

Artificial neural fuzzy system and monitoring the process via IoT for optimization synthesis of nano-size polymeric chains

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Abstract. Synthesis of acrylate-based dispersion resins involves many parameters including temperature, ingredients concentrations, and rate of adding ingredients. Proper controlling of these parameters results in a uniform nano-size chain of polymer on one side and elimination of hazardous residual monomer on the other side. In this study, we aim to screen the process parameters via Internet of Things (IoT) to ensure that, first, the nano-size polymeric chains are in an acceptable range to acquire high adhesion property and second, the remaining hazardous substance concentration is under the minimum value for safety of public and personnel health. In this regard, a set of experiments is conducted to observe the influences of the process parameters on the size and dispersity of polymer chain and residual monomer concentration. The obtained dataset is further used to train an Adaptive Neural network Fuzzy Inference System (ANFIS) to achieve a model that predicts these two output parameters based on the input parameters. Finally, the ANFIS will return values to the automation system for further decisions on parameter adjustment or halting the process to preserve the health of the personnel and final product consumers as well.

Keywords: hazardous material; healthcare; internet of things (IoT); optimization; process monitoring

1. Introduction

Internet of Things (IoT) is the monitoring and processing data acquired from sensors through infrastructure of internet (Ashton 2009, Lu and Neng 2010, Xu *et al.* 2014). It has found applications in healthcare systems (Yin *et al.* 2016), agriculture (Dlodlo and Kalezhi 2015, Tzounis *et al.* 2017), mining (Qiuping *et al.* 2011) and chemical processing (Ley *et al.* 2015, Vijayakumar and Ramya 2015, Kim *et al.* 2017, Prabhu *et al.* 2019). The ongoing application of IoT makes it the future of internet. The application of IoT is very diverse from a domain as big as entire world to domain as small as single process and synthesis line in a factory. This method composed of two sections; one is the collecting data from the sensors and data acquisition devices and second is the processing and analyzing data to make proper decisions. Analyzing and processing data is performed using several methods including artificial neural network (ANN), machine learning (ML) and other analyzing and prediction methods (Aggarwal and Kumar 2019).

Ley *et al.* (2015) discussed potential application of Internet of Chemical Things (IoCT) in the future of chemical experiments and claimed that chemistry will change to adopt IoCT. Further, it is discussed that IoCT would fill the vacancies in measuring process and experiment parameters which might be missed in human measuring.

Prabhu *et al.* (2019) discussed the use of IoT for chemical reactions and how it improves reliability and transparency of the experimental data through simultaneous data sharing with all scientists. They further employed a designed IoT model to inspect Ph-oscillating reaction and milk spoilage. Wen *et al.* (2020) reviewed recent development in wearable chemical sensors and systems helping health condition monitoring. They suggested that chemical sensors would eventually become self-power multifunctional systems which will work with the aid of IoT. Prabhu *et al.* (2020) in their paper comprehensively described use of micro-controllers and single-board computers to improve experimental design and screening experiments conditions. In this regard, they provide details of design and implementation of seven experimental routines with the help of microcontrollers and single-board computers as a part of IoT. Li *et al.* (2019) designed a wearable wrist-watch shaped sensor to measure a type of hazardous gas in the air which cause asthma attacks. They suggested that use of such devices could help the patient and also public health with continues monitoring hazardous gas through chemical sensor, smart phones and the internet.

Collecting and reporting data is one of the parts of IoT systems. One another part is the analyzing and decision making process. Using machine learning and artificial neural networks is the most effective and simplest way to comprehend the results of a dataset and sending instant feedbacks. In most cases, if-then logics works for industrial applications. However, with the aid of neural networks it become possible to choose between many options in an accurate and reliable way granted that the networks are appropriately trained (Yegnanarayana 2009). Nascimento *et*

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al. (2000) utilized neural network to acquire process parameters in chemical engineering problem to cope with nonlinear behavior of correlations between inputs and outputs. They used NN to calculate regions in which an output parameter fall into a desired range. It was observed that using these method several options of input configuration is obtained instead one possible option in solving nonlinear equations. Prediction of chemical reactivity was performed using supervised neural network in the research study by Coley *et al.* (2019). They used a massive dataset collected from patents to train their designed network to predict the organic reactions from their solvent, reagents and reactants. The model was able to predict reactivity with over 85% accuracy. They concluded that this artificial intelligence method could assist chemists in design of processes. Narayana *et al.* (2022) utilized ANN to predict and optimize heavy metal removal in adsorption processes. They used several experiments to train a neural network to observe the best condition for high rate removal. Moreover, the NN method is compared to design of experiment (DoE) method which showed the better performance and accuracy of neural network optimization. Neural network were also utilized in many other application from nanocomposites (Do *et al.* 2020) to mechanics of materials (Elangovan *et al.* 2010, Hussain *et al.* 2019, Safaei *et al.* 2019, Ankamwar and Sur 2020, Matouk *et al.* 2020, Alsultan 2021, Garg *et al.* 2021, Habibi *et al.* 2021a, Heirati *et al.* 2021, Orak and Sajedi 2021, Yanzhen *et al.* 2021).

Healthcare systems are very sensitive and delicate in which they must have high reliability in screening and reporting conditions. Using NN and IoT, it become possible to make vital decisions in emergency and normal conditions. Methods other than NN in engineering calculations take considerably greater time and efforts to reach a conclusion (Al-Furjan *et al.* 2021a, b, c, d, e, f, Dai *et al.* 2021a, Ghabussi *et al.* 2021, He *et al.* 2021, Huang *et al.* 2021, Huo *et al.* 2021, Moayedi *et al.* 2021, Shao *et al.* 2021, Shariati *et al.* 2021, Zhang *et al.* 2021a, Chen *et al.* 2022). Some methods uses semi-numerical solutions to solve equations and make a decision (Hou *et al.* 2021, Huang *et al.* 2021a, Jiao *et al.* 2021, Liu *et al.* 2021a, Ma *et al.* 2021, Moradi *et al.* 2021, Xu *et al.* 2021, Zhao *et al.* 2021, Yu *et al.* 2022). Other methods uses fully numerical procedure to solve a problem (Fazaeli *et al.* 2016, Ghazanfari *et al.* 2016, Habibi *et al.* 2016, 2017, 2018a, b, 2019a, b, c, d, Massoumi *et al.* 2018, Safarpour *et al.* 2018, Amelirad and Assempour 2019, Ebrahimi *et al.* 2019a, b, 2019, Esmailpoor Hajilak *et al.* 2019, Hashemi *et al.* 2019, Moayedi *et al.* 2019, Mohammadgholiha *et al.* 2019, Mohammadi *et al.* 2019, Pourjabari *et al.* 2019, Safarpour *et al.* 2019a, b, Shokrgozar *et al.* 2019, Amelirad and Assempour 2021). In any condition these methods are not able to respond quickly and to consider all input factors (Al-Furjan *et al.* 2021a, b, c, d, Dai *et al.* 2021a, Guo *et al.* 2021, Habibi *et al.* 2021g, h, i, j, Liu *et al.* 2021a, b, Najaafi *et al.* 2021, Safarpour *et al.* 2021, Zhang *et al.* 2021a, b). Chung and Jung (2020) employed deep learning method based on convolutional neural network (CNN) to analyze data and suggest healthcare recommendation. The study demonstrated 13% enhancement in prediction in

comparison to other methods. Jiang *et al.* (2017) categorized applications of artificial intelligence (AI) methods in healthcare system. They divided the healthcare data into structures and unstructured in which different types of AI are employed. They also reviewed application of AI in three different levels of diagnosis, treatment and prognosis of disease. Raghupati and (2017) used neural network to find correlation between chronic disease and behavioral habits. With the aid of AI, it was concluded that fruit and vegetable consumption and physical exercises were against chronic conditions while alcohol and smoke had negative influence. Alam *et al.* (2019) designed an internet of medical things (IoMT) system to recognize emotions through non-invasive sensors to be further used in mining of affective state. Adamović *et al.* (2018) used ANN method to predict rate of chemical and healthcare waste production in European Union.

In this study, we aim to screen the process parameters via Internet of Things (IoT) to ensure that, first, the nano-size polymeric chains are in an acceptable range to acquire high adhesion property and second, the remaining hazardous substance concentration is under the minimum value for safety of public and personnel health. In this regard, a set of experiments is conducted to observe the influences of the process parameters on the size and dispersity of polymer chain and residual monomer concentration. The obtained dataset is further used to train an Adaptive Neural network Fuzzy Inference System (ANFIS) to achieve a model that predicts these two output parameters based on the input parameters. Finally, the ANFIS will return values to the automation system for further decisions on parameter adjustment or halting the process to preserve the health of the personnel and final product consumers as well.

2. Internet of things (IoT) system

In order to acquire data a system of sensors is designed using a standard Arduino electrical board. The system gathered data from multiple sensors in the process line including Mass Controllers (MCs), DLS and residual monomer analyzers and Temperature Indicator and Transferring (TIT) sensor. The configuration of the system is illustrated in Fig. 1. All the data measured and sensed by these 5 sensors are transferred to an electronic board in a regular pattern each second. The data further transferred to a computational server where analyzing of data is performed and decision on controlling process is made. The decision making in the computational center is based on supervised trained AI network which was prepared and trained to optimize the process using the best prior experienced conditions. There also designed the ability to add more dataset as input and retrain the model as desired or when the decisions of the system are not reliable or not true in some conditions. In such circumstances, the operator is warned and the process of training will be started based on new added datasets.

The difference between this system and traditional systems is employing AI in the process to making decisions without interference of human. Traditional controlling systems obey some specified rules previously written as if-

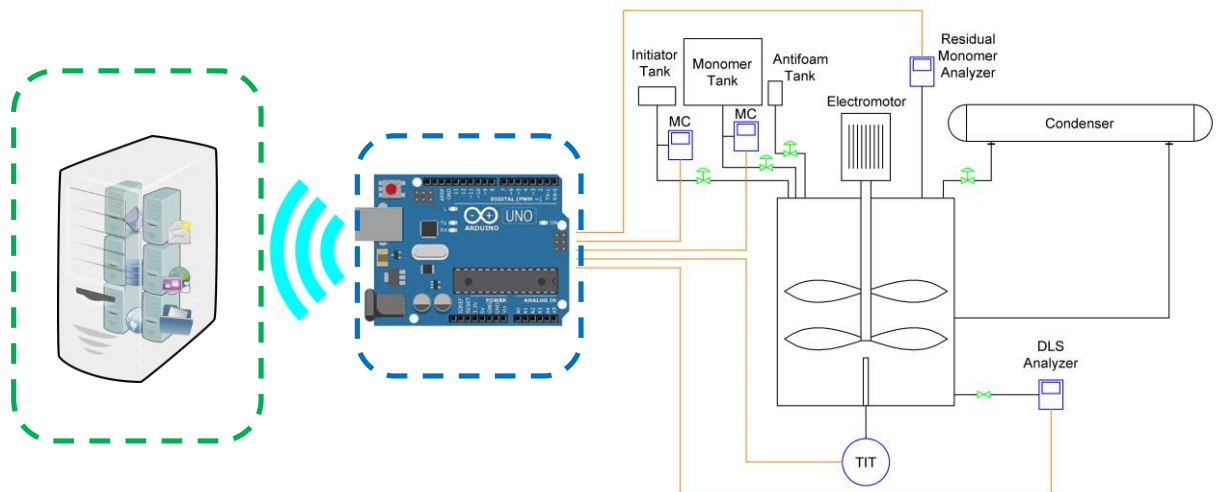


Fig. 1 IoT system to observe, collect and decision making in the acrylate-based dispersion resins synthesis

Table 1 Data acquired from process sensors

Run	Temperature [°C]	Rate of adding monomer [gr/sec]	Rate of adding initiator [mg/sec]	Poly Dispersity	Residual monomer [%]
1	61.2	34.7	366	0.96	0.107
2	60.3	35	362	0.32	0.109
3	60.4	32.1	335	0.98	0.100
4	59.8	52.3	535	0.46	0.156
5	59.5	21.9	233	0.62	0.072
6	64.8	41.5	426	0.51	0.119
7	65.1	36.4	375	0.85	0.099
8	65.2	35.7	370	0.64	0.096
9	65.9	33.8	350	0.34	0.094
10	65	62.9	648	0.68	0.175
11	70.2	28.4	297	0.6	0.070
12	68.9	27.6	294	0.59	0.075
13	69.7	29.3	306	0.36	0.081
14	69.4	32	338	0.3	0.085
15	71.2	31.5	325	0.74	0.078
16	76.8	44.6	460	0.8	0.105
17	75.6	40.8	428	0.39	0.102
18	75.2	43.2	452	0.59	0.099
19	75.2	39.7	416	0.38	0.095
20	75.4	46.1	475	0.94	0.110
21	81.8	36.4	384	0.98	0.079
22	81	36	378	0.94	0.082
23	81.6	35.2	364	0.58	0.079
24	81.6	33.9	349	0.42	0.081
25	80.6	31.5	332	0.89	0.074
26	85.4	38.5	396	0.37	0.084
27	85.6	37.9	399	0.43	0.079
28	86.4	36.8	387	0.72	0.078
29	87	36.5	381	0.78	0.082
30	87	35.4	367	0.66	0.072

Table 1 Continued

Run	Temperature [°C]	Rate of adding monomer [gr/sec]	Rate of adding initiator [mg/sec]	Poly Dispersity	Residual monomer [%]
31	90.6	32.4	344	0.44	0.064
32	90.8	36	374	0.6	0.069
33	91	39.4	405	0.74	0.082
34	91	41.2	430	0.74	0.087
35	91.2	35.1	366	0.99	0.069

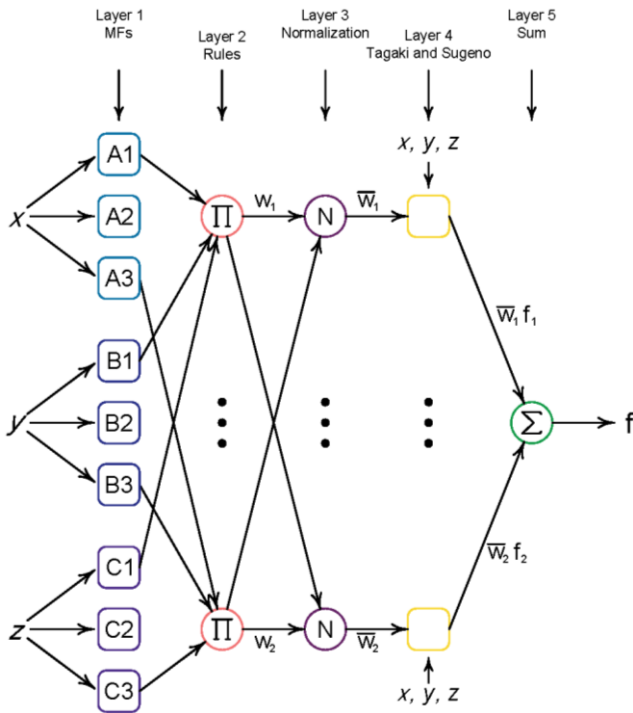


Fig. 2 Schematic of ANFIS layers for three inputs and one outputs

than rules. However, the AI system can be trained to makes better decisions on many parameters without limitations. The training process although have vital impact on the performance of the system.

3. Data acquisition

Some of the sample data gathered by designed IoT system is presented in the Table 1. The values of poly dispersity should be close to unity to have proper adhesion properties. However, the values above 0.2 is acceptable in the final product. In addition, the amount of residual monomer, because of its toxicity and danger to health safety must be kept under 0.1%wt. Otherwise, some other processes have to be performed to reduce the amount of the monomer. In any condition, the product with residual monomer higher than 0.1%wt would not release to the market. The amount of initiator is kept to around 1% of the monomer. Moreover, experiments demonstrated that in temperature between 60 to 90°C acceptable quality is obtained.

The data given in Table 1 are roughly divided into seven temperature values: 60, 65, 70, 75, 80, 85 and 90°C. All other data were simultaneously acquired by the IoT system. At first glance. It is observed that in lower rate of adding monomer and higher temperatures the hazardous residual monomer fall into safe range (<0.1%). However, for higher adding rate and lower temperature the condition is cautionary. There cannot be observed a clear correlation between poly dispersity and input parameters. Thus, we decide to design a neuro-fuzzy system to illustrate a richer correlation between parameters and design a model to predict and control the process in a more sophisticated and intelligence method.

4. Neural-fuzzy model

The ANFIS model is introduced in this section for calculating effects temperature and rate of adding monomer and initiator on the poly dispersity and residual monomer. In this regard, temperature and rate of adding monomer and initiator are regarded as input data and poly dispersity and residual monomer are the outputs. The neural network used in this this study is schematically presented in 0. As seen, this network has three inputs X , Y and Z and one output f . Membership functions in Layer 1 indicated by A_i , B_i and C_i ($i = 1, 2, 3$) converts input data to their membership values:

$$\mu_{A_i}(X), \mu_{B_i}(Y), \mu_{C_i}(Z) \quad (1)$$

In 0, the correlation between MFs and fuzzy rules are shown. Since each of the three inputs has three MFs function there are $3 \times 3 = 9$ rules in this network. However, rules can be modified based on the logic between them. These rules are applied in the Layer 2 (rules) to obtain the overall *firing strength* of each node in this layer:

$$w_i = \mu_{A_i}(X) \times \mu_{B_i}(Y) \times \mu_{C_i}(Z) \quad (2)$$

In Layer 3, all the firing strengths are normalized to adequately apply their effect portion on the final results. The normalization is performed according to following relation:

$$\bar{w}_j = \frac{w_j}{\sum_k w_k} \quad (3)$$

for $j = 1$ to number of Rules.

In Layer 4, influence of the actual values of the input data is calculated on the output for each rule. In this layer,

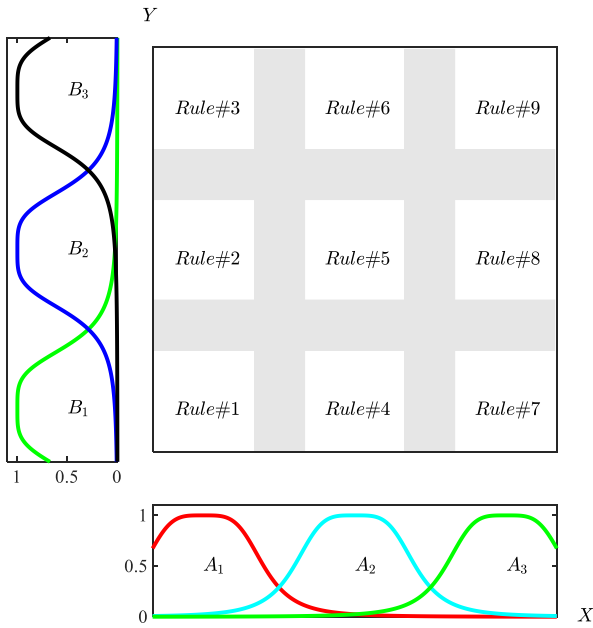


Fig. 3 Fuzzy subspaces for ANFIS with three inputs and nine rules

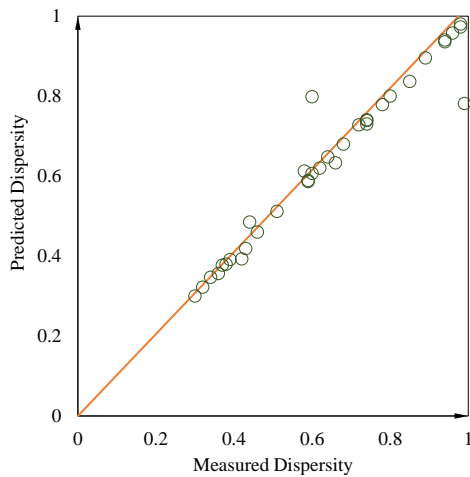


Fig. 4 Dependency of poly dispersity on the process parameters temperature and rate of adding monomer

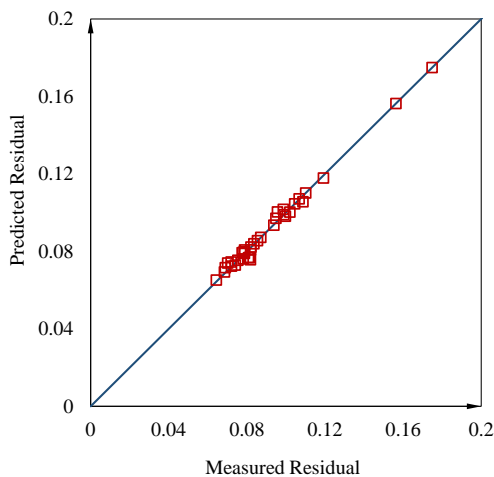


Fig. 5 Dependency of monomer residual on the process parameters temperature and rate of adding monomer

every single input data directly affect the output regardless of other provided input. This method was presented by Takagi and Sugeno’s rule Takagi and Sugeno (1985), Jang (1993). The effects is considered to have be linear:

$$f_j = p_jX + q_jY + r_j \tag{4}$$

Effects of all the input data on the output is a weighted combination of all data:

$$f = \sum_{k=1}^{NR} \bar{w}_k f_k \tag{5}$$

where NR represents number of all rules. The role of neural network is to adjust the weight values and coefficients of linear functions in Layer 4 to minimize the error of the network. Thus, an iterative method is used to obtain a model with acceptable error. Afterward, the network considered to be trained and will be ready to be tested and calculate output for new data.

5. Results and discussion

The input data in the ANFIS network described above is the temperature, rate of adding monomer and rate of adding initiator of the process. The outputs are poly dispersity and residual monomer for each a separate ANFIS model is designed. The dataset is prepared based on the acquired values from IoT. Triangle membership functions are considered for fuzzification of the input data with the following general relation:

$$f(x; a, b, c) = \max\left(\min\left(\frac{x - a}{b - a}, \frac{c - x}{c - b}\right), 0\right) \tag{6}$$

The parameters a , b and c are determined assigned by ANFIS app in Matlab.

From 35 set of data samples. 30 sets are used to train the network and 5 remaining are testing data to ensure about reliability of the network. After iteration, the overall error is 2.3% and 1.4% for poly dispersity and residual monomer, respectively, as demonstrated in Fig. 4 and Fig. 5. As seen, the train network predicts results with high accuracy.

The trained network surface for the thickness reduction is shown in Fig. 6. As seen in Fig. 6(a), there is a clear correlation between monomer residual and input parameters temperature and rate of adding monomer. With increase in temperature the hazardous residual monomer decreases. On the other hand, lower adding rate of monomer also reduces the residual. Therefore, these two parameters can be considered as controlling parameters in the process with a well-shaped behavior as illustrated with the aid of surface function. The decision making of the artificial design network is based on this surface for different conditions. However, this surface cannot be the main surface for decision making.

There is another output parameter, poly dispersity, which affects the control of process. As seen in Fig. 6(b), these two input parameters also alter the poly dispersity. Although, there is seen a fluctuated behavior of this output, some ranges of acceptable input values of temperature and rate of adding monomer can be determined. Clearly, high

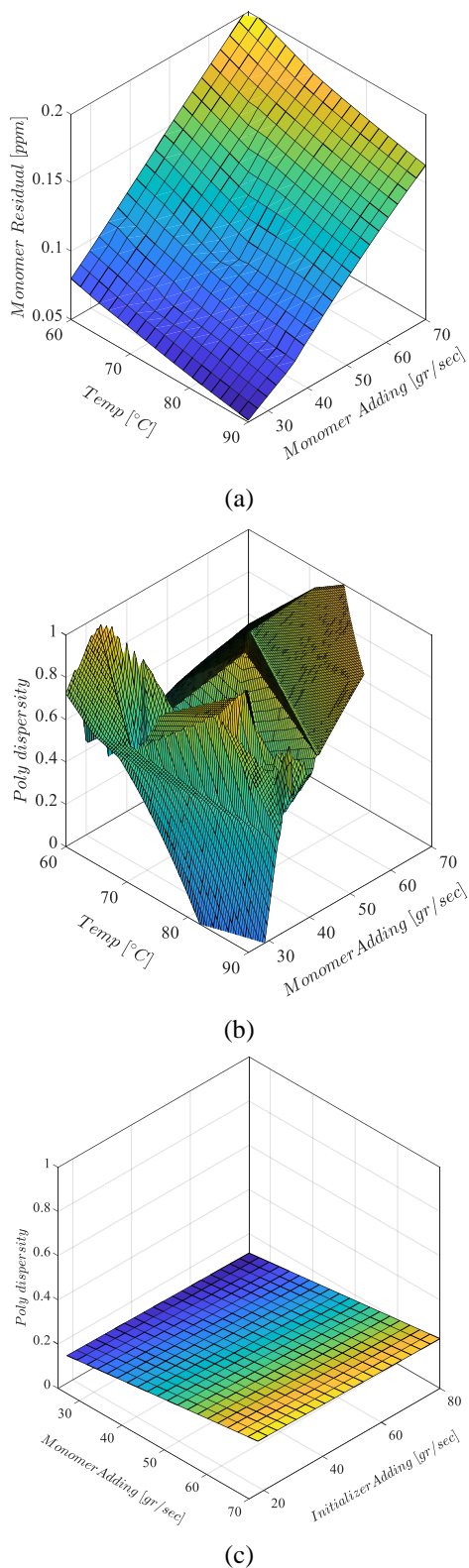


Fig. 6 Dependency of (a) monomer residual and (b) poly dispersity on the process parameters temperature and rate of adding monomer. The effect of the initializer concentration on the monomer residual is shown in (c)

temperature values along with low adding rate results in low and unacceptable values of poly dispersity, i.e., lower than 0.2.

Using these two surfaces, the intelligence system decides how to change temperature and adding rate to keep two important outputs in desirable ranges. These, decision making is not available in traditional control of the process where if-then commands control the process in most controlling systems. Therefore, a valuable result of using IoT system is the capability of using AI methods in controlling chemical process to ensure having a high quality and safe products with online checking and controlling beside instant proper decision making. One question here is that the obtained AI model is reliable? We have clear answer to this question. Based on the reliability of the input data we could train reliable AI models. With inaccurate data or neglecting influencing factor we may train AI systems with low reliability. However, experiences in other fields similar to self-driving cars make us confident that these methods have to be utilized in the chemistry and process controls. There also some other methods which are in some parts analytical and in some section are numerical to reach solve similar problems (Adamian *et al.* 2020, Al-Furjan *et al.* 2020a, b, c, d, e, f, g, h, i, j, k, Alipour *et al.* 2020, Bai *et al.* 2020, Cheshmeh *et al.* 2020, Ebrahimi *et al.* 2020, Ghabussi *et al.* 2020, Ghazanfari *et al.* 2020, Habibi *et al.* 2020, Jermstittiparsert *et al.* 2020, Li *et al.* 2020a, b, Liu *et al.* 2020a, b, Lori *et al.* 2020, Moayedi *et al.* 2020a, b, Oyarhossein *et al.* 2020, Safarpour *et al.* 2020, Shariati *et al.* 2020a, b, c, Shi *et al.* 2020, Shokrgozar *et al.* 2020, Wang *et al.* 2020, Zare *et al.* 2020, Zhou *et al.* 2020). However, the computational costs in these methods are very high (Al-Furjan *et al.* 2020a, b, c, d, e, f, g, h, i, j, k, l, m).

6. Conclusions

Synthesis of acrylate-based dispersion resins involves many parameters including temperature, ingredients concentrations, and rate of adding ingredients. Proper controlling of these parameters results in a uniform nano-size chain of polymer on one side and elimination of hazardous residual monomer on the other side. In this study, we designed an Internet of Things (IoT) system to acquire online measurement data of both input and output parameters to ensure that, first, the nano-size polymeric chains were in an acceptable range to acquire high adhesion property and second, the remaining hazardous substance concentration is under the minimum value for safety of public and personnel health. The obtained dataset is further used to train an adaptive neural network fuzzy inference system (ANFIS) to achieve a model that predicts these two output parameters based on the input parameters. The main results of the study can be encapsulated in the followings:

- IoT system can provide more online data to investigate all-time condition of the process. The data can be saved on servers.
- The gathered data can be analyzed using ANFIS system to make proper instant decisions. This analysis cannot be conducted in the traditional if-then controlling systems
- The models with high accuracy is utilized and can be adopted with more data available
- Higher temperature and lower rate of adding monomer

results in better product in terms of health safety of the product.

- The decision making in AI model is performed considering several parameters of both input and output data.

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