Machine Learning and Optimisation to Improve Energy Utilisation

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***Abstract*— The world is moving towards a conservative approach to fulfilling its energy needs due to inevitable uncertainty and disruptions in the supply chain. In addition, climate change, the availability of materials, and making them sustainable through recycling are other topics of high interest. Energy is a common item among all the industries, and demand for it keeps increasing due to developmental activities. In this work, we aim to improve the efficiency of utilising the available energy in the material processing industries. Mining the ore, extracting the material of interest, melting the material, and manufacturing the required components are typical processes in these industries. The manufacturing of the components also includes a heat treatment process. For example, the heat treatment process demands 20% of the total energy in a non-ferrous foundry. Pre-heating and heat treatment operations consume a significant amount of energy in the ferrous-based industry. We intend to investigate the processes in these industries and create a machine-learning model of the processes involved. Later, we use the machine learning models to build an optimization framework that provides the optimal process operating parameters to achieve the best output while using the least amount of energy.**

Keywords- machine-learning; Optimisation; heat-treatment; energy-efficiency.

I. INTRODUCTION

Heat treatment processes are an important stage in materials processing in which component properties are modified to suit a particular application. In this process, mechanical and physical properties, such as ductility, hardness, toughness, wear resistance, and strength are changed without changing the designed shape and size of the component [1]. In general, heat treatment processes are carried out to improve strength in the case of loaded members and wear resistance in the case of moving parts, however, it can also be used to improve the machinability, formability of materials. The changes in the properties of the material are made possible thanks to the changes which occur at molecular structure/microstructure level. The structure of the material is a function of two factors; (1) Grain size (2) Grain structure. These two components of microstructure of a material define its mechanical and physical properties. Also, heat treatment process is often coupled with pre and post heating process which enable us to utilize energy effectively besides improving the product performance.

In total, it can be observed that there are several parameters involved in heat treatment process such as, chemical composition of alloy, dimensions and shape of the component to be heat treated, micro structural, physical and mechanical properties, energy required for the heat treatment process, etc. Depending on specific objective, some of the parameters will be input before/during heat treatment and others will be output parameters. Irrespective of our objectives if we end up with more than 4 parameters, which vary then a complex problem needs to be solved to realize the effect of each parameter on the set out put parameters. To address this issue regression models are used. A brief literature review of the regression models used to map input to output parameters in heat treatment process is presented in the following section.

The rest of the paper is organized as, details of regression model and its results are presented in Section III, details of optimization framework and its results are presented in Section IV and the conclusions are presented in Section V.

II. LITERATURE

In the case of metals, Johnson [2], Avrami [3] proposed analytical models. Using their work, numerical simulations were developed to study heat treatment process. The simulation results reduced the effort of extensive experimentations (hence reduction in energy consumption) however they lack accuracy [4]. For example, Maisuradze [5] proved that the simulations predict strength parameter inaccurately in a heat treatment process. To address this issue computer aided simulations are developed which give a better accuracy than the simulations [6] – [9].

In general, an important task in a heat treatment model development is to predict the micro-structural properties accurately as they predominantly influence output quality parameters. In this way it is easy to suggest the initial/input parameters of a heat treatment. In this regard, data driven solutions are proven to accelerate the problem solving [10] [11]. Related works in this field include, Homer et al. [12] and Zhu et al. [13] investigated grain boundaries in polycrystalline material using machine learning tools, Raccuglia et al. [14] created a classification model to predict successful and failed experiments using vast amount of experimental data on materials. Agrawal et al. [15] [16] created a machine learning model which predicts fatigue strength of steel using composition and processing parameters. In [17] regression models are used to predict four mechanical properties after heat treatment process. The authors have used five different regression models of which random forests performed well in predicting the mechanical properties and they developed mathematical expressions out of it.

Heat treatment and other processes of glass also results in change in microstructure and hence mechanical properties. Structural and physical properties of strontium borate glass are evaluated against chemical composition using regression analysis by Masai H et al. [18]. Samuel B. O. et al. [19] have developed an optimization technique using which they modelled glass material for composites of particular flexural strength using Taguchi and general regression. In case of glass, a lot of attention is given to the manufacturing processes such as cutting, grinding, etc. In [20] [21], the authors have created a Neural Network (NN) model to predict material removal rate and surface roughness parameters in a laser machining process. Shimaa et al. [22] created a machine learning model of abrasive jet machining of glass in which material removal rate is correlated with process variables of machining process. Bezzera et al. [23] developed a machine learning model using NN to predict shear stress-strain behavior of CFRP material.

There is a lot of research literature in which investigations are carried out on implementing optimization methods with regression models as basis for prediction. Although regression models developed on machine learning techniques perform as per the expectations, the developed models suffer from a dis-advantage. The solution space of the machine learning models may refer to a local maxima or minima, over/under fitting and slow convergence. These disadvantages can be identified and overcome by implementing an optimization technique to rigorously search the solution space for a specific solution that fits our application [24] [25] [26]. In recent research works, deep learning models such as Deep Neural Networks (DNN), Convolutional Neural Networks (CNN), and Recurrent Neural Networks (RNN) are used for forecasting energy demand forecasting. Works of [27] [28] [29] have shown that using more than one type of deep neural networks for forecasting energy demand gives accurate result. Khan A. et al. [30] used machine learning algorithm along with cuckoo search method for forecasting energy requirement. Almalaq, A. et al. [31] used Long short-term memory networks with Genetic Algorithm (GA) to create prediction and optimisation models of energy consumption of buildings. Wen L. et al. [32] used LSTM with particle swarm algorithm (PSO) to correlate load dispatch in a community micro grid with solar power assistance. Similar work is done by Ceylan H. et al. [33] by using GA to estimate energy demand of Turkey using economic indicators.

Some other related works include [34] [35] in which researchers have used PSO to optimally configure the weights of NN to create an accurate model of energy consumption.

Although the reported literature includes the use of GA and PSO, there are several such heuristic algorithms namely, Tabu Search, Simulated Annealing, Travelling Salesman, etc. A review of the algorithms is presented in [36]. Of all these algorithms, GA and PSO are predominantly used because of their exceptional performance when applied to engineering problems. These two methods are broadly similar however they differ in their basic nature of search technique. GA is based on evolution whereas PSO is based on swarm intelligence. A detailed comparison study of these two techniques is presented in [37]. Also, R. Kshirsagar et al. [38] proved that PSO can be derived as special case of GA for a class of engineering problems. GA is a suitable algorithms for non-linear problems.

In this work we used simulation model results of a case study in glass industry to create regression model and an optimization frame work is created using the regression model. The frame work is a multi-objective and multi-constraint based prediction model which is capable of generating input parameter values for a particular output required.

III. REGRESSION MODEL OF HEAT TREATMENT

The case study we considered to analyse is a heat treatment process of glass bottles made of soda-lime material. Cooling part of the heat treatment process is selected for simulation. In the cooling part of the heat treatment we aim to study the changes in material quality and energy consumption in relation to the parameters annealing temperature (^{0}C), Cooling rate (^{0}C/min) and Exit temperature (^{0}C). All the other possible parameters are kept constant for this study. These three parameters are the independent parameters of the process.

For the purpose of creating data related to heat treatment of glass, we have setup maximum and minimum values of independent variables of heat treatment process of glass bottles. The details of the independent parameter values are presented in Table I.

TABLE I. LIST OF INDEPENDENT PARAMETERS AND THEIR VALUES OF HEAT TREATMENT OF GLASS

S.No	Parameters	Level 1	Level 2	Level 3
1	Annealing/Initial Temperature (^{0}C)	545	565	605
2	Cooling rate above S.T (^{0}C/min)	3	6	9
3	Exit Temperature (^{0}C)	70	110	150

Using the values of each independent/input parameters, we have created a full factorial design of experiment which results in 27 experiments. These experiments are carried out in a computer simulation using ANSYS. The simulation is a cooling simulation where the work piece is at annealing temperature and cools down to exit temperature at the given cooling rate. In each simulation, the value of maximum stress and energy required are evaluated. Results of simulation along with input parameters of each simulation are presented in Table II.

TABLE II. SIMULATIONS RESULTS. VALUES OF INPUT AND OUT PARAMETERS

Input parameters			Output parameters (Simulation results)	
Initial temperature (^{0}C)	Cooling rate(^{0}C/min)	Exit temperature(^{0}C)	Max Stress (von-Mises) Pa	Energy (J)
605	6	150	476420	73309
545	6	70	476350	76573
545	9	150	714670	63029
545	3	110	238230	70496
605	6	70	476350	86364
545	3	70	238200	77017
545	3	150	238270	63975
545	6	110	476390	70045
545	6	150	476420	63516
545	9	70	714440	76090
545	9	110	714540	69560
565	3	70	238200	80276
565	3	110	238230	73756
565	3	150	238270	67236
565	6	70	476350	79837
565	6	110	476390	73309
565	6	150	476420	66780
565	9	70	714510	79355
565	9	110	714620	72825
565	9	150	714490	66295
605	3	70	238200	86795
605	3	110	238230	80276
605	3	150	238270	73756
605	6	110	476390	79837
605	9	70	714440	85886
605	9	110	714540	79355
605	9	150	714660	72824

Using these results (listed in Table II), a data set is created with three input parameters namely Initial temperature, Cooling rate and Exit temperature, two output parameters namely maximum stress value and energy. NN is used to create a regression model. Details of the NN is presented in Figure 1.

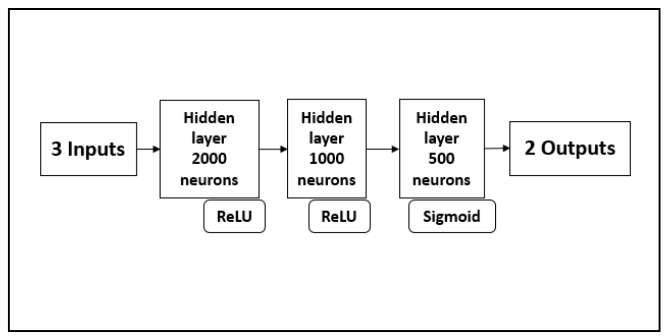

Figure 1. Flow chart of optimisation algorithm.

It can be noted that a specific architecture (as shown in Figure 1) is used in this work to create NN. As explained in [25], there is no logical way to decide the number of neurons and number of hidden layers in NN architecture for a particular type of problem or data set. In this report the architecture shown in Figure 1 is realised after several attempts made, by changing the number of hidden layer, number of neurons in the hidden layers and examining the results after several training iterations. The NN code is set to iterate till the loss function evaluated on training set is same as testing set and percentage error evaluated between predicted values and the actual values is less than 1%. This exercise confirms that the created model is accurate and does not over fit the data.

Data is normalised before feeding it to NN. It is normalised using the formula given by (1).

$$X_{norm} = \frac{X - X_{min}}{X_{max} - X_{min}} \qquad (1)$$

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Here, X_{norm} – normalised value, X_{min} – minimum value of a particular variable , X_{max} – maximum value of a particular variable , X – actual value of the variable (from Table II). It can be noted that the data in normalised form is unit less.

TABLE III. ACTUAL OUTPUT PARAMETERS, ESTIMATED OUTPUT PARAMETERS AND PERCENTAGE ERROR

Output parameters (Simulation results)		Output parameters (Neural network Model predictions)		Percentage error	
Max Stress (von-Mises) Pa	Energy (J)	Max Stress (von-Mises) Pa	Energy (J)	Max Stress (von-Mises)	Energy
476420	73309	474945	73260.8	0.31%	0.07%
476350	76573	473229	76579.8	0.66%	0.01%
714670	63029	716380	62957.3	0.24%	0.11%
238230	70496	239977	70599.4	0.73%	0.15%
476350	86364	473776	86353.2	0.54%	0.01%

The NN is trained by dividing the data into training and testing set. The division is carried out randomly. 80% of the data is used to create the NN model. Rest of the 20% of the data is used to validate the model created by training data. Mean squared error is measured on both testing and training data set. Training of the NN is carried out till mean squared error measured on both testing and training are equal so that the prediction model does not over fit the data. Percentage error between the predicted values and the actual values is within 1%. Percentage error evaluated over five data points is presented in Table III.

IV. OPTIMISATION MODEL USING HEAT TREATMENT MODEL

Regression model created (in Section III) to predict Von-Mises stresses and energy is used in GA to create optimization frame work. It enables us to find out the values of input parameter values for the required output. In the frame work, objective function is created using regression models created using NN. The objective function is given by (2).

Objective function = Minimize {abs(Stress evaluated by regression model-Required stress value)+abs(Energy evaluated by regression model-Required energy value}) (2)

Note that the parameters used in (2) are in normalized form, hence the issue of incomparable engineering units in a single equation does not arise. Also the parameters used in (2) namely "Required stress" value and "Required energy" value are set by the user. The range of parameters is 0 to 1. The regression model and the optimization process works well for interpolation.

The objective function is created as a minimization problem in which GA tries to find out a stress and energy value which is equal to required stress and energy values. The iterative steps in GA are as follows

- Step 1: Create an initial population. Here the initial population is nx3 matrix where n is the population length and 3 is the number of input variables in GTS data. Each value in the matrix is chosen randomly that lies between 0 and 1. This is because, regression model created is based on normalized data.
- Step 2: Evaluate stress, energy values for each population set (each row of nx3 matrix) using regression model and then evaluate objective function given by (2).
- Step 3: As the objective is to minimize (2), the rows of population set is sorted in ascending order with respect to objective function.
- Step 4: Top half of the population is selected as fit population. Cross over is carried out on the fit population by selecting two random chromosomes. Another half of the population is replaced with newly formed chromosomes.
- Step 5: Mutation is carried out by replacing randomly selected gene in a randomly selected chromosome.
- Step 6: repeat from step 1 to 5 with new set of population formed in Step 5 until the percentage error between the actual vs predicted values is within the set value.

Flow chart of the Algorithm explained in the above 6 steps is presented in Figure 2.

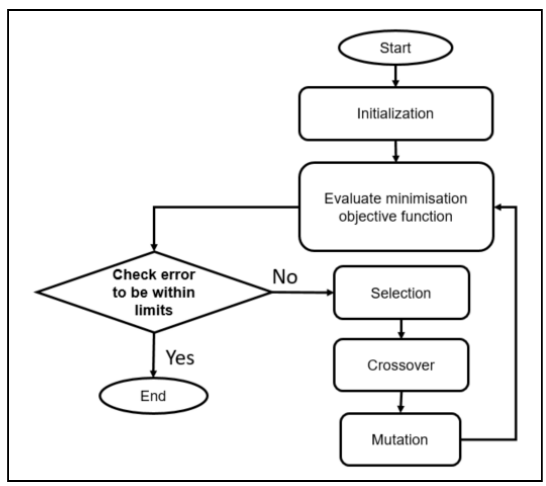

Figure 2. Flow chart of optimisation algorithm.

To start the algorithm, we have set required stress value and energy value as presented on Table IV.

TABLE IV. RESULTS OF OPTIMISATION FRAMEWORK

S. No.	Max Stress (von-Mises) Pa	Energy (J) (Set value)	Temp (GA result)	Exit temp (GA result)	Cooling rate(^{0}C/min) (GA result)	Max Stress (von-Mises) Pa	Energy (J) (NN result)

	(Set value)					(NN result)	
1	333494	74912	593.216	130.294	4.31758	332858	74903.1
2	285847	74912	573.789	112.013	3.74986	286081	74812.2
3	285847	65405.6	548.204	143.704	3.80564	285242	65338.5
4	476435	65405.6	553.14	147.554	6.00404	476384	65379.8
5	667023	84418.4	601.384	75.5933	8.3983	666715	84426.1
6	667023	79665.2	598.011	101.057	8.36115	662141	79657.9

Using trial and error, we identified that a population size of 50 results on definite convergence. So the population size is set to 50 and the algorithm is iterated till the required accuracy is achieved. At the end of the iterations, top chromosome set after sorting is identified to be the best solution. This exercise is carried out for all the 6 set of stress and energy values and corresponding input values obtained using GA are presented in Table IV with label "GA result".

To validate the obtained values using GA, "GA result" set are input to neural network model and stress and energy values are calculated. The values are presented in Table IV with label "NN result".

TABLE V. PERCENTAGE ERROR OF ACTUAL VALUES AND THE VALUES OBTAINED BY OPTIMISATION FRAMEWORK

Optimization frameworks results		Set values		Percentage error	
Max Stress (von-Mises) Pa	Energy (J)	Max Stress (von-Mises) Pa	Energy (J)	Max Stress (von-Mises)	Energy
332858	74903.1	333494	74912	0.19%	0.01%
286081	74812.2	285847	74912	0.08%	0.13%
285242	65338.5	285847	65405.6	0.21%	0.10%
476384	65379.8	476435	65405.6	0.01%	0.04%
666715	84426.1	667023	84418.4	0.05%	0.01%
662141	79657.9	667023	79665.2	0.73%	0.01%

Percentage error of between "GA result" and "NN result" is evaluated and tabulated in Table V. Maximum value of percentage error falls below 1% in this case also.

V. CONCLUSIONS

Heat treatment process of glass is studied in this work. A specific pattern of heat treatment and cooling is required to achieve desired properties in the glass material. For the purpose of study, independent/input parameters list is created with their maximum and minimum values. A full factorial design of experiments set is listed for computer simulations. Output parameters namely stress, energy are evaluated using the simulations. A multi-objective and multi-criteria optimization framework is created using regression model and genetic algorithm. Results obtained using both regression model and optimization model are well within 1% error. Although only one case study is used to carry out the analysis, the optimization framework we proposed can be used for any industry problem.

The framework proposed in this manuscript allows to set the output parameters and evaluate input parameters. GA is used for the evaluation. The framework also allows to constrain the range/value of few input parameters and evaluate others. In this way it is possible to obtain a range of input parameters which fit the operating conditions. So for a particular value of energy consumption and stress value and exit temperature, it is possible to obtain various values of cooling rate and initial temperature. An example is presented in Table VI. In this way, an optimal input parameter-set can be evaluated for a particular operating conditions. Several such input parameter-set can be evaluated using the proposed framework.

TABLE VI. MULTIPLE INPUR PARAMETER-SET FOR A PARTICULAR VALUES OF OUTPUT PARAMETERSSS

Initial temperature (^{0}C)	Cooling rate(^{0}C/min)	Exit temperature(^{0}C)	Max Stress (von-Mises) Pa	Energy (J)
545.971	4.80058	112.333	381141	70158.8
547.31	4.79042	113.755		
552.531	4.86698	119.288		
566.68	4.76859	132.511		
574.075	4.88605	139.3		

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