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Choice Modelling Of Styrene Tertiary Polymer under Various Monomer Compositions for Industrial Customer

Zahid H. Khokhar, Mamdouh A. Al-Harthi, Abdulazeez Abdurraheem

***Abstract*— Styrene tertiary polymer was made from two formula recipes at various temperatures for various reaction times. More than sixteen polymer products are made for each recipe formula many times. Observations show that each and every sample product polymer is suitable but it is necessary to locate the best one for industrial customer and choose for consumer market. Fuzzy rule based model is constructed by forming universe of discourse of temperature, reaction time, monomer ratio with hardness, rubber, glassy or fibre of polymer. Results show that this approach is good for further locating the best sample for production as per demand of customer.**

***Index Terms*—Styrene, Polymer, Industrial Customer, Innovation Market, Fuzzy Modeling.**

I. INTRODUCTION

In polymer extrusion industry, multiple problems occur due to inadequate raw material supply for extrusion. Percentage of additives is misunderstood. Machine cleaning becomes hard. Extruder may choke. Heavy blockage due to unexpected characteristics of raw material may happen. A process should pass through identifiable phases before any selection of suitable material locating among many and choosing the best.

Polystyrene is abundantly used in extrusion industry and many composite materials are added into it to modify its properties and characteristics as a whole for better resultant output product. This all needs better decisions, on-time capture of problem with system understanding and the raw material used during the process. Fuzzy logic is an effective paradigm to handle imprecision. It can be used to take fuzzy or imprecise observations for inputs and yet arrive at crisp and precise values for outputs. Also, the Fuzzy Inference System (FIS) is a simple and commonsensical way to build systems without using complex analytical equations. Implementation of fuzzy logic to control the processes is also an act of time [1]-[3].

Recently, some poor raw materials are disturbing plastic industry. The selection of the adequate material for process is a need of time. Many materials have been developed in the laboratory to use in industrial process one by one which consumes time.

It is very difficult to compare performance of various compositions of monomers on the basis of resultant product in hand of customer. Material capacities evaluation at different temperatures, monomer concentration ranges in batch experiments are done at small scale to save time to select better or exact product for different industrial consumer customer. Data is inconsistence as comparison of performance with each other is a major work if done by parts. Optimizing will also be a good task to serve further this field.

II. OBJECTIVE, SCOPE AND BACKGROUND

In this study our objective is to fuzify the observed data from our own experiments which have been done in laboratory for industrial application to understand the process and product. It presents the future lines to work out this problem in some understandable way to guide industrial consumer to select raw material based on end product.

This study develops a base which encourages towards using other data available for different raw materials and relationizes those with each other to form some typical correlation for different industrial applications as menu. A material selection guide may be prepared in this regard undergoing various laboratory and industrial experiences.

To apply fuzzy logic approach it is well worthy to present following selected discussions in this section regarding fuzzy logic or artificial intelligence approach applied to industrial processes or any relative fuzzy logic applied to control the production related process.

In industrial plants potential revolution to manufacture technology to get better polymer is always welcomed and a review of metollocene catalysis for manufacturer of polyolefin’s is provided [4]. All existing industrial plants may concentrate on the aspects of polymer reaction engineering, their mathematical modeling understanding the characteristics of polymer product with similar approaches for styrene tertiary polymer to enhance its quality use for industrial consumer customer. Reference [5] analyzed the use of the cluster analysis method in the fuzzy logic concept for the optimization of the cross-selective sensor arrays. This approach enables to purposefully form the sensor elements arrays with definite chemical functionality optimized for the solution of the specific applied problems.

Reference [6] used the fuzzy logic method improved by adaptive learning of a fuzzy inference system, based on anfis, to demonstrate a software analyzer design for parameters evaluation of ternary heavy metal ions removal. Reference [7] studied a fuzzy-logic based expert system for diagnosis and control of an integrated wastewater treatment. Reference [8] studied heats of immersion on activated carbons and their estimation by fuzzy methods. Reference [9] and [10] studied no exponential relaxations in sensor arrays: forecasting strategy for electronic nose performance by use of the cluster analysis method in the fuzzy logic concept for the optimization.

Both [11] and [12] studied fuzzy modeling estimation of mercury removal by wetland components. The majority of work discussed is not directly related to fuzzification of data mining but some of studies show that the method is useful and can be used for any case data study. Directly or indirectly, fuzzy method is used for numerous processes and applications. The above studies are few to mention.

We are not the first to introduce fuzzy into solving polymerization process problems. A lot of work has been done using different stochastic based techniques. Reference [13] studied the application of fuzzy logic in the control of polymerization reactors. Reference [14] applied artificial neural network models to control a time variant chemical plant. Reference [15] studied the trajectory tracking in batch processes using neural controllers. Reference [16] reviewed application of artificial neural networks to polymer composites. Reference [17] studied the adaptive heuristic temperature control of a batch polymerization reactor. Reference [18] investigated an industrial case study incorporating prior knowledge into artificial neural networks. Reference [19] studied data-driven model based control of a multi-product for semi-batch polymerization reactor. Reference [20] evaluated neural networks-based controllers in batch polymerization of methyl methacrylate. For interested quality of polymer product, considering characterization of number average molecular weight and polydispersity index, a strategy is applied to an open loop unstable steady state CSTR styrene polymerization for its good estimation and control [21]. Reference [22] studied development of a constant surface pressure penetration Langmuir balance based on axisymmetric drop shape analysis combining a pendant-drop surface balance, a rapid-subphase-exchange technique, and a fuzzy control algorithm. The reaction kinetics / penetration/ adsorption at constant PI are then studied monitoring A(t), i.e., determining the relative area change necessary at each instant to compensate the pressure variation due to the interaction of the surfactant in the subsurface with the surface layer. The study was of protein adsorption kinetics at the solution-air interface.

A modelling work with key parameters identification is done for batch emulsion copolymerization of a system containing styrene. Simulation and validation for the application is done for various conditions and is generalized for semi batch process [23]. Reference [24] studied ANN-based soft-sensor for real-time process monitoring and control of an industrial polymerization process. Polystyrene is abundantly used in extrusion industry and many nice composites are added into it to modify its properties and characteristics as a whole for better resultant output product. Polymerization is a process of reacting monomer molecules together in a chemical reaction to form three-dimensional networks or polymer chains.

III. MATERIALS, METHODS AND EXPERIMENTAL WORK

In polymer extrusion industry, multiple problems occur due to inadequate raw material supply for extrusion. Percentage of additives is misunderstood in many laboratory table researches. Forward and backward percentage verification may lesion the situations to reconcile to show better picture of the process and product. Polystyrene is abundantly used in extrusion industry and many composite materials are added into it to modify its properties and characteristics as a whole for better resultant output product.

Table 1. Experiments Done at Laboratory at Different Temperature For Different Time and Product Observed Characteristic

Time, min	Temperature, °C	Styrene Tertiary Polymerization Reaction	Product Appearance Observations
1	120	Completing	Hard
3	120	Completes	Rubbery
6	120	Experiment Completed	Rubbery
1	130	Completing	Hard
3	130	Completes	Rubbery
6	130	Experiment Completed	Glassy
1	140	Completing	Hard
3	140	Completes	Rubbery
6	140	Experiment Completed	Glassy

The reaction system under consideration is liquid and solid phase, whereas gas phase may be involved and the type is

$$A + B + O \rightarrow fDn,$$

Where A, B, and O are reactants in formula and f is any positive real number with D as styrene tertiary polymer product of n phase. Fig 1 shows a sliced pie quantitative product distribution of experiment. The boundaries between two products are not permanently defined although pie is sliced to present clear picture. The borders are porous and product quantity variation may occur depending upon time and temperature with significant contour profile. The

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percentage formation of observed product formed is also shown in the figure.

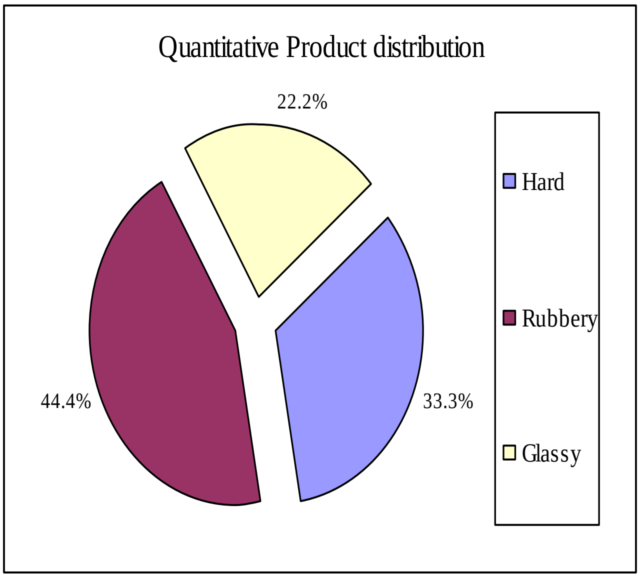

Figure 1: Sliced Pie Product Distribution Produced In the Laboratory Experiments

Reactor is a part of a carefully designed and constructed reacting system and it is not necessary to detail its procedures and particular dimensions of each section here due to scope of work. Steady state conditions prevail that is no accumulation of mass, momentum and energy with respect to time. After completion of all experiments the product is saved and conserved for observations. Temperature and time record is available for each and every product formed for the fixed formula of reactant materials. These notes are used to mine the data to construct the required system to put into fuzzy model. Fuzzy rule based model is constructed by forming universe of discourse of temperature, reaction time, monomer ratio: recipe with hardness, rubber, glassy or fiber of styrene tertiary polymer. Recipe is fixed and each material in the recipe is constant for every experiments. Selected experiments done at laboratory at different temperature for different time and product observed characteristic are tabulated in table 1.

Styrene tertiary reaction is proceeding and completing. It is an interesting phenomenon to note that the intermediates can be used for some important applications as well as unstopped reactions may be used and tested for self healing purposes. Table 1 shows the selected cases of experiments.

Details of materials will be discussed elsewhere with further recipes and modifications. All mass transfer, heat transfer, chemical simplitude, dynamic/thermodynamic simplitude, physical and chemical forces, and thermal properties are assumed same and constant for each and every experiment without any abrupt change unless otherwise stated. Fig 2 shows the system of recipe for temperature and time input showing the styrene tertiary polymer formed as output.

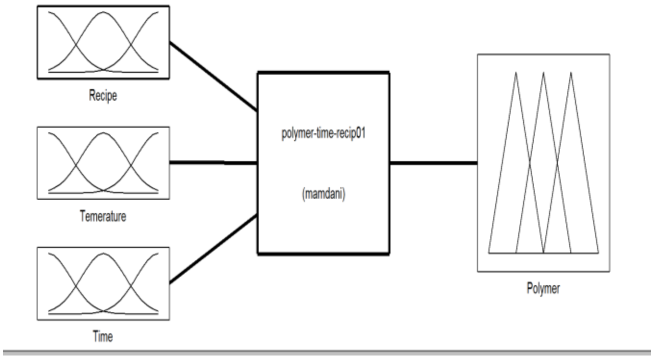

Figure 2: Universe Of Discourse of Inputs and Output FIS System

The reaction system has its all characteristics same during each reaction to form product from same formula of reactant for different temperature and for different time. All physical and chemical standards are met and implemented during experimentation with all care and safety. Labor efforts are also observed during experiments to recover the product. These all details are beyond the scope for this part of presented work.

IV. Fuzzy System Rules

For innovative studies and solving new problems, Matlab is a power full tool which is used to run fuzzy programming. Type of fuzzy input system was chosen as mamdani. Defuzzification was done by centroid method. Membership functions were selected trimf for each input FIS. Rules were made and supported by data produced from laboratory scale batch experiments. Table 2 shows the ranges used for data inputs and output. Polymer is set as 0 to 1 using membership function gauss2mf for parameters [0.1359 -0.04 0.1359 0.04] and [0.1359 0.46 0.1359 0.54] and [0.1359 0.96 0.1359 1.04] for hard, glassy and rubbery respectively.

Table 2. Type and Range of Different Variables of Given Universe Of Discourse

Variable	Type	Minimum	Maximum
Polymer	Output	0	1
Recipe	Input	1	1
Time	Input	0	6 min
Temperature	Input	120	140 ^{o}C

Following rules are applied to set the system. Some rules may be repeated as per their weight. For fixed recipe if temperature is low then polymer is hard, and if temperature is medium then polymer is glassy, and if temperature is high then polymer is rubbery. and if time is high then polymer is rubbery, and if time is medium then polymer is also rubbery for this range, and if time is low then the polymer is hard. That is, for constant reactant materials for each experiments, and if temperature is high then polymer is rubbery, and at medium temperature it is glassy, and at low temperature it is hard. and it is rubbery also at medium time, and at high time for the said range polymer is glassy.

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Dimensionless simplitude is shown in table 3. For all input and out variables, denominator is taken as maximum value whereas numerator is a product of division by minimum value to substraction of actual value and minimum value in all ranges of every variable. The above rules are implemented with full weight given to each rule and at various points where needed repetition of rule is done to adjust the weight. Range is set. Establishment of fuzzy rules are implemented for set ranges for inputs and out put for the fixed recipe of reactant material as deduced from experimental data recorded.

Table 3. Dimensionless Simplitude Type and Range of Different Variables of Given Universe Of Discourse

Variable	Type	Minimum	Maximum
Polymer	Output	0	1
Recipe	Input	1	1
Time	Input	0	1
Temperature	Input	0	0.1667

V. RESULTS AND DISCUSSIONS

Plastic industry is disturbed from the usual reason as well as by some cheap raw materials. The selection of the adequate material for process is a need of time. Many materials have been developed in the laboratory to use in industrial process one by one which consumes time. Material capacities evaluation at different temperatures, monomer concentration ranges in batch experiments are done at small scale to save time to select better or exact product for different industrial consumer customer. It presents the future lines to work out this problem in some understandable way to guide industrial consumer to select raw material based on end product.

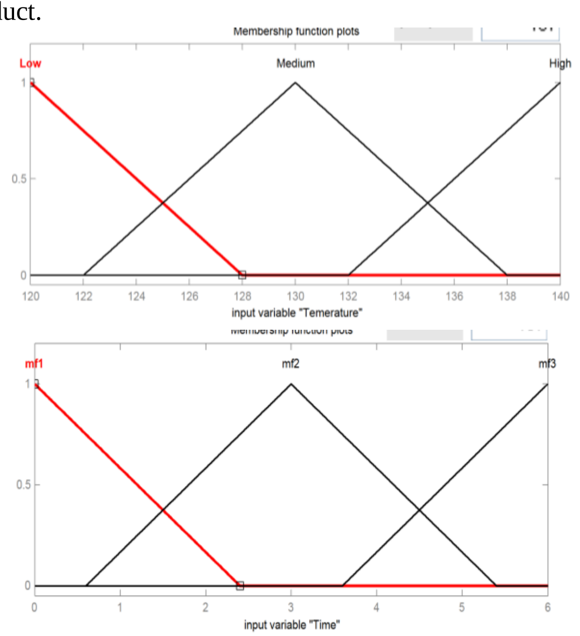

Figure 3: Membership Functions, For Fuzzy Interface System Input Universe Of Discourse, Variable Range Setup For Constructing and Verifying Rules, Trimf For Temperature and Time For Styrene Tertiary Polymer

From two basic fuzzy interface systems, mamdani and sugeno, former type is selected and with recipe, time and temperature are set as input variables whereas polymer production as out put variable forming universe of discourse of temperature, reaction time, monomer ratio: recipe with hardness, rubber, glassy or fibers of polymer. Membership functions of type trimf are defined for all inputs using centriod defuzzification whereas for output membership function gauss2mf. . Ranges are defined for all variables as shown in Table 1. Rules are defined on the basis of data of laboratory experiments repeated many times for same recipe. Those rules are implemented with full weight given to each rule where needed repetition of rule is done to adjust the weight. Establishment of fuzzy rules are implemented for set ranges for inputs and out put for the fixed recipe of reactant material as deduced from experimental data recorded.

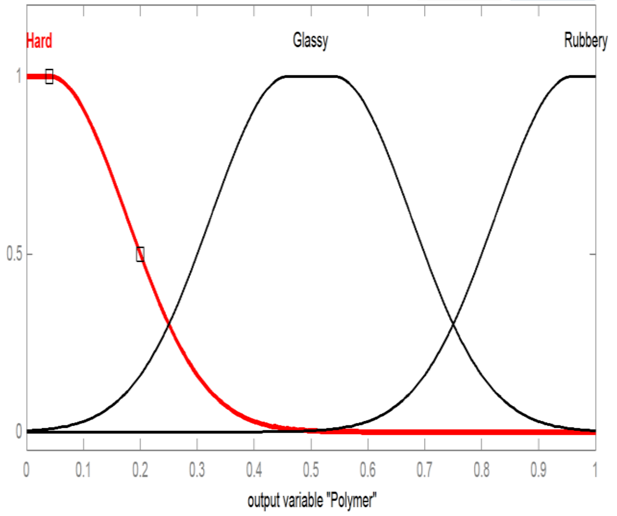

Figure 4: Membership Functions, For Fuzzy Interface System Universe Of Discourse, Output Variable Range Setup For Constructing and Verifying Rules, Gauss2mf For Styrene Tertiary Polymer Output

Fig 2 shows the block diagram of system constructed and followed. Recipe, temperature, and time input variables are fed to mamdani fuzzy interface system out of which one that is recipe is fixed and output is received at the other side. Variables can be changed, modified and their range can be set to a different number at any time to study the effects of range change on out put specially to construct a complex system, more than one recipe of reactant materials can be introduced. The range change step is a validation step to check the rules fed to system and for scale up and scale down the system and with set rules range change resulted in good agreement.

Causal importance involved in this system is also important. Implementation of rules is done and plots of their membership functions for input and output variables to construct universe of discourse are shown in Fig 3 and Fig 4 respectively. It is also an interesting part of this system that setting the lower, medium and upper part of ranges in these plots can be done. Fig 5 shows the fuzzy model rules on FIS system mamdani, for run time analyses of product shape and characteristics feelings for comparisons of styrene tertiary polymer product with recorded observed data to locate and choose appropriate product as per requirements of industrial customer.

This facility makes the problem setting accurate and near to actual situation and state of solution. Range of time and temperature is set into lower, medium and upper. The polymer product range is also set into lower, medium and higher hard, glassy, and rubbery correspondingly. These divisions of input variables then use to create rules combing with output variable lower and higher range distribution. Numerous possibilities played on these plots to satisfy the data and theory and to find acceptable link between them.

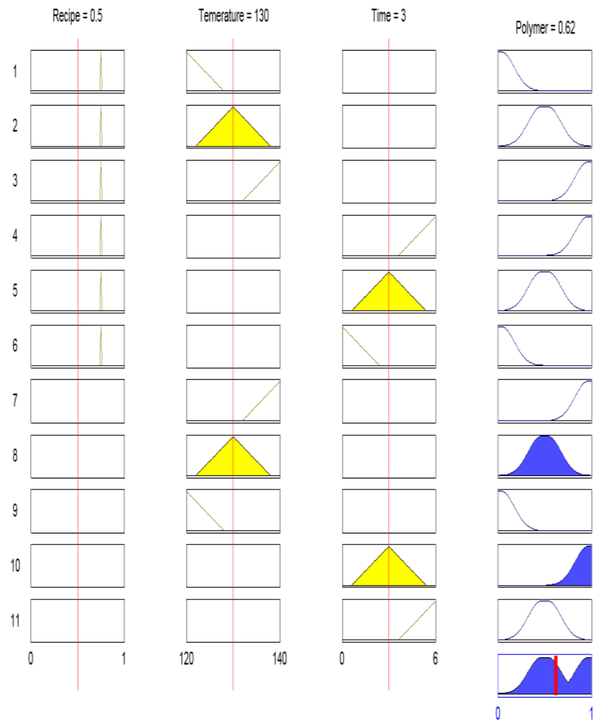

Figure 5: Model Rules On Fuzzy Mamdani FIS System, For Run Time Analyses of Product Shape and Characteristics Feelings Comparisons of Styrene Tertiary Polymer Product with Observed Data to Locate and Choose Appropriate Product as Per Requirements of Industrial Customer

The pattern from hard to glassy behavior is seen from the lines for this recipe. Any modification or requirement may be met easily by controlling time or temperature for choosing the best required product for industrial use. Fig 6 for 120°C and 140 °C, with line of 130°C being acted as a medium separator, a peak and a dip respectively form an area of keen interest. As the polymer formation is critical for 0.5 to 0.6, the time 5 to 6 min is also very critical to control the process. Similarly, Fig 7 a concluded chart shows that the critical check point for choosing the best polymer is from 0.5 to 0.6 and there is a dip which is crucial to look at. This time span is main concerned and controlling factor to form appropriate polymer and introduce desirable change with required characteristics and application oriented par.

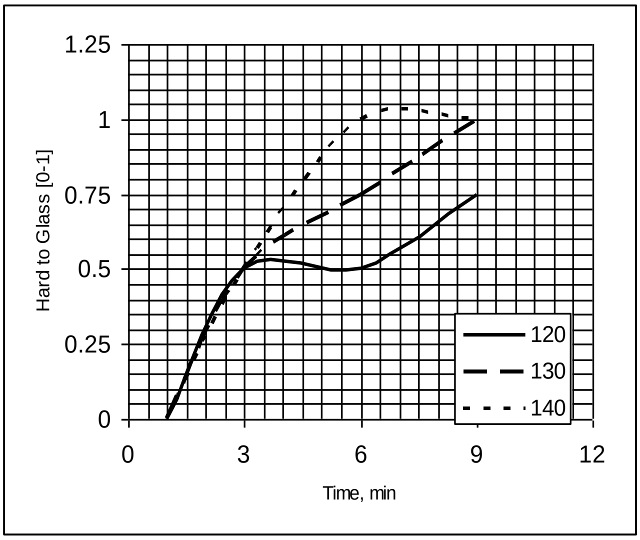

Figure 6: Comparisons of Styrene Tertiary Polymer Product Recorded For Three Different Temperatures for Different Time to Choose Appropriate Product

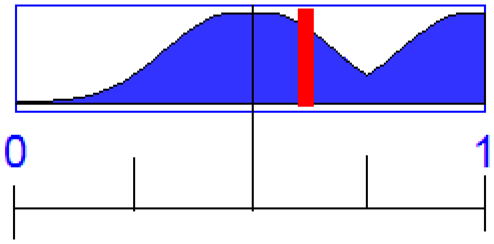

Figure 7: Styrene Tertiary Polymer Product Critical Range Check Point for Appropriate Product, Hard To Glass, 0-1.

The finding of both axis of critical area of the process and defining the issues of that area to enhance the product quality is an innovative task which is preliminarily done. Whether the time is controlling or the product formation is controlled by composition controlling of monomers, whichever is suitable at the time of decision, is a tool of quality enhancement. This approach is good and is extendable to other results as well as including the other formulae on the basis of process or any other suitable parameter. Further extension and application to other systems is a promising task to do. Also it will be a good guide to do any experiment for same or different system to avoid unnecessary experimentation. Experiments can be done on different ranges and with our fuzzy system the results for other bigger or smaller ranges can be predicted and further set of experiment can be designed accordingly. Observations show that each and every sample product styrene tertiary polymer is suitable but it is necessary to locate and choose the best one for industrial customer and consumer market.

VI. CONCLUSION AND RECOMMENDATION

This pre preliminary innovative study of selection of product of styrene tertiary polymerization process using different raw materials for industrial customer is a first step to set up a series of studies in this way. Capability of locating

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the best materials and choosing one out of those suitable for one's application is gained after many practices. Also experimental scale up and scale down can be done for different set of ranges following the modelling results designing further series of experiments categorically. Other methods along with fuzzy may give some more understanding of the system. A material selection perfect package may be prepared in this regard undergoing various laboratory and industrial experiences.

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Author Biography

First Author: Zahid H. Khokhar
Email: zahedhk@gmail.com, zahidhkhokhar@yahoo.com
Second Author: Mamdouh A. Al-Harthi
Email: mamdouh@kfupm.edu.sa
Third Author: Abdulazeez Abdurraheem
Email: toazeez@gmail.com, aazeez@kfupm.edu.sa