

A MODELING AND OPTIMIZATION TOOL FOR THE EXPANDABLE POLYSTYRENE BATCH PROCESS

Mikko Heikkinen¹, Ville Nurminen², Teri Hiltunen¹ and Yrjö Hiltunen¹

¹University of Kuopio, Department of Environmental Sciences
P.O. Box 1627, FIN-70211 Kuopio, Finland

²StyroChem Ltd
P.O. Box 360, FIN-06101 Porvoo, Finland

Mikko.Heikkinen@uku.fi (Mikko Heikkinen)
Ville.Nurminen@styrochem.com (Ville Nurminen)

Abstract

The Expandable Polystyrene (EPS), material of the insulation productions and packages, is commonly produced in a batch process. The control of the batch process is based on predefined process recipes and the process parameters such as mixing properties. The EPS production has to be able to satisfy the aims and quality requirements of the markets, which causes additional demands on process control. In this paper we demonstrate the optimization and modeling application for the EPS-batch process. The application consists of a production optimization tool and a simulation tool for the process parameters based on the Multi-Layer Perceptron network (MLP) with retrain properties. The software can be used at the operational level as well as at the process management level. The features are programmed into standalone software built up in the Matlab environment and it is tailored for the needs of the EPS production company StyroChem Ltd. The results show that the application can offer an efficient tool to economize production and storage costs.

Keywords: batch process, modeling, simulation, process optimization, Multi-Layer Perceptron (MLP).

Presenting Author's biography

Mikko Heikkinen, born in Sotkamo, Finland, November 24, 1975, graduated from the University of Oulu, Finland, as M.S. (eng.) in 2003. His main research interest includes process engineering, process modeling, industrial data processing, and data mining. He is currently preparing the Ph. D. degree in process informatics.



1 Introduction

Many studies have shown the importance of data-based modeling methods such as neural networks in the field of an industrial process [1-7]. However, getting these intelligent mathematical methods for the industrial daily-use has been challenging. Processing the raw data as well as modeling and simulation is problematic if the conditions of the process change. Furthermore, artificial neural networks, such as the Multi-Layer Perceptron (MLP) model, are considered difficult to use at the operational level.

A batch process is commonly used for producing Expandable PolyStyrene (EPS). Batch processes are typically based on predefined process recipes. If the process conditions, chemicals and recipes are constant, the product should always be the same in theory. In practice, the EPS polymerisation reaction in the batch reactor is a very sensitive process and is affected by numerous variables, which makes the process difficult to control. Moreover, EPS production has to be able to satisfy the aims and quality requirements of the markets, which causes additional demands on process control. Thus, there is clearly room for intelligent mathematical methods and computational modeling systems such as artificial neural networks (ANN) in the control of the EPS process and optimization of the production.

The selling EPS production is divided into fractions of the bead size. For example, the bead size for the insulation product is different from the bead size for the cup. Each of the batches produces the load of beads, where the mean bead size is controlled, but the shape of the bead size distribution is typically Gaussian. Therefore, the production of the campaign is a sum of the Gaussian bead size distributions. Thus, the biggest challenge is to produce the optimal bead size fractions for the markets.

Archived process data is an important resource for knowledge management of the process, and it can be used for the optimization and improvement of productivity. Several studies have demonstrated that ANN can provide an efficient method for modeling industrial data [1-7]. In particular, studies, which use standardized protocols, are most likely to benefit from automated artificial neural networks analysis [1-9]. One of the most popular ANN methods, the Multi-Layer Perceptron network (MLP) [1-3, 6] has been successfully applied in many areas of research and for process optimization. Previous study [6] demonstrated the efficiency of the MLP for EPS batch process. However, there are not many real applications based on ANN methods in industrial use.

In this paper we demonstrate the optimization and modeling application for the EPS-batch process. The application consists of a production optimization tool and a simulation tool for the process parameters based on the Multi-Layer Perceptron network. The optimization and the modeling features are programmed into standalone software built up in the Matlab environment. The software is tailored for the needs of the EPS production company StyroChem Ltd.

2 Methods

2.1 The EPS batch process

The studied process was a typical suspension polymerisation batch process, which is commonly used for producing EPS (Expandable PolyStyrene). The reactor has a powerful mixer and the cooling system in the inner wall. The main raw materials are styrene, water, pentane, stabilisation agents and additives. The general structure of the EPS reactor is illustrated in Figure 1.

The duration of each batch takes about 12 hours. At first, the main chemicals are added into the reactor and the process is heated up to the polymerisation temperature. The polymerisation stage is executed in a pressure-temperature range below the boiling point of the styrene-water suspension system. After the polymerisation stage the process continues into the impregnation stage, where the blowing agent (pentane) is impregnated into the beads. The impregnation stage assumed to be negligible in the means of bead size distribution. The final stages are cooling and sieving. The end product is a load of solid EPS beads.

CHEMICALS:
styrene
water
pentane
stabilisation agents
additives

STAGES IN THE REACTOR:
1. Polymerisation
2. Impregnation
3. Cooling

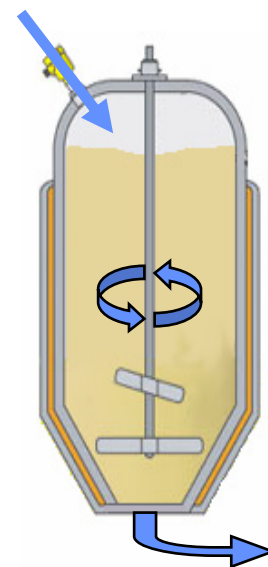


Figure 1. The polymerisation batch process.

It is common knowledge that the basic variables in the term of the bead size are the mixing properties and the amount and quality of the suspension stabilizers. However, suspension polymerisation of styrene is a very sensitive process and numerous variables affect it. Some of these variables cannot be measured or followed by in a reasonable way. For example, analyzing all impurities from all raw materials is too heavy a task for any industrial laboratory. Some variables are quite easily measurable, but have not been traced due to the assumption that they would not have a significant contribution to the process. To be able to model the process the studied system required elimination of the variables, which were assumed to be inessential.

The shape of the bead size distribution of each batch is almost Gaussian. As shown in Figure 2, the mean bead size can be controlled by a dosage of chemicals and mixing conditions, but the bead size distributions are normally Gaussian.

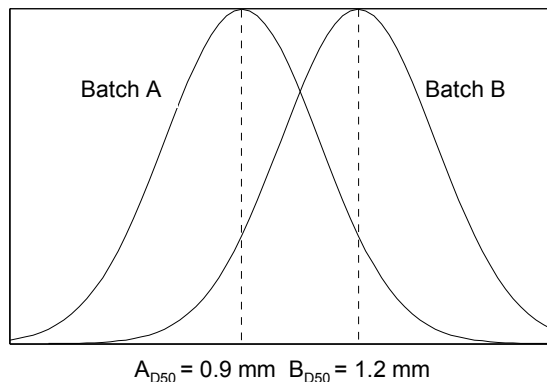


Figure 2. The shapes of the bead size distribution are nearly Gaussian. The mean bead size (A_{D50} and B_{D50}) can be controlled by chemical dosages and mixing conditions.

2.2 The process data

The process data can be divided into three groups: recipes, results and process parameters. The recipes, such as the amount of stabilisation agents, are specified individually for each batch. The most important information, concerning the end product, is the bead size distribution. The bead size distribution is specified in a laboratory by laboratory sieves. The recipes and the measurements made in a laboratory are archived into Microsoft Excel™.

2.3 The Multi-Layer Perceptron

Multi-Layer Perceptron (MLP) is widely used network model. The MLP model is very general and can, in theory, represent almost anything. It

consists of one input layer, hidden layers (typically one or two), and an output layer. The input signals are processed through successive layers of neurons in a forward direction on a layer-by-layer basis. The input layer simply feed directly the corresponding values from the input pattern into the first hidden layer. Each neuron of a hidden layer and an output layer computes a linear combination of the outputs of the neurons of the previous layer. The coefficients of the linear combinations (plus biases) are called the weights. A simplified example of a MLP model is illustrated in Figure 3.

Supervised networks, such as MLP networks, must be trained to a given problem. The most popular training techniques are a backpropagation algorithm. It compares the output values with the correct answer to compute the value of some predefined error-function. The training, an iterative process, determines a set of weights, which minimizes the error between the actual and expected outputs for all input patterns.

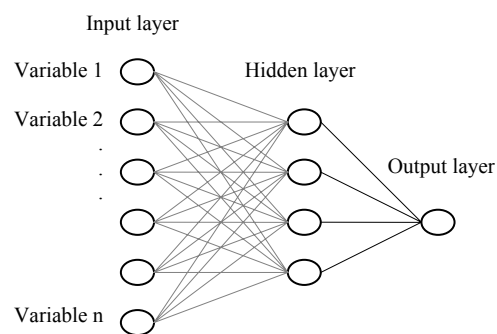


Figure 3. A simplified example of a MLP model with an input layer, one hidden layer and an output layer. The input variables 1...n are applied to the input layer, which has a number of nodes equal to the number of data variables.

3 The application

The application is coded in Matlab software platform (Mathworks, Natick, MA, USA), and compiled for the stand-alone software by the Matlab compiler. The purposes of the application are optimization of the production, and simulation of the process parameters. In addition, the software has versatile visualization properties for viewing data. The main structure of the software is illustrated in Figure 6.

The software consists of 3 graphical interfaces: the production optimization interface, the training interface for the MLP model, and the simulation interface. These interfaces are shown in Figures 4, 5 and 7.

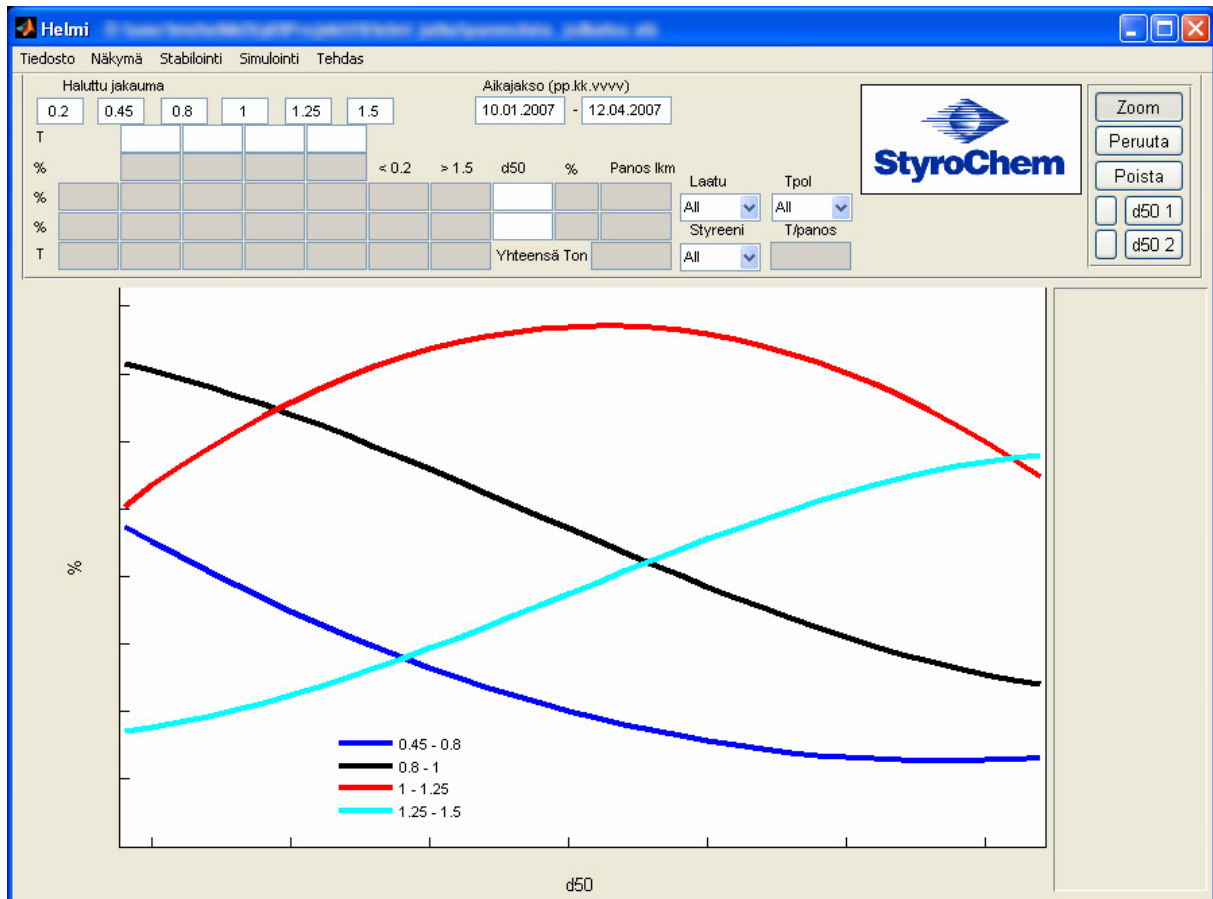


Figure 4. The graphical interface of the production optimizing tool. The mean square errors (curves) are fitted into the historical data (small dots). The dashed lines show two optimal distributions of the bead size to satisfy the production tons (T) based on information of the markets.

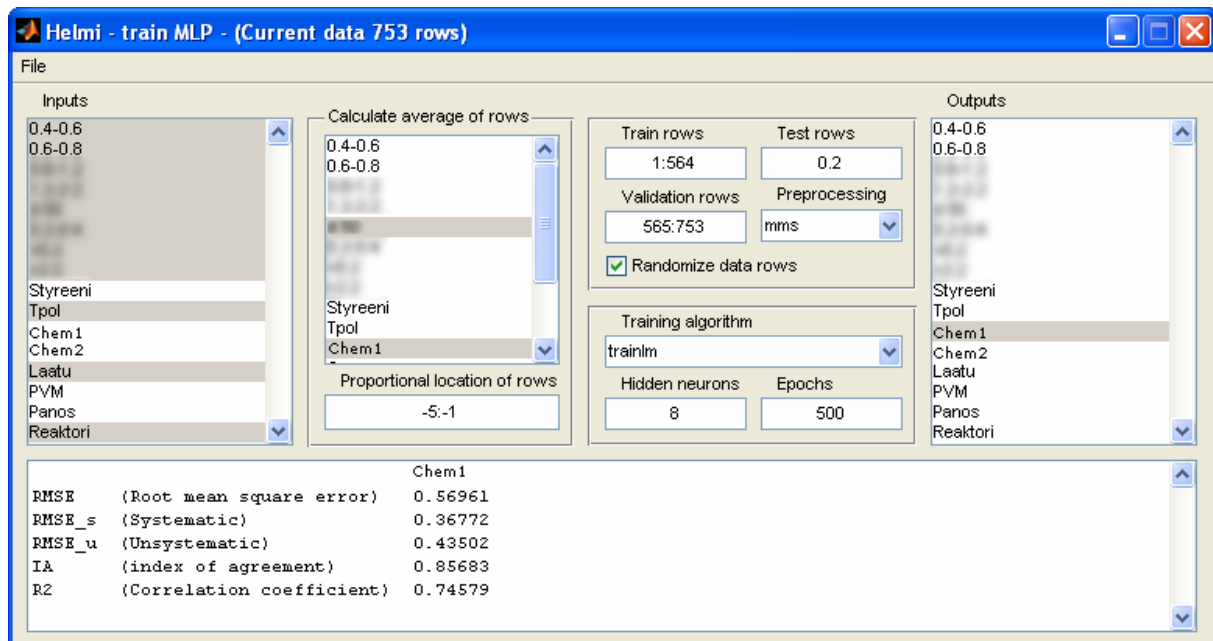


Figure 5. The graphical interface for training of the MLP-model. The inputs and outputs variables can be selected from the menu bars. In addition, the user can set some of the basic training parameters such as the training algorithm and the number of hidden neurons.

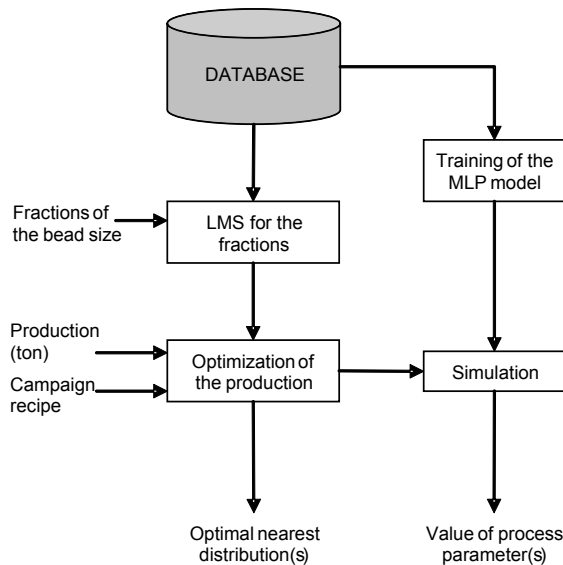


Figure 6. The main structure of the application

3.1 Optimization of the production

The main idea of the optimization is to define the optimal feasible production for the marketing demands. The marketing demands are compared to the historical data of bead size distributions of the batches. Before the comparing, the data are fitted in a function of a mean bead size (D_{50}) by Least Mean Square (LMS) method.

The distribution of the bead size in the production campaign is a sum of Gaussian distributions. The aim of the optimization of production is to predefine the optimal mean bead size for one or two Gaussian distribution, which satisfy the marketing demands and minimize the amount of production. The marketing demands are predefined in tons or in percentage for different fractions. The optimization chain can be described as follow:

1. Set the fractions (the products to sell) of the bead size
2. Set amount of production (in tons or in percentage) of the fractions to be produced
3. Set the campaign recipe (type of EPS)
4. LMS for the fractions
5. Define the optimal feasible production by use of one or two distributions

The distribution of bead size is divided for fractions to be sold. This prospective information is utilized for planning the production and marketing of EPS. In addition, the fraction parameters defined in the optimization window can be used in the modeling phase for simulate the process parameters. The simulation supports the optimization purpose.

3.2 Training the MLP model

The data rows for the training phase are selected in an optimization interface (shown in Figure 4). For example, it is useful to cut the outliers, because they could disturb the accuracy of the model. In a training interface (shown in Figure 5), the user can set the inputs and outputs variables for the model from the menu bar. In addition, there is a possibility to add new input variables by calculating averages of the previous rows of variables. Some basic parameters for the training of the MLP model such as a number of the hidden neurons, a training algorithm, the training rows, and the validation rows can be set in the interface. A complete setup of the parameters, concerning the MLP model, is assembled in a separate text file.

Validation of the MLP model can be done by scatter plots, the root mean square errors, the index of agreement, and the correlation coefficient. Finally, the model is saved for the simulation purpose.

3.3 Simulation

In the simulation interface (shown in Figure 7) the user can simulate the MLP model. The output, such as the dosage of the chemical X, will appear until all the inputs are set. The inputs are filled in automatically, if values of the inputs are defined in the process optimization interface. Thus, the calculations made in the optimization interface can be used for inputs in the MLP modeling phase.

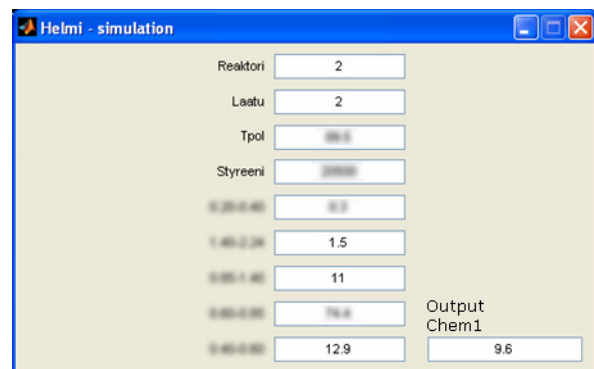


Figure 7. An example MLP simulation in the simulation interface. The inputs are in the middle of the simulation interface and the output is on the lower right corner of the window.

4 Discussion

Data-based modeling methods, such as neural networks, have shown the efficiency in many fields. However, in process industries, getting these intelligent mathematical methods for the industrial daily-use has been challenging. Data preprocessing,

which is an essential stage in the modeling, must be done manually in general. In addition, the use of neural networks methods, such as the MLP model, can be difficult in practical use, because the complexity of parameters and modeling functions.

The main purpose of the study was to integrate process management with process control into functional software. The results of the study show that the application is an efficient tool for optimization of a batch process and modeling process parameters. A prerequisite for the efficient use of the application are user-friendly graphical interfaces with versatile visualization properties. The software can be used at the operational level as well as at the process management level. In addition, the software is generic because the data is updated automatically from the databases, and the MLP model can be retrained quickly.

EPS production of a batch process based on predefined recipes achieves the required bead size distribution, which is nearly Gaussian. The production can follow the requirements of the market easily by using more than one recipe at the same time. The application can calculate the optimal production by combining the distributions. These calculations can be used as inputs in the MLP-modeling phase where process parameters such as chemical dosages are estimated. The marketing can set amount of the production (tons) for each fraction, and the software defines the optimal process parameters. Thus, production will economize on process and storage costs. That was proved in a test use of the software in company StyroChem.

Archived process data is an outstanding resource for the knowledge management of the process, but in practice measurement errors and other mistakes in the data can disturb the analyses. Consequently, the result of the MLP model depends on the accuracy of the data. Besides, in the training phase of the MLP model, there are some parameters to be set, which are very critical for the performance of the model. Therefore, basic knowledge of the modeling principles is needed in the training phase of the MLP model. This is an important issue for future research.

5 Conclusion

The present application integrates production optimization and process modeling. The results indicate the MLP analysis with functional data preprocessing tool provides an efficient method for data analysis in the process industry. Therefore, this kind of intelligent data-driven approach is a fruitful way of developing tools for the batch process optimization.

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