

**Incorporation of Phenomenological Models
in a Hybrid Neural Network
for Quality Control of Injection Molding**

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Abstract

Injection molding is characterized by complex dynamics, which makes quality difficult to control. This is because the exact relations between the machine inputs, material properties, and molded part quality are not known precisely. Hence, the existing models for quality prediction have a limited accuracy and difficulty in application to general molding applications [1, 2]. This paper investigates the integration of analytical process knowledge and artificial neural networks as a solution for quality prediction of molded parts, with accuracy increased towards quality control targets of three defects per million (6σ). This paper describes the hybrid system based on the neural network and process knowledge then compares its performances with conventional neural models for prediction of the injection pressure.

Key Words

hybrid neural networks; on-line quality control; injection molding process control; design of experiments

Introduction

Injection molding is a widely used process for high volume production of thermoplastic resin parts. It can produce complex parts with different combination of plastics and fillers and has a high efficiency ratio between applied material and the end product. Despite major advantages of injection molding, there are significant difficulties in controlling quality of the molded part. These difficulties arise not only from the complex dynamics of the process and unpredictable behavior of the material under temperature-pressure fluctuations, but also from the lack of consistent relationships between the material properties, machine parameters, mold geometry and molded part quality.

There are several sources of variation in the injection molding process which include material properties, process machinery, mold design, environmental fluctuations, and human interaction [3]. If these factors had precisely defined and deterministic effects on the process, the quality of the molded part could be easily controlled. However, there are many interactions between stochastic factors, resulting in frequent irregularities in process parameters so the ideal state of constant quality does not exist. Examples of such irregularities include mold and melt temperatures that can drift from their set values, changes in polymer properties from batch to batch, and the machine and tool performance, which alter as they wear. Besides these major factors there exists small natural fluctuations making the process even more unpredictable.

There are several different approaches to quality control and process optimization (such as expert systems, continuous process control, regression modeling, and design of

experiments) that are used in industry today [4-7]. Unfortunately, none of these approaches deliver 100% quality assurance. Difficulties in regulation arise mainly from non-linear character of the process and interactions between inputs that make the relationships between machine parameters and part quality not obviously defined. At the same time, the number of variables adds difficulty in evaluation of the significant parameters. Thus, a more capable quality control system requires a process model that not only describes the relationship between the process parameters and the resulting part quality, but is also capable to learn and express the process nonlinearities and complexities. Because of the stochastic correlations between the process parameters and characteristics of part quality, such a model should also be adaptable to the changing process conditions.

Neural Networks Approach

Artificial neural networks (ANN) offer an alternative approach to forecast part quality. Emulating a biological neural network, ANNs are trained by representative examples. Once a neural network has been trained, the quality characteristics of the molded part can be predicted from the measured process data during production. ANNs are inherently nonlinear with a network structure capable of modeling nonlinear systems. The basic element of neural network structure is a neuron, depicted in Figure 1.

A neuron accepts a signal or set of signals from input or other neurons, sums together the weighted signals, adds a bias value, and passes this summed value through a transfer function. This transfer function specifies how the neuron will scale the response

to incoming signal, and produces the output. Most common transfer functions (f) used in back-propagation learning methods are sigmoid functions, such as log-sigmoid (eq.1)

$$f(N) = \frac{1}{1 + e^{-N}} \quad (1)$$

and hyperbolic tangent sigmoid (eq.2).

$$f(N) = \frac{e^N - e^{-N}}{e^N + e^{-N}} \quad (2)$$

These functions are smoothly defined over the interval of possible input values. During training, the weights and biases are updated using the approximate steepest descent rule. This optimization continues until the error is small enough for application. After the network is trained, the system is tested with a different set of data. Several reviews of neural network techniques used in process and quality control are available elsewhere [8-12].

As was shown in previous works [1, 2, 13-20], artificial neural networks have provided better results (accuracy of 96%) than other methods (such as multiple regression modeling, statistical process control) due to their ability to deal with nonlinear effects and interactions. On-line predictions of mass, sink marks, and surface quality characteristics of molded parts using ANNs were obtained, for example, by Hauessler [1]. The correlation coefficients for the calculated and measured quality characteristics obtained by neural networks were approximately 15% higher than similar coefficients obtained by a multiple regression model. The results of these works show the advantage of the neural networks in terms of expression of process non-linearities, and that ANNs can be used as a powerful tool in process regulation.

In related research, Wortberg [14] utilized the skeletonization method in combination with ANNs to analyze melt inhomogeneities, varying boundary conditions and wear of the machine. Woll et. al. [2, 16] developed a cascade control strategy using an artificial neural network to analyze cavity pressure patterns, then update machine set points to maintain a desired pressure pattern set point as a part quality signature. DeMirci [20] developed a system for the control of flow front progression during injection molding processes. In this case, the control scheme developed is based on a neural network that was trained with data obtained from a first-principles based process model rather than actual molding experimentation. The control strategy was developed such that one can specify a desired flow progression scheme and the controller will take corrective actions during the molding process to realize this scheme.

In these research efforts, the goal is typically to achieve 100% quality assurance as described by Haeussler [1]. However, the accuracy of correlations available from ANNs remain inadequate given quality targets of three defects per million. Also, the model usually requires significant training, which may involve many molding iterations. Yonehara [13] examined different network topologies and different training strategies for a large set of fifteen input variables. While some improvements were made with respect to learning rates, large sets of training data were still required. This is often not acceptable for on-line applications. Finally, the neural network approach assumes the process to be a 'black box' with unknown relationships among different parameters, and does not provide insight into the process behavior.

The integration of process knowledge into neural networks might be one of the best ways to solve the problem of 100% quality inspection. In the application to injection

molding, such a hybrid system may speed up the convergence, improve accuracy, and eliminate the links that do not affect part quality.

Implementation

To investigate and compare the performances of the hybrid and conventional models, several network topologies were built and trained for the same data subsets. This data is the result of an extensive experimental investigation performed at GE Plastics (Pittsfield, MA). The part, a Hewlett – Packard printer Output Tray, was molded on a 550 ton Krauss Maffei machine (Figure 2) with a high speed data acquisition system. The single-cavity mold was filled with a grade of ABS (Cyclocac GPM5500).

The experimental data set contains 69 subsets, each of which includes from 5 to 20 runs. The machine inputs that were adjusted during the experiment include plastication time (sec), dwell time (sec), hold time (sec), back pressure (MPa), shot size (m), cushion (m), injection velocity (m/sec), hydraulic pressure (MPa), and melt temperatures (C). The part attributes determined for each part were weight, surface quality (presence of burn marks, sink marks, blush, flash formation), the width and length, and the presence of the short shot. Data for this investigation was extracted from the experimental data set in such a way that it contains 69 representative runs with varying machine inputs.

Description of the process model

The dynamic model of the filling process for a rectangular strip geometry [21] includes the local mass conservation equation (eq. 3), the momentum balance in the axial direction (eq. 4) and the local energy balance (eq. 5).

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v) + \frac{\partial}{\partial z}(\rho v) = 0 \quad (3)$$

$$0 = \frac{\partial}{\partial z} \left(\eta \frac{\partial v}{\partial z} \right) - \frac{\partial P}{\partial x} \quad (4)$$

$$\rho C_p(T) \left(\frac{\partial T}{\partial t} + v \frac{\partial T}{\partial x} \right) = \frac{\partial}{\partial z} \left(\kappa(T) \frac{\partial T}{\partial z} \right) + \eta \dot{\gamma}^2 \quad (5)$$

In these flow equations, x is the axial coordinate, z is the gap-wise coordinate, and (v, v) are the velocity components in the local (x, z) directions, t is time, T is the temperature, P is the pressure, ρ is mass density, η is viscosity, $C_p(T)$ is the specific heat, and $\kappa(T)$ is thermal conductivity of polymer melt.

The flow dynamics of the polymer during filling and post-filling stage is highly dependent on the shear viscosity of the polymer melt. Polymers exhibit a non-Newtonian, shear-thinning behavior with increasing shear rate and also are highly temperature and pressure dependent. If polymer viscosity is a function of temperature and shear rate only, then it can be calculated by the following empirical equation:

$$\eta = \frac{\eta_0}{\left(1 + \frac{\eta_0 \dot{\gamma}}{\tau^*} \right)^{1-n}} \quad (6)$$

where η_0 is the zero-shear-rate viscosity (eq 7), the parameter n is the power-law index, and τ^* is the stress level at which the viscosity transitions from the Newtonian limit to the power-law asymptote corresponding to large shear rates [21].

$$\eta_0 = B \exp\left(\frac{T_b}{T_p}\right) \cdot \exp(\beta P) \quad (7)$$

B is the reference viscosity coefficient, β is the pressure dependence coefficient, and T_b characterizes the temperature sensitivity of η_0 .

The value of the shear rate of the polymer in the plate can be approximated as:

$$\dot{\gamma} = \frac{6Q}{w \cdot h^2} \quad (8)$$

where Q is the melt flow rate, w and h are width of the flow front and wall thickness respectively.

The cavity pressure P_c can be calculated from the Hagen-Poiseuille equation (9) for the polymer flow of a non-Newtonian fluid between plates as

$$P_c = \frac{12\eta \cdot Q \cdot H_{Lc}}{w \cdot h^3} \quad (9)$$

where H_{Lc} is the distance between cavity pressure transducer and the flow front. The Poiseuille flow equation can be used under an assumption that the polymer flow is steady. The equations 6-9 are based on the assumption that the polymer flow is fully developed, laminar viscous flow.

Description of the Conventional Model

In this work, the melt pressure was chosen as a focus of investigation for two reasons. First, melt pressure is an observable and continuous characteristic related to the molded product quality; the melt pressure results from many input parameters and is available to a high resolution. Second, many quality attributes, for instance, short shot and aesthetics, are not directly observable as a continuous response; therefore they are subject to interpretation and not suitable for this investigation.

Melt temperature, ram velocity, and shot size were chosen as inputs for the conventional network. The melt temperature was varied between 210 and 259 C (410 and 498 F), ram velocity between 0.12 and 0.71 m/sec (0.5 and 2.8 in/sec), and shot size between 0.75 and 0.88 m (2.96 and 3.47 in). The injection pressure had observed values distributed between 5.7 and 14.9 MPa (826.9 and 2167 Psi).

To choose the most appropriate network, several network topologies were constructed of different complexity and various activation functions, started from different random weight configurations and different training subsets. The network that showed the smallest mean squared error along with smallest standard deviation for test points was chosen as a model for the next stage of investigation. The results indicated that the best architecture for the conventional model in this instance is a fully connected network with two hidden layers, which contains three and one hidden nodes respectively, and log-sigmoidal (logsig) activation function in both layers (Figure 3).

Description of the Hybrid Model

Figure 4 presents the process model when the shear rate, viscosity, and pressure are estimated from velocity, melt temperature and shot size by using empirical equations given above (eqs. 6-9). The viscosity coefficients are given in table 1, as measured from a typical capillary rheometer.

On the basis of this model, the hybrid neural network was built and trained. Melt viscosity, ram velocity, shot size, and estimated pressure were the inputs for the hybrid network, with injection pressure as the output. The design intent is that the topology and internal coefficients of the hybrid model will permit the fastest convergence when the

network contains just one hidden node with a linear (purelin) activation function, as presented in Figure 5.

Neural Networks Configurations

Before training, all data inputs were scaled according to their activation function, such that every value falls within a given range. For instance, the target outputs for neural network with sigmoidal function lie in a range from zero to one, thus all input data should be scaled down to this interval. Another reason for scaling each variable into a fixed range is that they cover different ranges. For instance, the shot size data varies in range from 0.12 to 0.7 (m), while the melt temperature data covers the interval from 210 to 259 (C). The errors due to the higher valued variable will have a greater effect during training if unscaled. Thus, ensuring that every variable covers the same range also ensures that errors on each variable contribute the same portion to the change of network weights. The variables v were scaled within the range from zero to one, producing a new value r , according to the equation:

$$r = \frac{v - \min(v_{1...n})}{\max(v_{1...n}) - \min(v_{1...n})} \quad (10)$$

The target outputs were also scaled to a range that in within the bounds of the sigmoid function. The common practice in scaling of the outputs [22, 23] is to use only the relatively linear part of the sigmoid function that lies between 0.1 and 0.9. Thus, all output data was scaled to this range:

$$tar = 0.1 + \left(\frac{v - \min(v_{1...n})}{\max(v_{1...n}) - \min(v_{1...n})} \cdot 0.8 \right) \quad (11)$$

where tar is the new value of output.

When the neural network is initialized, the weights and biases must be given some initial values from which the training process may begin. These initial values should be chosen in such a way that the learning be performed as fast and accurately as possible. Usually, the initial weight setting contains the small random numbers uniformly distributed around zero. In this work, since the relationships between the input parameters and the pressure are known a-priori from the phenomenological models and the experimental data is available, the initial weights were estimated according to the character of these relationships. For instance, our process knowledge indicates that the injection pressure will rise as the polymer viscosity increases. Therefore, the initial value of the weight on the link from viscosity to pressure should have a positive sign. Furthermore, the approximated value of the weights can be found from the estimated slope of the viscosity-pressure data. From the existing experimental data it was defined that the initial values of the weights should be set within the range from 0.1 to 0.3. Using similar methods, all other initial weights were determined. Their approximated values are given in Table 2.

Results and Discussion

Using the systems described above, multiple training sets were utilized to estimate the effectiveness of conventional and hybrid neural networks. Since the model should reflect a real molding process where the number of different data sets is limited, multiple training experiments were performed using one, four, and sixteen sets of randomly selected molding data. The hypothesis is that the hybrid network should

outperform the conventional neural network, as can be confirmed by testing both networks with the remaining (69- n) data points.

The graphs of observed pressure vs. predicted pressure for training on one, four and sixteen points are shown in figures below. In the ideal case, when the data does not contain noise and the network is perfectly accurate, the observed injection pressure is always equal to the predicted value as presented by the diagonal line. However, this ideal case is difficult to achieve due to frequent irregularities in the process as well as uncharacterized process dynamics due to the complex interactions between input parameters. To compare the performance of the conventional and hybrid networks, the mean squared error measure was used as an indicator of accuracy. To remove dependency on input selection, the network performance was investigated across multiple runs which were randomly instantiated. The sum of the squared errors (SSE), together with the standard deviation across multiple runs, can then be confidently used as measures of model performance. The average number of epochs to train the network and the average computing time (cpu) were also used as parameters for comparing the speed of convergence.

Simulation studies for twenty different (randomly chosen) training sets have shown that the incorporation of the process knowledge to the quality model can significantly enhance the performance of the neural network. Figure 6 graphs the predicted pressure as a function of observed pressure for the conventional and hybrid networks. The training with only one point shows that the conventional system always predicts the test point. This is, of course, expected as the conventional network is trained on only one point and thus has no access to information regarding sensitivities. The

hybrid network, however, is able to perform a generalization since its internal phenomenological models provide some additional information about the melt pressure behavior. As such, the hybrid model uses the one training point to ‘tune’ its internal models and provide reasonable estimates of melt pressure.

The training on four points also shows the advantage of the hybrid model compared with the conventional model. Figure 7 presents the observed vs. predicted pressure for conventional and hybrid networks with four points. With more data points, the behavior of both the conventional and hybrid networks are improved. The conventional network now has access to multiple data points and can thus estimate the global behavior of the injection molding process. However, the accuracy of the result is highly dependent on the selection and relationships of the four points which are randomly selected. Because of this dependency, both the error magnitude and standard deviation are significantly lower for the hybrid network, which can use its internal knowledge to balance and extrapolate from the chosen points.

For example, if the four training points are uniformly distributed throughout the data set, the networks result in an SSE of 1.11 and 0.62 for the conventional and hybrid systems, respectively (Figure 7). However, if all four points are located in a local area of the data set, the conventional network shows a significant reduction of accuracy (SSE=2.51), while the hybrid network is capable to predict pressure with approximately the same accuracy (SSE=0.65). After twenty different runs with randomly chosen training points, the results indicated that the accuracy of the hybrid model increased by 54% (with respect to the sum of squared errors) and standard deviations decreased by 61% when compared to the performance of conventional networks.

With additional data, however, the advantages of the hybrid network become less clear. In fact, the conventional network shows the best results when the system is trained on a significant amount of data (16 points). In this case, the conventional model has enough process data to perform training, and, since the relationships between the input parameters and output-pressure are not strictly defined, also has more degrees of freedom than the hybrid model. This is because the hybrid network involves implementation of artificial built-in constraints that reduces the number of degrees of freedom. For instance, the temperature-pressure relationship in the molding process may be more clearly defined than the viscosity-pressure relation in the hybrid model (e.g. an analytic relationship of eq. 9). Thus, the multiple layers of neurons provides greater model flexibility for the conventional network to outperform the hybrid network after adequate training on a large data subset (Figure 8).

Table 3 summarizes the results of pressure prediction of the two quality models. Results of the conventional and hybrid network performance in terms of accuracy have been previously discussed. The sum of squared errors are plotted as a function of number of training points in Figure 9, with the whiskers indicating the calculated standard deviation across multiple training sets. The results indicate the trade-offs between conventional and hybrid neural network approaches. Given a small amount of data, the hybrid network was able to quickly estimate the molding response to a reasonable degree of accuracy. Given a large amount of data, the conventional neural network was more able to replicate the observed process behavior.

Accuracy is one measure of model performance. There are two additional behaviors which should be discussed. First, the hybrid network with its controlled topology permits interpretation of internal state variables. For instance, the hybrid model discussed in this paper estimated a representative shear rate of approximately 200 sec^{-1} , which is valuable information for material development, selection, and lot to lot characterization. Second, the hybrid network also exhibits the fastest convergence. This leads to the significant reduction of average number of epochs (by approximately 55%) and computing time (by 50%) when the network is trained on one and four points.

Conclusions

The complexity of the injection molding process makes it difficult to develop a model for quality prediction that delivers 100% quality assurance. This work has shown the successful integration of process knowledge into a neural network for the prediction of melt pressure. The results of training the conventional and hybrid models with a back-propagation learning rule demonstrated the ability of the hybrid neural system to predict pressure more accurately when training is performed using a minimal amount of data (one and four points). When significant data was available, conventional neural network designs did outperform the hybrid topologies.

The next stage of investigation is the development of a hybrid system for prediction of other quality attributes, such as width and length. These hybrid networks will involve the development of a more sophisticated model with a description of the residual stress and shrinkage dynamics. Additional research is also required for the development of novel process tuning and regulation strategies that interpret and leverage

such hybrid networks. If successful, this research will open new possibilities in developing an on-line control system that directly relates desired changes in molded part quality to necessary changes in machine inputs.

Nomenclature

a	Output of neural networks or hidden layer
b	Biases of neural networks
B	Reference viscosity coefficient
β	Pressure dependence coefficient
C_p	Specific heat
f	Activation function of neural networks
h	Thickness of the wall
H	Total length of polymer
k	Thermal conductivity of polymer
n	Power-law index
N	Input for transfer function
P	Injection pressure
P_c	Cavity pressure
ρ	Mass density
R	Input to the neural networks
r	New value of variable v after scaling
t	Time
T	Melt temperature
tar	New value of the output after scaling
T_b	Temperature sensitivity
Q	Average melt flow rate of the polymer
γ	Shear rate
τ^*	Modified-Cross model parameter
η	Viscosity of polymer melt

η_0	Zero-shear-rate viscosity
(u, v)	Velocity components in the local (x, z) directions
v	Input , output variable
V	Injection velocity
W	Weights of neural networks
w	Width of plate shape mold
x	Shot size

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Table 1. Rheological Coefficients

<i>B</i>	3.44e-6 PaSec
τ^*	5.18e4 Pa
<i>n</i>	0.319
<i>Tb</i>	1.04e4 K

Table 2. Initial Values of Network Weights

Input	Weight Sign	Weight Value
velocity	>0	0.2 ... 0.3
shot size	>0	0.3 ... 0.4
temperature	<0	-0.4 ... -0.5
viscosity	>0	0.2 ... 0.3
estimated pressure	>0	0.4 ... 0.5

Table 3: Comparison of Conventional and Hybrid Networks Predictions

	One Point		Four Points		Sixteen Points	
	conventional	hybrid	conventional	hybrid	conventional	hybrid
sum sq. error	3.102	1.045	2.004	0.909	0.459	0.697
st. deviation	1.518	0.435	0.84	0.328	0.206	0.536
epochs	77.5	28.1	162	76.1	889.7	943.1
cpu	3.6	2.3	9.1	3.8	43.3	26.3

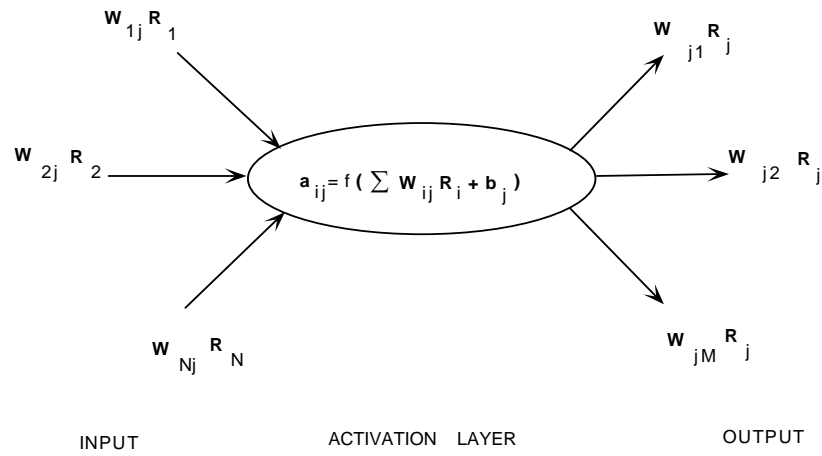


Figure 1: Microstructure of Neural Networks

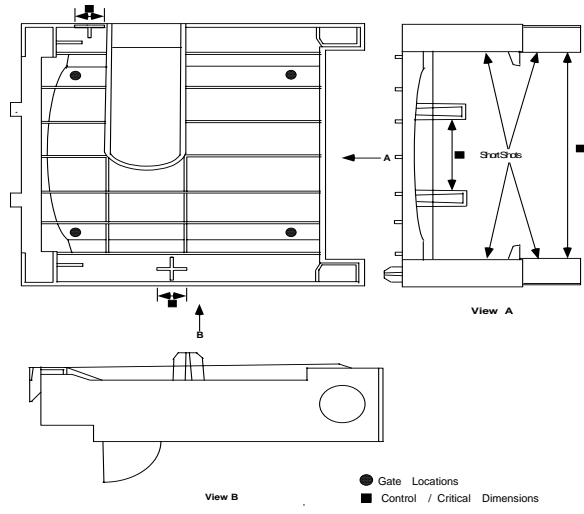
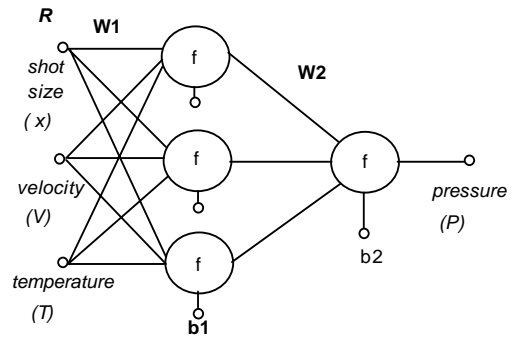
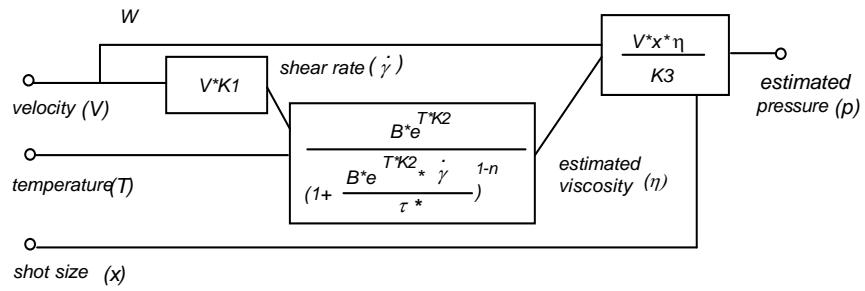


Figure 2: HP Printer Output Tray



$$a1 = \text{logsig} (W1 \cdot R + b1) \quad a2 = \text{logsig} (W2 \cdot a1 + b2)$$

Figure 3: Conventional Neural Network



B, τ^*, n - experimental coefficients

Figure 4: Hybrid Model for Prediction of Injection Pressure

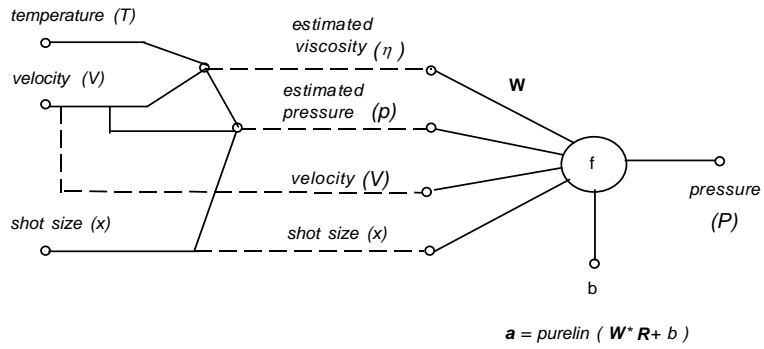


Figure 5: Hybrid Neural System

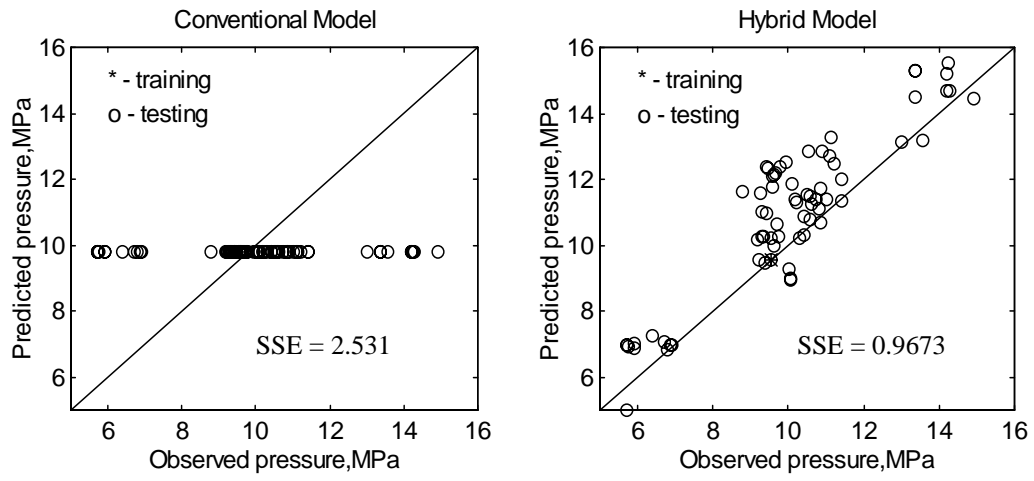


Figure 6: The Observed vs. Predicted Pressure for Conventional and Hybrid Models, 1 Point

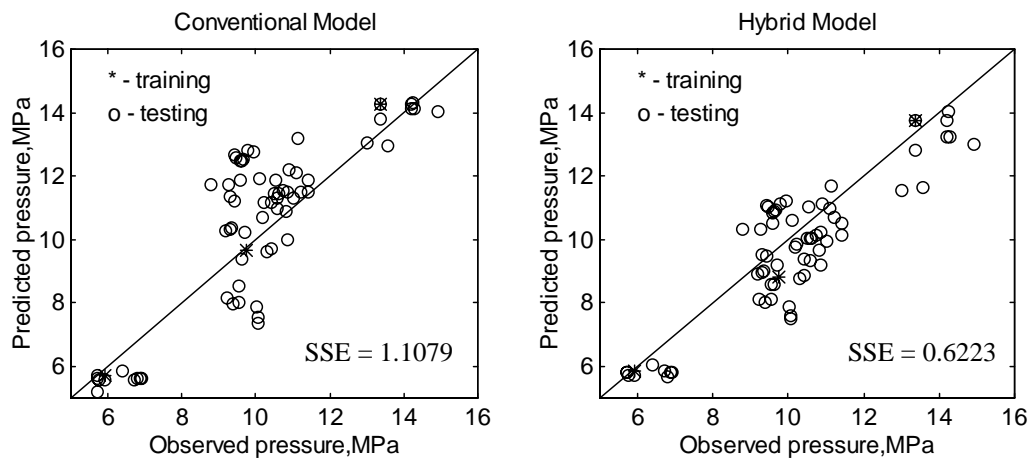


Figure 7: The Observed vs. Predicted Pressure for Conventional and Hybrid Models, 4 points

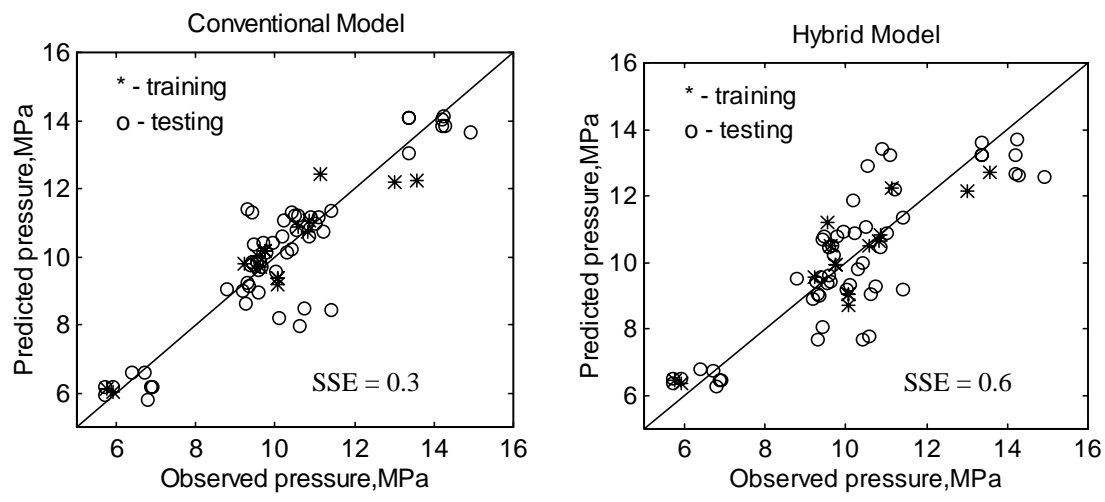


Figure 8: The Observed vs. Predicted Pressure for Conventional and Hybrid Models, 16 points

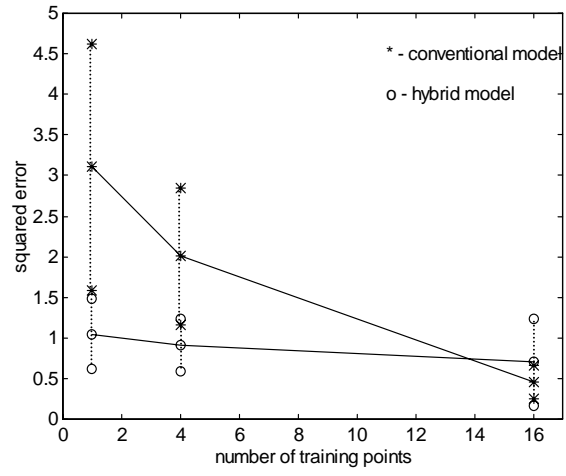


Figure 9: Sum of Squared Errors and Standard Deviations for Conventional and Hybrid Networks.