approach for synthesis of chemical reactor network involving multiple objective functions using combined Fuzzy algorithm and superstructure approach based on a proposed model that optimized at different temperature using GAMS software. After that the results obtained from GAMS are further optimized using FUZZY Approach.

Grossmann et al have presented a new method for reactor network synthesis using uncertain parameters which expressed as bounded variables [1]. Chitra and Govind used a geometrical interpretation for design of only isothermal complex reactions [2]. Achenie and Biegler were the first to use algorithmic and mathematical programming by formulating the reaction system as NLP to get the optimum solution of desired reactor network [3]. The most widely and more effective approach employed in reactor network synthesis is superstructure-based methods which is greatly developed by Biegler for both simple and complex isothermal and non-isothermal reaction system [4]. Superstructures represent all possible reactor configurations and their interconnections. By formulating the problem as an optimization task, these methods efficiently explore the vast design space and identify the most favorable reactor net-

work. The superstructure approach allows engineers to consider various reactor types, operating conditions, and connection possibilities, thereby providing flexibility and a holistic perspective in the optimization process [14].

Another commonly utilized method for chemical reactor network synthesis is graph-theoretic approaches such as Attainable region method developed by Hildebrandt and Glasser [6,9]. Graph theory offers a powerful framework to model and analyze interconnected reactor networks. The concept of AR theory is based on geometry, which means that we always aim to represent our system and the data it generates using vectors. AR method use linear programming (LP) to express the rate vector field in concentration space [9].

Genetic algorithms provide a powerful optimization technique inspired by biological evolution. By iteratively generating a population of potential reactor network configurations and applying selection, crossover, and mutation operations, genetic algorithms explore the design space extensively [10]. Soltani proposed a new algorithmic approach for synthesis of reactor network (RN) using combination of stochastic algorithm (ICA) and mathematical method (QLP) with the aid of genetic algorithm (GA) principles [8,14]. They have proven effective in handling complex and nonlinear reactor network synthesis problems, providing near-optimal solutions through intelligent search mechanisms.

Mixed-Integer Nonlinear Programming (MINLP) combines continuous and discrete variables to represent reactor types and their operating conditions. MINLP methods formulate the reactor network synthesis problem as a mathematical optimization problem and apply sophisticated algorithms to search for the optimal solution. These methods offer the advantage of accurately modeling nonlinear kinetics and constraints, enabling precise optimization of the reactor network [7]. Kokossis and Floudas proposed a general superstructure model which contains all possible combinations using one CSTR with one PFR and two CSTR with two PFR containing recycle and bypass stream for each reactor [5]. He applied his model on both isothermal and non-isothermal operating conditions [18]. Samoilov used the principle of reactors arrangement by using mathematical model to decrease the catalyst weight required in diesel fuel hydrotreating units [20].

In summary, the continuous advancement of methods used in chemical reactor network synthesis has opened new horizons for process design and optimization. Superstructure-based methods, graph-theoretic approaches, genetic algorithms, heuristic methods, and MINLP techniques all contribute to the diverse toolbox available to engineers and researchers. The choice of method depends on the specific problem requirements, solution complexity, available computational resources, and desired optimization goals. By selecting the appropriate method and leveraging its strengths, researchers can achieve efficient and sustainable reactor network designs to meet the increasing demands of chemical process engineering.

This research paper aims to deepen our understanding of the different methods employed for chemical reactor network synthesis and their respective applications. By critically evaluating their advantages, limitations, and recent developments, this study aims to highlight the current state-of-the-art and inspire further advancements in the field.

## 2. Problem statement

In order to solve each optimization problem involved in chemical reactor network synthesis, certain data given is required. Since RN synthesis is an optimization problem, this data includes:

1. Mass or molar flow rate of inlet stream, its temperature, and concentration of each component.
2. Reaction mechanism, reaction rate equation, the value of reaction rate constant in case of isothermal reaction, and the Arrhenius equation in case of non-isothermal reaction.
3. Constraints provided in case of volume limitations or molar flow rate upper and lower bond of each stream regarding design consideration. Constraints although include residence time limitations to avoid coke formation in case of highly exothermic reaction which although should include another temperature constraint [8].

Reactor network synthesis is an optimization problem which may has only one specific objective function or it may have multiple objectives at the same optimization problems such as minimum volume requirements, maximum concentration(yield) of the desired product, and maximum selectivity of the desired component compared to the undesired ones within the outlet stream [11].

Solving RN problem provide us with the following valuable information:

1) The optimum reactor network which shows how reactors can be connected in optimum manner.
2) The volume of each reactor, and its type.
3) Yield of desired component, its selectivity, conversion of the limiting reactant.
4) Flow rate, temperature (in case of non-isothermal), and concentration of each component, for each stream in the superstructure model proposed [17].

## 3. Methodology

GAMS (General Algebraic Modeling System) is widely used in the optimization of complex reactor network synthesis. Reactor network synthesis involves determining the optimal configuration, design, and operation conditions of a network of interconnected reactors to meet specific production goals. The complexity of reactor networks arises from multiple factors such as the number of reactors, various reaction pathways, competing reactions, and different feedstock and product specifications. GAMS provides a powerful platform to model and solve these complex optimization problems by representing the process constraints, objective functions, and decision variables in a concise algebraic form. GAMS allows for the incorporation of various mathematical programming techniques such as linear, nonlinear, mixed-integer, and dynamic programming, which enables researchers and engineers to explore a wide range of feasible solutions and identify the optimal design and operating conditions for the reactor network [16]. The versatility and flexibility of GAMS make it an invaluable tool for optimizing complex reactor network synthesis, leading to efficient and cost-effective production processes in the chemical and petrochemical industries [15].

The superstructure-based approach is a systematic framework used for isothermal and non-isothermal reactor network synthesis. It involves the formulation of a comprehensive superstructure that includes various possible reactor configurations, heat exchangers (in case of non-isothermal exothermic or endothermic reactions), and interconnecting streams [18]. First, we begin by defining the System including the reaction mechanism, the desired conversion, selectivity, temperature profiles, and any other relevant factors. After that develop a general superstructure model consisting of one PFR and one CSTR, the model should contain all possible combinations between the two reactors [12].

PFR is approximated as ten CSTRs connected in series, all reactors have the same volume as shown in Fig. 2 [5]. As solving the material balance equation of PFR contains differential equation so, approximation of PFR using CSTR is a very important step in reactor network synthesis using superstructure approach. Noting that as number of CSTRs used in this approximation are increased, we will get more accurate optimum network, but our problems become more complex and will take lot of time to be converged in GAMS software.

Below are the detailed steps followed during synthesis of chemical reactor network for given reactions based on the superstructure method followed by further optimization using fuzzy approach.

Step (1): Define the sets for components (i), mixers (m), splitter (s), reactors (r), reactions ($r_c$), and streams (str).

Step (2): Define the inlet stream and outlet stream of each reactor.

Step (3): Define the inlet stream(s) and outlet stream(s) of each mixer and splitter.

Step (4): You should specify the positive variables for GAMS to be as constraints. Positive variables include [flow rate of all streams, volume of all reactors, concentration of each component in all streams, and reaction rate of each reaction].

Step (5): Specify the data given that include reaction rate constant, molar flow rate of the inlet stream, concentration of each component in the inlet stream, and in case of non-isothermal reaction, we should define the Arrhenius equation that represents the temperature dependence of the reaction rate constants ($k_r$).

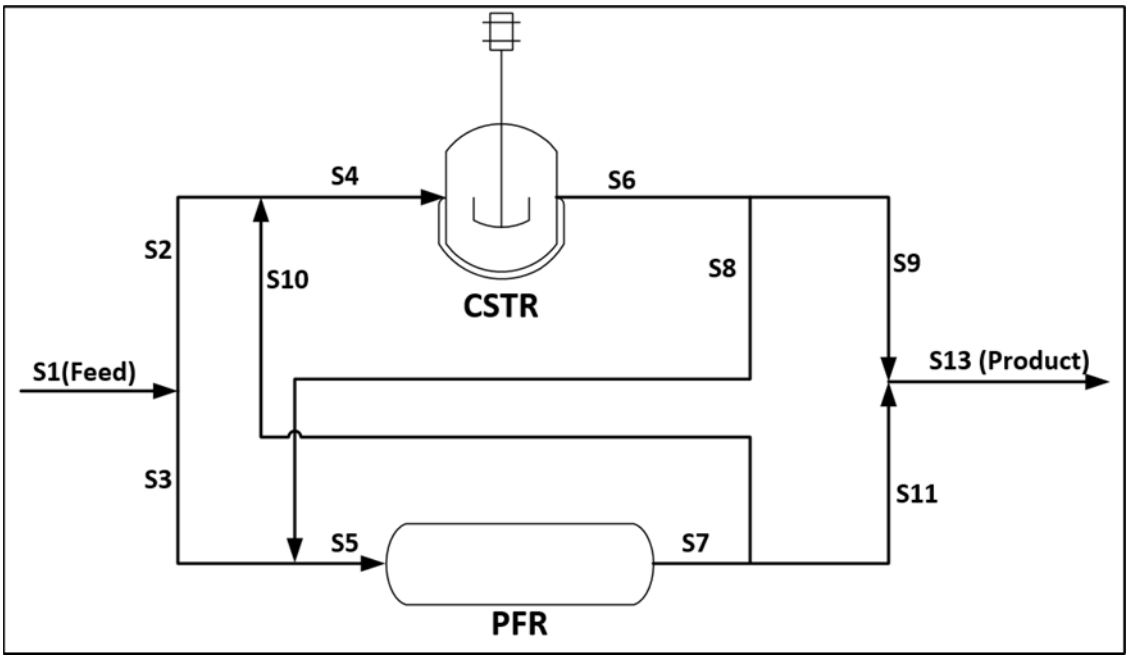



Figure 1. Schematic representation of proposed superstructure of one PFR and one CSTR.

Step (6): Write the overall and component material balance equations for each mixer(m).
For any mixer (m):
1) Overall material balance:

$$F_{str(out)} = \sum F_{str(in)} \quad (1)$$

2) Component (i) material balance:

$$F_{str(out)} * C_{i,str(out)} = \sum F_{str(in)} * C_{i,str(in)} \quad (2)$$

Where: $i$: represents each component in the reaction inlet and outlet.
Step (7): Similar to mixer, we can write the overall and component material balance equations for each splitter.
For any splitter (s):
1) Overall material balance:

$$F_{str(in)} = \sum F_{str(out)} \quad (3)$$

2) Component (i) material balance:

$$F_{str(in)} * C_{i,str(in)} = \sum F_{str(out)} * C_{i,str(out)} \quad (4)$$

Step (8): write the overall and component material (mole) balance and on each reactor.
For any reactor (r):
1) Overall material balance:

$$F_{str(in)} = F_{str(out)} \quad (5)$$

2) Component (i) material balance:
a) Reactant component:

$$F_{str(out)} * C_{i,str(out)} = F_{str(in)} * C_{i,str(in)} - V_r * (-r_i) \quad (6)$$

b) Product component:

$$F_{str(out)} * C_{i,str(out)} = F_{str(in)} * C_{i,str(in)} + V_r * (-r_i) \quad (7)$$

where: $V_r$: The volume of each reactor
$-r_i$: The rate of reaction of each component (i)

Step (9): Define the constrains and limitation of the variables of concern in our problems such as the volume of the reactor as it may be a limitation for the available area. Other constrains include the upper and lower bond of the flow rate of each stream in the network proposed. In this paper we assume, that the volume of CSTRs approximating the PFR, are equal, so the volume of PFR equals the sum of volumes of ten CSTRs. Noting that the total volume of the network, which we will use in the fuzzy approach, equals to summation of $V_{PFR}$ and $V_{CSTR}$.
Step (10): Define the objective function of the problem which may be minimizing the required reactor volume at given yield or maximizing the yield or selectivity of the desired product at given reactor configuration.

$$objective\ function = \max(yield\ or\ selectivity)\ or\ \min\ (total\ required\ volume)$$

Step (11): repeat the above calculation at different temperature conditions, in each case get the optimum reactor network that specify the objective function. Finally, check these results using the Fuzzy Approach (the MAX-MIN Algorithm) method the get the most optimum solution regarding other variables such as selectivity and conversion beside the volume and yield.

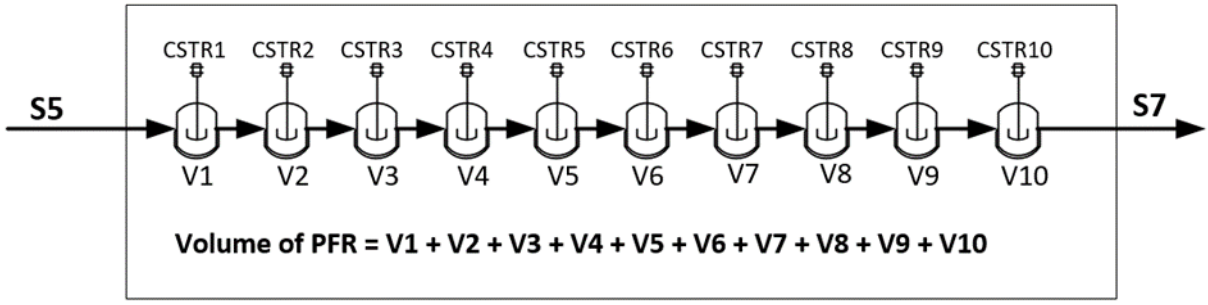



Figure 2. PFR approximation using ten CSTRs.

## 4. Fuzzy approach (MAX-MIN algorithm)

A decision is to be made by evaluating all the related rules at different levels in a knowledge base. The evaluations are out according to the max-min algorithm.

$$\mu_j(x) = \max\{min_{k\epsilon K}[\mu_{j1}(x), \mu_{j2}(x), \dots\dots, \mu_{jk}(x)]\} \quad (8)$$

where $\mu_{jk}(x)$ = Membership function of variable (x) in fuzzy set (k) representing the kth antecedent of the ith rule at the jth level.

The MIN operation yields a set truth values (τi) through evaluation of the membership functions of all the rules. Then, a single rule is selected by performing the MAX operation. i.e.

$$\tau = \max(\tau_1, \tau_2, \tau_3, \dots\dots, \tau_i) \quad (9)$$

This selected rule is activated or fired. The same operation is repeated at the succeeding level based on the information received from the preceding level. The objective function may be maximization of the variables such as yield, conversion, and selectivity or minimization of the variable such as volume and operating temperature. The following MAX-Normalization equation can be used in case of maximization problems for the more preferable variables.

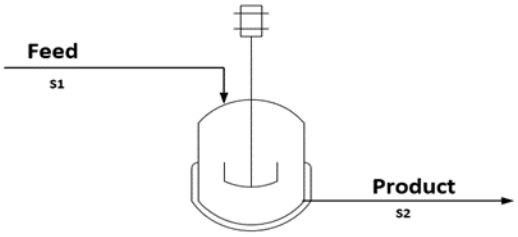
$$\mu = \frac{f - f_{min}}{f_{max} - f_{min}} \quad (10)$$

while in case of the less preferable variables such as total volume of the reactor, it should be minimized by MIN-Normalization equation as shown below.

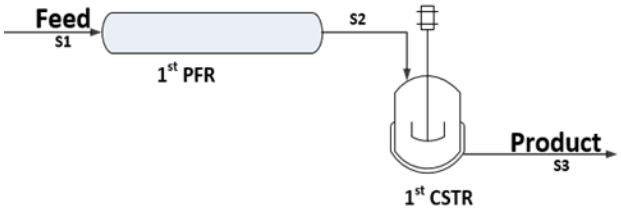
$$\mu = \frac{f_{max} - f}{f_{max} - f_{min}} \quad (11)$$

After optimizing the general reactor network superstructure as shown in Figure 1, we will obtain will obtain one of the below sub-networks as shown in Figure (3 a, b, c, d, e).

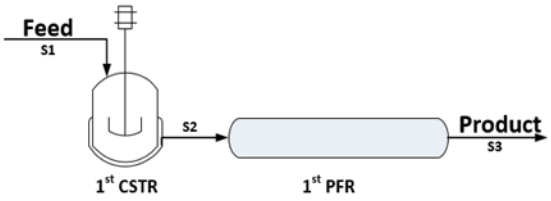

(3a) One PFR only.



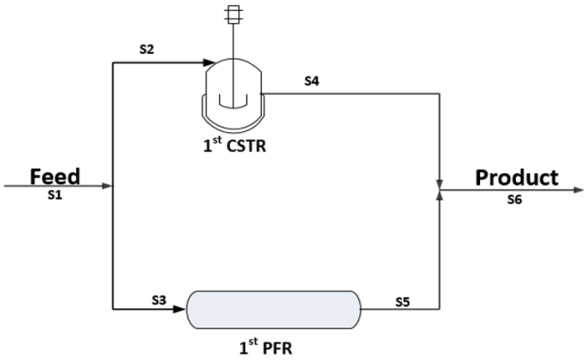

(3b) One CSTR only.




(3c) One PFR followed by one CSTR in series.




(3d) One CSTR followed by one PFR in series.




(3e) One PFR and one CSTR in parallel.

Figure 3. Examples of possible sun-networks may be obtained from our general proposed superstructure model.

## 5. Illustrative examples

### 5.1. Example (1): Synthesis of chemical reactor network for maleic anhydride production [19]

The following reactions represent the oxidation of benzene (A) using excess air to produce maleic anhydride (P) which is the desired product. There are some undesired reactions leading to production of H2O and CO2. The reactions can be described as follows:

$\boldsymbol{Reaction\ (1)}$: $C_6H_6 + \frac{9}{2}O_2 \rightarrow C_4H_2O_3 + 2CO_2 + 2H_2O$ (12)

$\boldsymbol{Reaction\ (2)}$: $C_4H_2O_3 + 3O_2 \rightarrow 4CO_2 + H_2O$ (13)

$\boldsymbol{Reaction\ (3)}$: $C_6H_6 + \frac{15}{2}O_2 \rightarrow 6CO_2 + 3H_2O$ (14)

As air is considered as the excess reactant, it does not affect the rate of reaction. The above reactions can be simplified as follows:

$A \rightarrow P$ $r1 = k_1C_A$ (15)

$P \rightarrow B + C$ $r2 = k_2C_P$ (16)

$A \rightarrow B + C$ $r1 = k_3C_A$ (17)

The reaction rate constants, having unit of (m3/kg.cat.·s) for the above reaction depend on the temperature as shown through these Arrhenius equations:

$k_1 = 4280e^{-\frac{12660}{T(K)}}$ (18)

$$k_2 = 70100e^{-\frac{15000}{T(K)}} \quad (19)$$

$$k_3 = 26e^{-\frac{10800}{T(K)}} \quad (20)$$

The feed enters the reactor with volume flow rate 0.0025 $m^3/s$ with benzene (A) concentration equals to 10 $mol/m^3$. The benzene is considered as the limiting reactant as air presents in excess amount.

As the reaction is catalytic, taking place in fluidized bed catalytic reactor, so this reaction network can be modeled as single plug flow reactor (PFR) which is approximated as ten CSTRs connected in series. The reaction is assumed to be isothermal. The objective of this problem is to determine the optimum reaction temperature at which there is minimum possible weight of catalyst, maximum yield, and maximum selectivity. Solving this problem using GAMS software, we get the Table 1.

Table 1. Results of GAMS optimum solution at different temperatures for example (1)

| T(K) | Yield | Selectivity | Conversion | Weight of catalyst (kg) |
|---|---|---|---|---|
| 600 | 3.8007 | 0.0926 | 0.6672 | 8.791 |
| 650 | 4.6709 | 0.1039 | 0.759 | 232.181 |
| 700 | 4.2832 | 0.099 | 0.7186 | 51.985 |
| 750 | 3.9308 | 0.0944 | 0.6813 | 14.133 |
| 770 | 3.8007 | 0.0926 | 0.6672 | 8.791 |
| 800 | 3.6172 | 0.0901 | 0.6472 | 4.504 |
| 850 | 3.341 | 0.0862 | 0.6162 | 1.637 |

The above table contains four variables. The first three variables (yield, selectivity, and conversion) should be maximized while the last variable (weight of catalyst) should be minimized. Using the FUZZY Approach, we can get the most optimum temperature after using Maximum-Minimum normalization as follows:

MAX-Normalization:

$$\mu = \frac{x - x_{min}}{x_{max} - x_{min}} \quad (21)$$

MIN-Normalization:

$$\mu = \frac{x_{max} - x}{x_{max} - x_{min}} \quad (22)$$

where: $\mu$: the normalization value of each variable; $x$: the value of each variable before normalization; $x_{max}, x_{min}$: the maximum and minimum value of each variable separately.

Solving this problem in GAMS contains 12 constraints, 70 variables, 310 non-zero elements, and we get the optimum solution in less than one second after 5 iterations.

### 5.2. Example (2): Case study- synthesis of multi-objective chemical reactor network [18]

Consider the following isothermal reaction scheme consisting of two stochiometrically independent reactions represented by

$$A \underset{k2}{\overset{k1}{\leftrightharpoons}} B \xrightarrow{k3} C \quad (23)$$

Component (B) is the desired product while component (C) is the undesired product. After producing a specific amount of component (B), it will further react to form undesired product (C). the first (desired) reaction is reversible while the second reaction is irreversible. All reactions are first order reaction with respect to the reactants.

The reaction rate constants depend on the temperature according to the following Arrhenius equations:

$$k_1 = 1.11 \times 10^4 e^{-\frac{8975}{T(K)}} \quad (24)$$

$$k_2 = 1.11 \times 10^4 e^{-\frac{12000}{T(K)}} \quad (25)$$

$$k_3 = 2.78 \times 10^3 e^{-\frac{6000}{T(K)}} \quad (26)$$

The inlet feed stream enters the first reactor with volume flow rate of 100 Liter/s. The feed contains component (A) only with no (B) or (C). the inlet concentration of the feed is 10 gmole(A)/Liter. The most appropriate temperature range for this reaction is 200-850°C.

The problem is considered as a multiple criteria decision-making problem for which we want to get the optimum temperature at which there are optimum reactor network with minimum volume, maximum yield (outlet concentration of component (B)), maximum selectivity, and maximum conversion. In some cases of low conversion, we may need to use recycle to enhance the reaction to maximum possible limit. As mentioned above, the PFR is approximated as 10 CSTRs connected with each other in series and the volume of PFR equals the summation of these ten reactors (all reactors have equal volume).

First, we assume the general superstructure reactor network as shown in Figure 1. We use this model to make mathematical formulation for this reaction system. Then using GAMS software helps us to get the optimum reactor network at multiple temperatures. Table (2) shows the results of optimum reactor network at each temperature. Finally, apply the Fuzzy approach using MAX-MIN normalization for each variable that needed to be optimized.

Table 2. Results of GAMS optimum solution at different temperatures for Example (2).

| T(C) | Yield | Selectivity | Conversion | Temperature(K) | Total volume(L) |
|---|---|---|---|---|---|
| 500 | 0.6568 | 0.4537 | 0.2104 | 773.15 | 236.956 |
| 550 | 0.7974 | 0.4993 | 0.2394 | 823.15 | 135.795 |
| 600 | 0.9399 | 0.5413 | 0.2676 | 873.15 | 82.982 |
| 650 | 1.0836 | 0.5828 | 0.2943 | 923.15 | 53.368 |
| 700 | 1.2222 | 0.6203 | 0.3193 | 973.15 | 35.910 |
| 750 | 1.3622 | 0.6606 | 0.3424 | 1023.15 | 25.029 |
| 800 | 1.5042 | 0.7037 | 0.3642 | 1073.15 | 17.996 |
| 850 | 1.6369 | 0.7425 | 0.3841 | 1123.15 | 13.327 |

Solving this problem in GAMS contains 9 constraints, 100 variables, 366 non-zero elements, and we get the optimum solution in less than one second after 20 iterations.

## 6. Results

Results obtained from GAMS for the first example of maleic anhydride reactor network synthesis can be furthered optimized using the Fuzzy Approach by following the above-mentioned procedures, we get the Table 3.

Table 3. Fuzzy approach results for Example (1)

| T(K) | Yield | Selectivity | Conversion | Weight of catalyst | μ |
|---|---|---|---|---|---|
| 600 | 0.3457 | 0.3616 | 0.3571 | 0.969 | 0.3457 |
| 650 | 1 | 1 | 1 | 0 | 0 |
| 700 | 0.7085 | 0.7232 | 0.7171 | 0.7816 | **0.7085** |
| 750 | 0.4435 | 0.4633 | 0.4559 | 0.9458 | 0.4435 |
| 770 | 0.3457 | 0.3616 | 0.3571 | 0.969 | 0.3457 |
| 800 | 0.2077 | 0.2203 | 0.2171 | 0.9876 | 0.2077 |
| 850 | 0 | 0 | 0 | 1 | 0 |

As shown from the Table 3, the optimum reaction temperature is 427°C (700K) at which we will use packed bed reactor (PBR) containing 51.9853 kg. catalyst and achieving yield (outlet concentration of maleic anhydride) equals to 4.2832 mol/m$^3$. The resulting selectivity

equals 0.099, and the percentage conversion of the limiting reactant (A) is 71.86%. these results are shown in Figure 4.

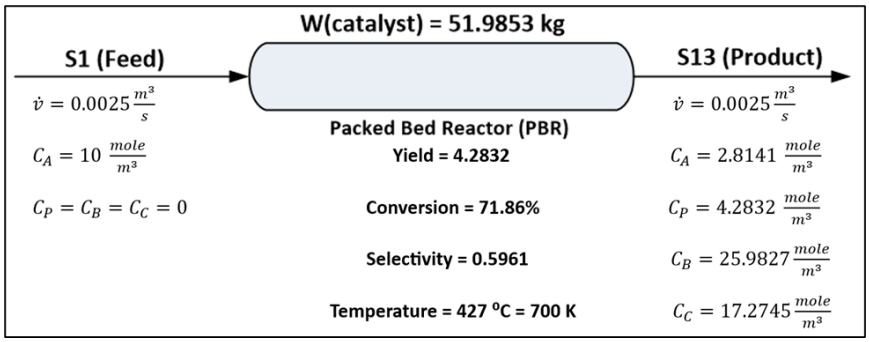



Figure 4. Optimum reactor network at optimum operating temperature for Example (1).

For the second example consisting of two independent reversible and irreversible reactions with one desired component of (B), GAMS results have been presented in Table 4. The table 4 contains five variables. The first three variables (yield, selectivity, and conversion) should be maximized while the last two variable (temperature and total volume of reactors PFR+CSTR) should be minimized.

Using the FUZZY Approach, we can get the most optimum temperature after using Maximum-Minimum Normalization as described above. The results of Fuzzy approach for the second example are presented in table (4).

Table 4. Fuzzy approach results for Example (2)

| T(C) | Yield | Selectivity | Conversion | Temperature | Total volume | μ |
|---|---|---|---|---|---|---|
| 500 | 0 | 0 | 0 | 1 | 0 | 0 |
| 550 | 0.1435 | 0.1579 | 0.1670 | 0.8571 | 0.4524 | 0.1435 |
| 600 | 0.2889 | 0.3033 | 0.3293 | 0.7143 | 0.6885 | 0.2888 |
| 650 | 0.4355 | 0.4470 | 0.4830 | 0.5714 | 0.821 | 0.4355 |
| 700 | 0.5769 | 0.5769 | 0.6269 | 0.4286 | 0.8991 | 0.4286 |
| 750 | 0.7197 | 0.7164 | 0.7599 | 0.2857 | 0.9477 | 0.2857 |
| 800 | 0.8646 | 0.8657 | 0.8854 | 0.1429 | 0.9791 | 0.1429 |
| 850 | 1 | 1 | 1 | 0 | 1 | 0 |

Results show that the optimum temperature is 650°C (923.15K) at which we will use CSTR with volume equals to (4.8517 Liter) followed by PFR (in series) with volume equals to (48.5158 Liter). The optimum yield is 1.0836 mol/L while the selectivity equals 0.5828 and the percentage of conversion is 29.43%. These results are shown in Figure 5.

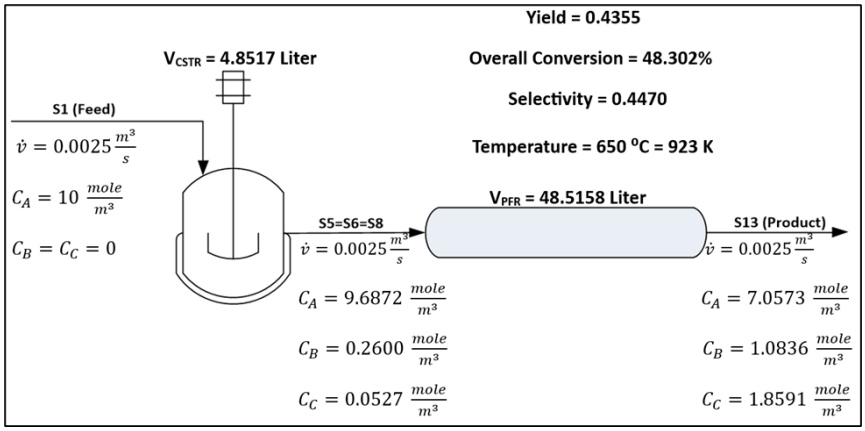



Figure 5. Optimum reactor network at optimum operating temperature for Example (2).

## 7. Conclusion

Results of this research paper have demonstrated the importance of using GAMS and a fuzzy approach in advancing the field of chemical reactor network synthesis and enhancing the efficiency and cost-effectiveness of production processes involving chemical reactions. The utilization of GAMS and a fuzzy approach for chemical reactor network synthesis based on a proposed superstructure model has proven to be a highly effective and efficient methodology. This research paper has highlighted the importance of optimization techniques in tackling the complexity of reactor network synthesis and the ability of GAMS to aid in this process. Additionally, the integration of fuzzy logic has provided a more robust and flexible approach, allowing for the consideration of uncertainties and allowing us to optimize multiple objectives decision-making problems. The proposed superstructure model has showcased its capability to simply represent all reaction pathways, different types of reactors used, and all possible streams that may enter or exit from each reactor with its composition and flow rate. By combining GAMS, fuzzy logic, and the superstructure model, researchers and engineers can explore a wide range of feasible solutions and identify the optimal design and operating conditions for chemical reactor networks.

***Nomenclature***

| | |
|---|---|
| *CSTR* | *Continuous stirred tank reactor* |
| *PFR* | *Plug flow reactor* |
| *RN* | *Reactor network* |
| *GAMS* | *General algebraic modeling system* |
| *GA* | *Genetic algorithm* |
| *NLP* | *Non-linear programming* |
| *MINLP* | *Mixed integer non-linear programming* |
| *ICA* | *Imperialist competition algorithm* |
| *QLP* | *Quasi linear programming* |
| *AR* | *Attainable region* |
| *m* | *Mixer* |
| *s* | *Splitter* |
| *r* | *Reactor* |
| $r_c$ | *Reaction* |
| *str* | *Stream* |
| *k* | *Reaction rate constant* |
| $F_{str(in)}$ | *Mole flow rate of inlet stream, mole/s* |
| $F_{str(out)}$ | *Mole flow rate of outlet stream, mole/s* |
| $C_i$ | *Concentration of each component (i), mole/liter* |
| $V_r$ | *Volume of reactor* |
| $r_i$ | *Rate of each reaction* |
| $\mu$ | *Membership function of variable (x)* |

**References**


[1] Grossmann IE, and Sargent RWH. Optimum Design of Chemical Plants with Uncertain Parameters. AlChE Journal, 1978; 24(6): 1021-1028. https://doi.org/10.1002/aic.690240612

[2] Chitra SP, and Rakesh G. Synthesis of Optimal Serial Reactor Structures for Homogeneous Reactions Part I, Isothermal Reactors. AlChE Journal, 1985; 31(2): 177-184. https://doi.org/10.1002/aic.690310202

[3] Achenie LEK and Biegler LT. Algorithmic Synthesis Of Chemical Reactor Networks Using Mathematical Programming. Ind. Eng. Chem. Fundam, 1986; 25: 621-627. https://doi.org/10.1021/i100024a024

[4] Achenie LEK and Biegler LT. A Superstructure Based Approach To Reactor Network Synthesis. Computer Chem. Eng., 1990; 14(1): 23-40. https://doi.org/10.1016/0098-1354(90)87003-8

[5] Kokossis AC, and Floudas CA. Optimization Of Complex Reactor Networks-I, Isothermal Operation. Chemical Engineering Science, 1990; 45(1): 595-614.

https://doi.org/10.1016/0009-2509(90)87004-C
[6] Hildebrandt D, and Glasser D. The Attainable Region and Optimal Reactor Structures. Chemical Engineering Science,1990; 45(8): 2161-2168. https://doi.org/10.1016/0009-2509(90)80091-R
[7] Balakrishna S, and Biegler LT. Constructive Targeting Approaches for Synthesis of Chemical Reactor Networks. Ind. Eng. Chem. Res., 1992; 31: 300-312. https://doi.org/10.1021/ie00001a041
[8] Hadi Soltani. Isothermal and Non-isothermal reactor network synthesis by combination of mathematical method and imperialist competitive algorithm. Chemical Engineering Science, 2021; 239: 116617. https://doi.org/10.1016/j.ces.2021.116617
[9] Kauchali S, and Biegler LT. Linear programming formulations for attainable region analysis. Chemical Engineering Science, 2002; 57: 2015–2028. https://doi.org/10.1016/S0009-2509(02)00101-X
[10] Gholizadeh Z, Soltani H, Javid M, and Azar MS. A New Robust Approach for Reactor Network Synthesis by Combination of Mathematical Method and NSGAII. International Journal of Chemical Reactor Engineering, 2019; 20190090. https://doi.org/10.1515/ijcre-2019-0090
[11] Pastore de Lima AE, and Maravelias CT. A Generalized Framework for Reactor Network Synthesis: A Graph Theoretic Approach. Computers and Chemical Engineering, 2022; 160: 107722. https://doi.org/10.1016/j.compchemeng.2022.107722
[12] Choi SH, and Manousiouthakis V, A stochastic approach to global optimization of chemical processes. Computers and Chemical Engineering, 1999; 23: 1351-1356. https://doi.org/10.1016/S0098-1354(99)00289-6
[13] Esposito WR, and Floudas CA. Deterministic global optimization in isothermal reactor network synthesis. Journal of Global Optimization,2002; 22: 59-95. https://doi.org/10.1023/A:1013842726210
[14] Ravagnani MASS, and Samed MMA. Reactor network synthesis for isothermal conditions. Maringá, 2008; 30(2): 199-207. https://doi.org/10.4025/actascitechnol.v30i2.5494
[15] Li SJX, and Tao S. Globally optimal reactor network synthesis via the combination of linear programming and stochastic optimization approach. Chemical Engineering Research and Design, 2012; 90: 808-813. https://doi.org/10.1016/j.cherd.2011.10.005
[16] Soltani H, and Shafiei S. Adiabatic reactor network synthesis using coupled genetic algorithm with quasi linear programming method. Chemical Engineering Science, 2015; 137: 601-612.https://doi.org/10.1016/j.ces.2015.06.068
[17] Hadi Soltani. Reactor Network Synthesis Using Coupled Genetic Algorithm with the Quasilinear Programming Method. Chem. Biochem. Eng. Q., 2016; 30 (2): 199-211. https://doi.org/10.15255/CABEQ.2014.2163
[18] Kokossis AC, and Floudas CA. Optimization Of Complex Reactor Networks-II, Nonisothermal Operation. Chemical Engineering Science, 1994; 49(7): 1037-1051. https://doi.org/10.1016/0009-2509(94)80010-3
[19] Seider WD et al. Product and Process Design Principles - Synthesis, Analysis and Evaluation. 4th edition, Wiley, 2017.
[20] Samoilov NA. Analysis, Modeling and Optimization of Reactors for Hydrotreatment of Diesel Fuel with Removing Organosulfur Impurities. Pet Coal, 2022; 64(4): 938-949. https://www.vurup.sk/wp-content/uploads/2022/11/PC-X_Samoilov_06_22.pdf

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