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Hybrid Neural Network and Particle Swarm Optimization Model Applied to Assist Production Planning in a Large Petrochemical Plant

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ABSTRACT: Process and production planning play an important role in petrochemical production systems. Planning models are essential to optimize the combination of multiple non-linear production processes involved and therefore improve the commercial competitiveness of the such plant. Artificial neural networks offer an effective petrochemical plant planning tool, especially when configured in hybrid form as a back propagation artificial neural network coupled with an optimizer to assist with feature selection. A plant with eight feedstock inputs and thirteen petrochemical products is evaluated, firstly to show the capabilities of a basic backpropagation network model in predicting product outputs. The involvement of a particle swarm optimizer assists in filtering the dataset to remove outlying data records and identifying the input variables that are influential in determining specific product output volumes. The hybrid back propagation network-particle swarm optimization model assists by determining the logical relationship between input and output variables and expressing them in the form of an index matrix. The matrix leads to improved predictions of production outputs and faster convergence of the planning model. The modified back propagation network achieved maximum, minimum, and average relative errors of 59.1%, 0.0%, and 9.9%, respectively. Prediction errors in that range are considered acceptable for the collective production processes of a large-scale petrochemical complex evaluated with a nonlinear planning program.

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1- Introduction

Petrochemical production processes rely on raw materials including crude oil, natural gas, and natural gas liquids to produce primary petrochemicals including methanol, olefins (ethylene, propylene, etc.), aromatics (benzene, toluene, xylene, etc.) [1]. These primary petrochemicals are themselves feedstocks for processes forming a wide range of other products. In particular, they are:

Converted into petrochemical intermediates and derivatives such as acetic acid, vinyl chloride, sulfuric acid, solvents, ethylene oxide, and many more.

Polymerized into a number of more complex and larger molecules, such as styrene into different polystyrene products, ethylene into polystyrene, and propylene into polypropylene.

Classifying and describing petrochemical products is difficult because there are so many of them and they are used to make many thousands of end products. The most common end products tend to include polymers and copolymers and various forms of plastic. However, elastomers and fibers are also in high demand. Petrochemicals are also major constituents of coatings and paints, packaging (particularly in the food and drinks industries), pharmaceuticals, solvents, detergents, dyes, pigments, synthetic rubber, and cosmetics [2]. Consequently, petrochemical industries are commercially important to many nations and they are widely traded internationally [3]. Petrochemical plants are typically associated with substantial intervention, turnaround, operating, and maintenance costs. Consequently, it is important to manage such plants with an efficient and practically achievable plan; failing to do so invariably leads to unnecessary production losses and sub-optimal commercial returns [4]. An effective production strategy facilitates more efficient use of available resources which, in turn, improves a plant's competitive market position. Understanding the strategic, tactical, and operational issues involved in linking markets, products, and resources is essential for any petrochemical plant to compete in today's global marketplace. [5]. Petrochemical industries were estimated to be worth more than $600 billion worldwide in 2015 and continue to grow [6]. Therefore, establishing an optimal production plan makes financial sense for plants to compete effectively in global petrochemical markets.

Artificial Neural Networks (ANNs) are mathematical systems structured to work as simplified animal brains. An ANN is composed of an interconnection of computational elements (referred to as neurons or nodes assembled in layers to simulate the way that neurons operate in biological brains. The development of ANN is based on essential

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computational elements. A key breakthrough in developing the perceptron was achieved by Frank Rosenblatt (1957). ANN is trained through experience using appropriate learning examples gaining their knowledge by detecting patterns and relationships in the data variables they process [7].

Efficient petrochemical production and product planning require both learning from experience and continuous optimization. Various optimization strategies have been applied in attempts to achieve more efficient petrochemical plants. These include efficient production planning, exploiting the benefits of economies of scale (e.g., through mergers and acquisitions), integration of petrochemical plants with refineries to diversify products, dynamic capacity adjustments, spatial reorganization of production train layouts, and optimal supply chain management. A number of goals, such as minimizing total costs, resource requirements, downtime, and environmental impacts, and maximizing profitability remain ongoing challenges for the petrochemical industry [6].

Generally, there are three ways to approach and improve process planning [8]: Manual: This type of planning is known as man-variant process planning and is the commonest type of planning used for production today:

Manual Process Planning: This type of planning is known as man-variant process planning and is the commonest type of planning used for production today. Planning the operations to be used to produce a part requires knowledge of two groups of variables:

The part requirements (as indicated by an engineering drawing).

The available machines and processes, and the capabilities of each process.

Automated Process Planning: Man-variant process planning (at times) becomes a boring and tedious job. It produces erroneous process plans. This, coupled with the labor intensity of man-variant planning, has led many industries to investigate the automation of process planning. A completely automated process planning system would eliminate all human effort between the preparation of an engineering drawing and a complete process plan for every manufacturing operation.

Generative Process Planning: Generative process planning may be defined as a system that synthesizes process information in order to create a process plan for a new component automatically. Process plans are created from information available in a manufacturing database with little or no human intervention.

Process planning automation typically involves developing software to apply effective algorithms that collectively can be configured to act as automated expert systems for certain applications [9]. However, expert systems have their limitations with respect to plant design and control options [10]. Attempts have been made to integrate intelligent process planning within the structural configurations of relational databases [11]. Learning and optimization can be achieved by combining the benefits of ANN and Particle Swarm Optimization (PSO) algorithms enabling them to effectively model systems that are both complex and nonlinear [12]. A Multi-Layer Perceptron (MLP) employing a Back Propagation (BP) learning algorithm is widely used for petrochemical applications [13]. This configuration is referred to in this study as a Back-Propagating Network (BPN). Weights and biases within a BPN network are progressively adjusted as the BP algorithm iteratively attempts to minimize a specified cost or error function. The Mean Squared Error (MSE) between the MLP predictions from its output layer versus observed output variable values are often used as the BPN error function to be minimized. The BP algorithm employs a gradient-descent method. Although BP is effective in some cases, often its convergence rate during training can be slow and it is prone to become trapped at local minima. Moreover, BP convergence tends to be dependent on the selection of the initial weight and bias values applied to the BPN connections. It is also influenced by the learning rates and error thresholds adopted.

These limitations tend to render BPNs inconsistent and unpredictable, for certain applications at least. Therefore, to improve BPN predictive performance, an alternative effective method to optimize BPN has been proposed [14]. The PSO algorithm can be effectively exploited to do this. Table 1 lists published engineering applications of BPN, PSO, and hybrid BPN-PSO concentrating on those focused on process planning.

This paper applies a BPN-PSO algorithm in a novel way to optimize and forecast production planning in a complex petrochemical plant. Industrially acquired, real data (eight input variables) are used to train and test the BPN performance in three distinct configurations. The multi-layered BPN predicted outputs are compared for accuracy with the actual measured data. The study indicates the hybridized BPN-PSO model can simulate the effect of a wide range of operating conditions on the production mass flow behavior of the petrochemical plant to a high degree of accuracy. This makes it an effective analytical tool for improving efficiency and productivity and reducing plant operational costs. The main innovation of this study, applying a BPN-PSO hybrid algorithm that combines PSO with a BPN to optimization of the performance of a multilayer neural network by adjusting the weightings applied to its nodes for organizing an effective petrochemical plant planning tool.

2- Method and Materials

The feedstock, processes, and products of a complex petrochemical plant are specified evaluated, and optimized for this study. The feedstock includes liquid gases and heavy naphtha, which is supplied mainly from a nearby oil refinery. In addition, various cuts of petrochemicals are also used as feedstock for the production of certain products. There are five main product production trains: olefin, benzene, polyethylene, polystyrene, and Acrylonitrile Butadiene Styrene (ABS). The plant is supported by several utility units supplying: water, steam, cooling (via a cooling tower), compressed air, and nitrogen.

In the olefin unit, different feed chemicals are introduced, and, following cracking, a range of primary petrochemical

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Table 1. Published research relating to the application of the ANN and PSO relevant to production and process planning.

No.	Topics	Description	Ref.
1	Simulation Process planning PSO	Applying PSO to optimize process planning	[15]
2	Process planning Expert system ANN	Rule-based expert system integrating an ANN	[16]
3	Constraints Production planning Petrochemicals	Constraint-based programming to optimize production planning and to maximize profitability	[17]
4	Multi-objective decisions Pareto optimization Petrochemical planning	Multi-objective mixed-integer optimization model	[18]
5	Hybrid ANN algorithms	Review of hybrid ANN structure and applications	[19]
6	Multi-objective linear program Petrochemical planning	Strategic model applied to a national company	[2]
7	Process planning Scheduling	Integrates process planning with scheduling	[20]
8	Integrating refinery with petrochemical processes Process planning	Planning of multi-site integrated refining and petrochemical processes exploiting stochastic algorithms.	[21]
9	Process planning	Multi-product process planning	[22]
10	BPN-PSO Multiple process streams	BP-PSO applied to multiple daily process streams	[23]
11	Teaching-learning-based-optimizer (TLBO) Petrochemical process planning	MLP optimized with an elitist TLBO algorithm	[24]
12	Multiple-level planning Petrochemical processes	Application and Limitations of the multi-level planning system for petrochemical industries in Saudi Arabia	[6]
13	Strategic planning model Integrated petroleum/petrochemical supply chains	Multi-objective, multi-period strategic optimization applied to supply chains	[25]
14	PSO application Integrated process planning and scheduling	Integrated Process Planning And Scheduling (IPPS) model optimized by PSO	[26]

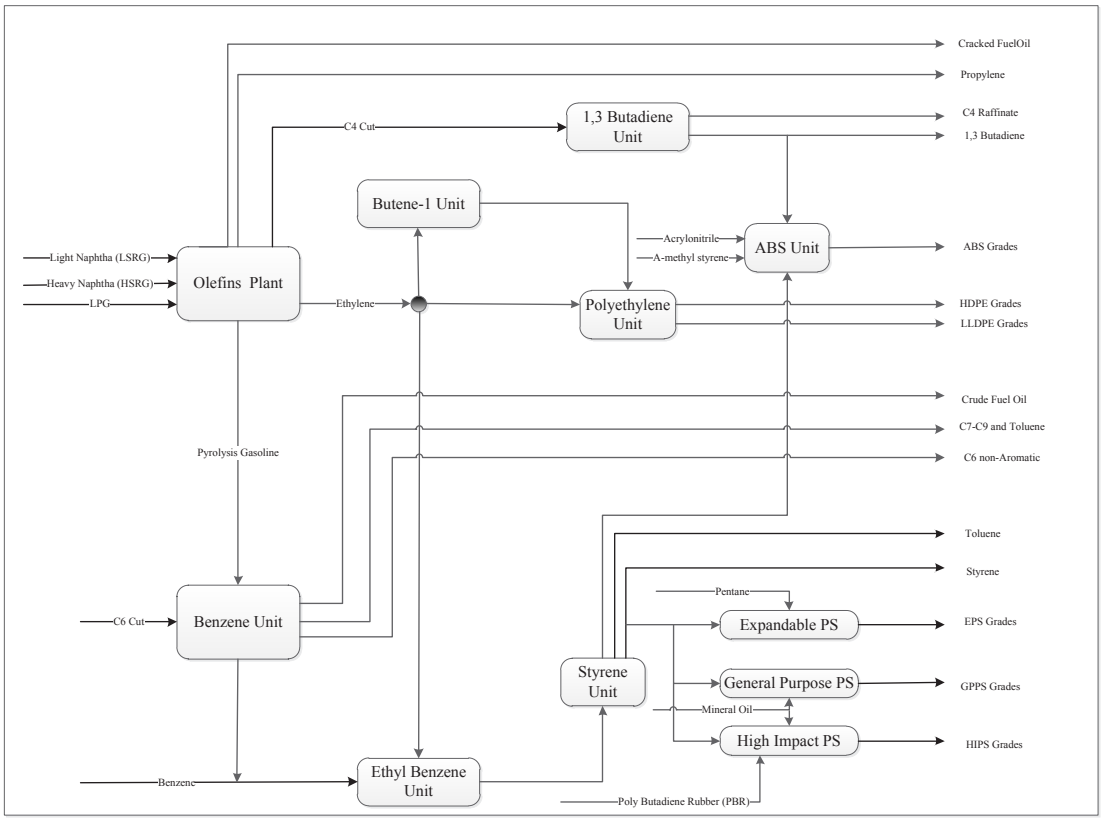
products including ethylene and propylene are separated. These products are either fed into other processing units to produce secondary petrochemical products or are sold directly as bulk primary chemicals. Tests are carried out on the olefin products to measure their binary bonds, conjugate bonds, and water contents to improve product specifications. The polyethylene unit produces two types of polyethylene: light and heavy. Laboratory tests are conducted to determine ethylene purity, the percentage of polymerization, and the quality of the products in terms of resistance, softening temperature, density, and granulation.

In the benzene unit, following catalytic reforming, benzene is purified and also used in the preparation of styrene and polystyrene in specialized process units. Three types of polystyrene are typically produced, a) general purpose b) resistant, and c) expandable. In addition, various grades of ABS are produced is a specialized ABS unit. The quality of these products, including a stretching test, is determined in the laboratory and the processes are adjusted to ensure that product specification requirements are satisfied and maintained.

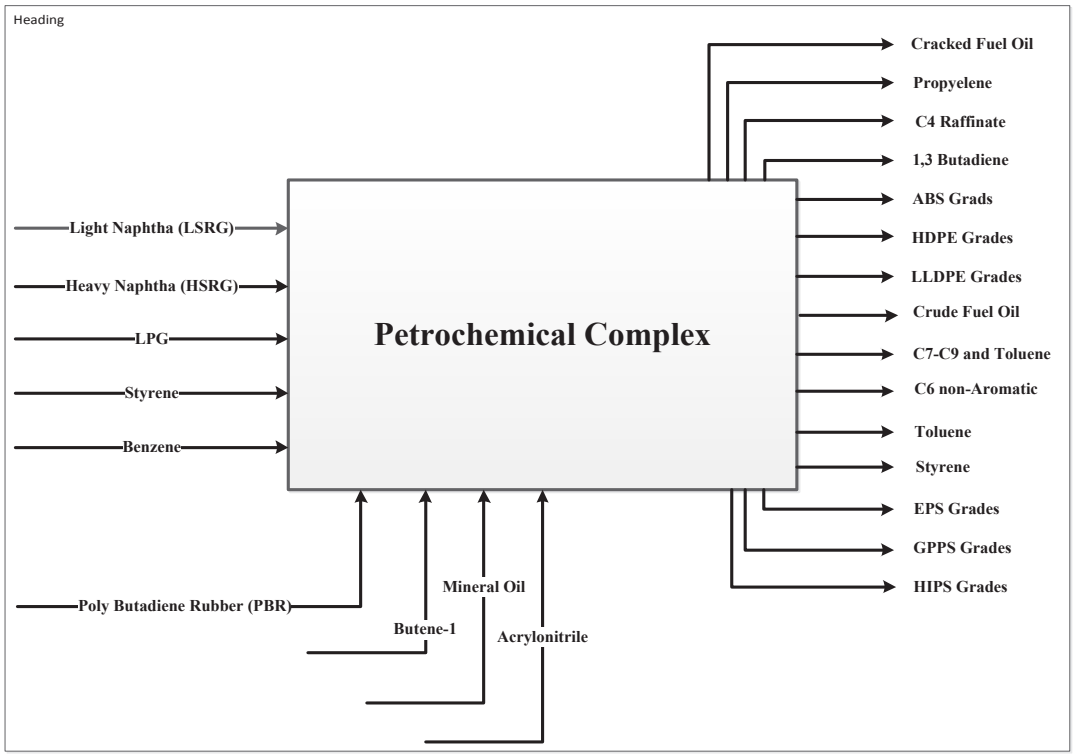
Purified water is produced in a dedicated water unit from soft fresh water. That unit applies reverse osmosis and ion exchange resins to generate ion-free water. That ion-free water is then used to produce steam and to provide water for cooling systems. A Combined Heat and Power (CHP) plant is employed to cogenerate electricity and produce steam at various pressure-temperature conditions. Fig. 1(a) displays a schematic flow diagram of the integration of the mentioned

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(a)



(b)

Fig. 1. (a) Block Flow Diagram; (b) black box model of the studied petrochemical complex

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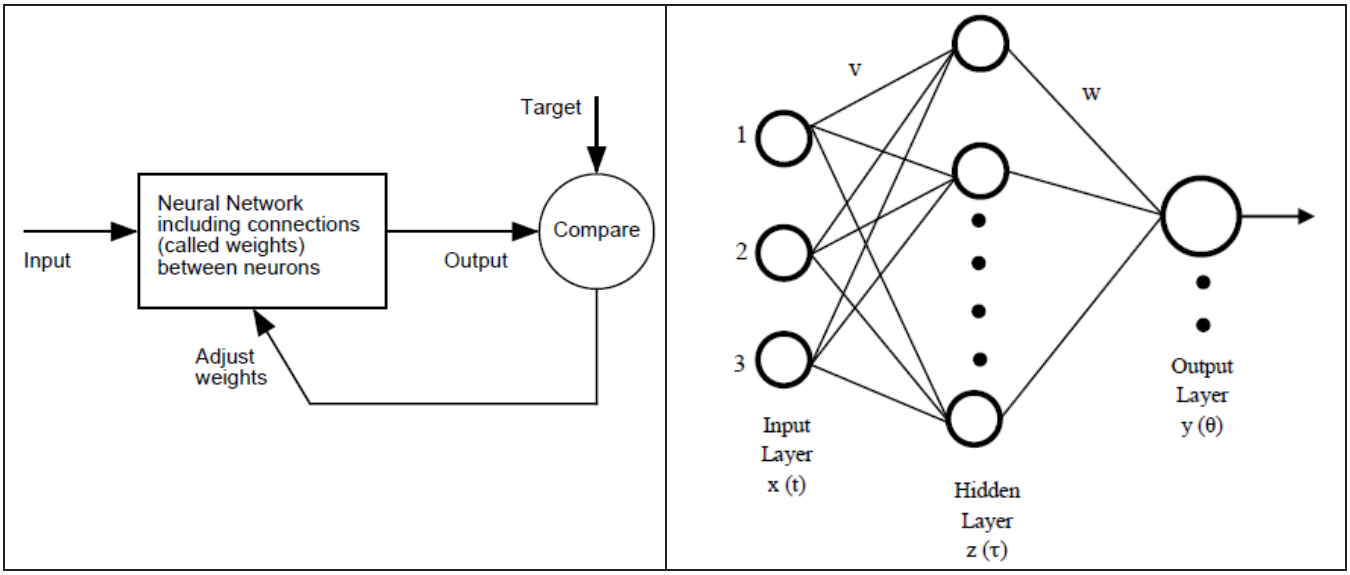


Fig. 2. Schematic representation of the architecture of a generic ANN model.

processes in the petrochemical plant evaluated.

3- Applied Hybrid Algorithm

3- 1- ANN algorithm

ANNs attempt to mimic the neural interconnection of animal brain structures in a simplified format. The Neural Network (NN) finds patterns or correlations in the large complex dataset (i.e., multiple variables including non-parametric distributions and limited correlations). NN can be configured to provide useful future predictions of dependent variables [27]. NN can be trained to solve problems that are difficult for simple regression and correlation statistical techniques to resolve accurately. Consequently, NN is widely used in engineering, finances, and many other practical applications (Demuth, 2021). ANNs, in particular MLPs, are widely used in the petrochemical and refining industries to model production flows and optimize production throughputs [28]. Complex Petrochemical plant production data is typically characterized by multiple dimensions, a degree of operational uncertainty, and noise. Consequently, it is difficult to accurately optimize and predict the energy usage of such plants. Therefore, a Data Envelopment Analysis (DEA) technique that integrates ANN (DEA-ANN) has been proposed [29].

Commonly, NN is trained so that a particular set of input variable values accurately predict a specific target output (Fig. 2). The NN control parameters are progressively adjusted, based on a comparison of the predicted output and the known measured value of the target. This is repeated until the NN predicts the output matches the target as closely as possible. Many such input/target variable pairs are evaluated to train an NN (Demuth, 2021).

In this study, a back-propagating MLP neural network (BPN) model using MATLAB software (Demuth & Beale, 2021) is employed as the basic ML engine. Although BPN is an effective ML algorithm, its training, usually with back-propagating or other gradient descent algorithms, tends to involve very slow convergence and becomes easily trapped at local minima.

3- 2- PSO algorithm

PSO is a highly effective evolutionary algorithm applying swarm intelligence that is effectively used to optimize processes in many industries, including production process planning and scheduling (Table 1). It applies velocity vector information alongside the best local and global particle quality information to update the current values of each particle in the swarm for each iteration of the algorithm. It uses this information to calculate an optimization function for each particle in the swarm. Moreover, the velocity vector associated with each particle is updated in each iteration based on the historical performance of each particle's position /values. This history stores the knowledge gained by each particle in the swarm that can be used for learning purposes as the PSO iterations evolve. Consequently, poor-performing particle positions can be eliminated/avoided by exploiting the swarm's social variable memories to adjust particle positions to move towards previous promising locations within the feasible solution space. This avoids the inefficiency of the algorithm repeatedly researching unpromising positions. The PSO method can be used and applied to solve a wide range of optimization problems. These include:

Unconstrained optimization problems

Constrained optimization problems

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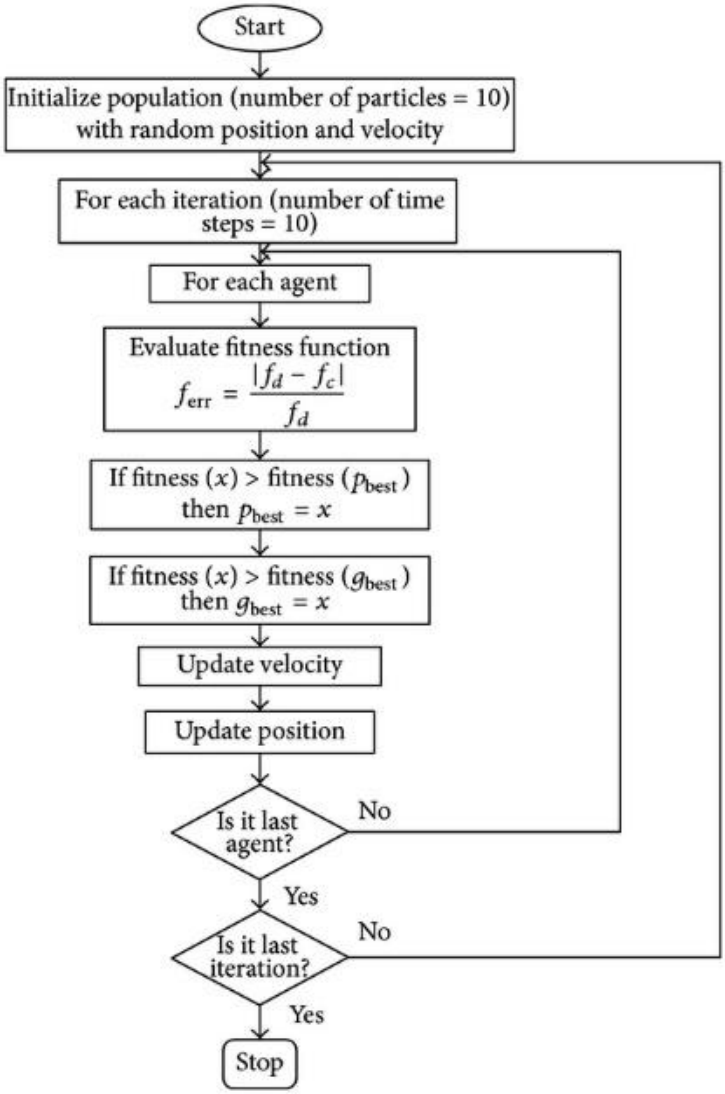


Fig. 3. Flowchart of PSO algorithm, where: pbest refers to the local best position for each particle, and gbest refers to the global best position for the particle swarm as a whole.

Nonlinear programming (such as polymerization processes)

Multi-objective optimization (predicting the best combinations of multiple products)

Stochastic programming (utilizing probabilistic information for certain input variables)

Hybrid optimization problems (improving the optimization of ML algorithms)

3- 3- Hybrid BPN-PSO algorithm

BPN-PSO is a hybrid ML-optimization algorithm that combines PSO with a BPN to optimize the performance of a multilayer neural network by adjusting the weightings applied to its nodes/neurons and layer biases. Whereas the PSO algorithm is highly effective at finding global solutions without becoming trapped at local optima, the BP algorithm has a tendency to find local optima rather than determine the global optimum in an optimization problem. By constructing a hybrid BPN-PSO algorithm, the PSO component is used to locate the global optimum more rapidly and thereby accelerate the training speed. When the optimizer fitness value does not change after a specified number of iterations, or the fitness function arrives at a value that is smaller than a predefined number, the solution space search algorithm can be changed to use a slower gradient descent method to explore solutions around the PSO global solution [14].

This study demonstrates how BPN-PSO can be effectively used to optimize production planning for a multi-product / process petrochemical plant.

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Table 2. List of eight influencing parameters in the planning of a problem case study

Row No.	Input Number	Input variable full name	Input variable abbreviation name	Variable unit
1	Input (1)	Mass flow rate of source reagent gas (SRG: including both heavy and light naphtha compositions)	MFSRG	ton/d
2	Input (2)	Mass flow rate of Liquid Petroleum Gas (LPG)	MFLPG	ton/d
3	Input (3)	Mass flow rate of Styrene (S)	MFS	ton/d
4	Input (4)	Mass flow rate of Benzene (B)	MFB	ton/d
5	Input (5)	Mass flow rate of Polybutadiene Rubber (PBR)	MFPBR	ton/d
6	Input (6)	Mass flow rate of butene-1	MFB1	ton/d
7	Input (7)	Mass flow rate of Mineral Oil (MO)	MFMO	ton/d
8	Input (8)	Mass flow rate of Acrylonitrile (ACN)	MFACN	ton/d

Table 3. Example of ten days of feedstock input data (8 input variable mass flow rates) for the petrochemical plant.

Daily Data Records	Input							
	SRG	LPG	PBR	BEN	STYRENE	ACNE	MO	BUTENE-1
1	975.38	241.039	10.5	130.4	187.3	0	7.73	34.48
2	1029.04	247.089	10.5	135.9	149	24	7.65	35.64
3	1041.4	241.941	15.4	134.3	72.8	0	7.72	33.75
4	1036.06	245.858	12.6	130.8	184.1	27	12.6	34.5
5	1032.85	256.595	10.5	131.1	167.7	8	7.63	35.77
6	1035.05	245.759	10.5	132.3	134.3	12	7.64	35.87
7	1030.16	267.202	14.7	126.4	180.7	3.2	7.68	34.4
8	1021.64	265.542	15.75	120.1	222.3	43	7.68	35.28
9	1005.73	288.238	10.5	116	125.7	26	7.65	35.46
10	1008.12	291.085	11.62	109.8	140.1	14	7.74	35.4

4- Problem Formulation

The model evaluated in this study is designed to reflect the inputs and outputs of a real and operational complex petrochemical plant (Fig.1 (b)). It involves the following eight influencing parameters shown in Table 2 (decision or input variables):

All values of the eight input variables values are compiled from the studied petrochemical plant control system (DCS) for each day across a single year, establishing a dataset with 366 data records. Table 3 lists example data record input values for ten days of operations observed at the plant.

The model is evaluated in four steps:

Step 1- Data analysis and pre-processing

Step 2- Evaluating all data records with a basic ANN (BPN) tool

Step 3- Data record classification into two categories using the PSO algorithm: those input combinations that are effective and those that are ineffective in optimizing the petrochemical plant's product slate.

Step 4- Evaluating the data with a modified BPN tool

Model inputs (left side) and outputs (right side) are distinguished.

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Table 4. List of thirteen output products in the planning of problem case study

Row No.	Output Number	Output variable full name	Output variable abbreviation name	Variable unit
1	Output (1)	Mass flow rate of POLYETHYLENE	MFPE	ton/d
2	Output (2)	Mass flow rate of HIPS	MFHIPS	ton/d
3	Output (3)	Mass flow rate of GPPS	MGPPS	ton/d
4	Output (4)	Mass flow rate of EPS	MEPS	ton/d
5	Output (5)	Mass flow rate of ABS	MABS	ton/d
6	Output (6)	Mass flow rate of TOLUENE	MFTOL	ton/d
7	Output (7)	Mass flow rate of BD	MFBD	ton/d
8	Output (8)	Mass flow rate of PENTANE	MFPEN	ton/d
9	Output (9)	Mass flow rate of PROPYLENE	MFPROPYLENE	ton/d
10	Output (10)	Mass flow rate of C4 Raffinate	MFC4R	ton/d
11	Output (11)	Mass flow rate of CFO	MFCFO	ton/d
12	Output (12)	Mass flow rate of Fuel Oil	MFFO	ton/d
13	Output (13)	Mass flow rate of C7-C9	MFC7C9	ton/d

Each data record incorporates daily production quantities for thirteen output products. These variables are presented in Table 4:

Fig. 1 (b) identifies the 8 inputs and 13 outputs used to model the petrochemical plant. The process can be expressed by a simple material balance formulation (Eq. (1))

$$\sum_{i=1}^{8}(input)_i = \sum_{j=1}^{13}(output)_j \quad (1)$$

5- Results and Discussion

5- 1- Data analysis

The data analysis step examines the quality of the data and how each input variable is statistically distributed. This analysis utilizes Excel's statistical functions and the results are presented in Table 5. None of the input variables follow a symmetrical normal distribution and they display substantially different degrees of dispersion.

Table 6 lists Pearson's correlation coefficients (R) between the independent variables (the inputs) and the dependent variables (the outputs). If R is 1.0, it indicates a direct or perfect positive relationship between two variables. Whereas if R is -1, it indicates an inverse or perfect negative relationship between the two variables. On the other hand, when R is zero, there is no linear relationship between the two variables. It is apparent from the results displayed in Table 6 that R values between the variables show a main range of poor to moderate positive and negative correlations among the input and output variables.

Propylene, CFO, fuel oil and C7-C9 products show relatively high positive R values with the SGR input variable. Also, ABS shows a moderate negative R value and Toluene and a moderate positive R value with Benzene. However, the correlations between all other output products and input feeds are low as reflected in the mean of the R values for each input variable with all the output variables (Table 6). This confirms the necessity of using nonlinear models, such as BPN, to analyze the petrochemical plant processes and define the complex relationships between input and output variables. Table 6 displays the maximum residual coefficient calculated between each dependent and independent variable. The high maximum residual coefficients for input variables SRG and LPG highlight the unreliability of exploiting mathematical relationships between the input and output variables collectively to predict this petrochemical plant's production performance based on variations in the input feed values.

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Table 5. Data distribution analysis for each input variable (ton/d) was actually compiled from the plant DCS.

Index Topic (Input parameters)	SRG (ton/d)	LPG (ton/d)	PBR (ton/d)	BEN (ton/d)	Styrene (ton/d)	ACN (ton/d)	MO (ton/d)	Butene-1 (ton/d)
Standard Deviation (S)	144.87	44.77	8.28	47.74	114.13	10.87	4.04	11.55
Variance	23266.15	2121.75	68.44	2279.68	12988.05	117.73	16.37	133.17
Variation range	1076.12	306.56	47.25	225.10	521.70	43.00	48.40	40.00
Coefficient of Variation (CV)*	0.15	0.19	0.52	0.49	0.73	1.16	0.46	0.60
Skewness	-4.76	-2.60	0.98	-0.61	0.62	0.77	3.40	0.28
Kurtosis	26.60	11.06	1.22	-0.08	-0.06	-0.38	29.95	-1.25
Min.	35.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Max.	1111.45	306.56	47.25	225.10	521.70	43.00	48.40	40.00
Mean ($\bar{x}$)	987.10	238.26	15.80	98.18	156.16	9.37	8.69	19.17
Median	1010.68	244.20	13.00	108.00	144.20	0.00	7.85	14.38

* $CV = S/\bar{x}$

5- 2- BPN model

The basic BPN architecture includes an input layer with eight nodes, a hidden layer with 10 nodes, and an output layer with 13 nodes, with each node in the output layer representing a specific product output (Fig. 4). A sigmoid transfer function is applied between the input and hidden layer, and a linear transfer function is applied between the hidden layer and output layer of the BPN. The BPN is trained with the Levenberg-Marquart algorithm. The transfer functions and the training algorithm were selected based on trial and error tests of the BPN. All input variables were normalized to a scale range of 0 to 1.

The data records were split into three subsets: training, validation, and testing subsets. Based on trial and error testing, the 366 total data records were split between the subsets: 256 data records (70% of the total) to the training subset; 55 data records (15% of the total) to the validation subset; and, 55 data records (15% of total) to the testing subset.

Fig. 5 shows the measured versus predicted output values for the basic BPN model applied to the training, validation, and testing subsets and all the data records compiled for the studied petrochemical plant. The predicted output values track the measured output values quite well for each subset and the total dataset, as revealed by the R values between about 0.96 and 0.98 recorded for each subset evaluated. The predicted values from the BPN model are compared with the recorded (actual DCS) values for the thirteen output variables and the errors between those measurements are recorded. The target of the model is to minimize collectively the sum of the errors associated with all 13 output variables for each data record. The predicted versus target values are plotted in Fig. 5. As shown in Table 7 and Fig. 4, the BPN model has 8 input variables and 13 output variables. All variables are expressed in mass flow units of tons per day. The clustering of data in Fig. 6 is a consequence of the output variables extending over different tons per day ranges. For cases where predicted values (Y) are equal to target values (T) (Fig. 5), the data point falls along the $Y = T$ line displayed with zero prediction error (target value- predicted value = 0).

The performance curve of the BPN with 10 neurons in the hidden layer is shown in Fig. 7 in terms of the Mean Squared Error (MSE) of its objective function. MSE is:

$$MSC(\%) = \frac{1}{n}\sum(CS\ data value - Calculated\ value\ by\ BPN)^2 \times 100 \quad (2)$$

Fig. 6 indicates the iteration at which the validation performance reached a minimum. The training continued for 9 more iterations before training stopped. This figure does not indicate any major problems with the training. The validation and test curves are very similar. If the test curve had increased significantly before the validation curve increased, then it would suggest that some overfitting had occurred.

The impact of MSE and R on each subset with different numbers of neurons in the one hidden layer of the BPN is displayed in Table 7. Five different numbers of neurons in the

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Table 6. Results of Pearson Correlation Coefficients

Independent variable	SRG	LPG	PBR	BENZENE	STYRENE	ACRYLONITRILE	MINERAL OIL	BUTEN-1
Dependent variable	Pearson Correlation Coefficients							
POLYETHYLENE	0.54	0.51	0.05	-0.11	-0.14	-0.18	0.09	0.30
HIPS	-0.07	-0.11	0.14	-0.10	0.18	0.07	0.09	-0.10
GPPS	-0.08	0.25	0.01	-0.09	-0.16	-0.19	0.30	0.33
EPS	-0.01	-0.13	0.06	-0.03	0.25	0.24	0.03	0.12
ABS	-0.20	-0.11	-0.04	-0.47	0.59	0.13	0.03	0.16
TOLUENE	0.35	0.05	-0.06	0.57	-0.40	0.20	0.00	-0.02
BD	0.06	-0.01	-0.06	0.09	0.06	-0.01	0.01	0.05
PENTANE	0.08	0.13	-0.08	0.10	-0.27	-0.17	-0.01	0.05
PROPYLENE	0.89	0.77	0.04	0.28	-0.47	-0.16	0.13	0.21
C4 RAFFINATE	-0.07	-0.09	-0.07	-0.19	0.13	-0.10	-0.04	0.10
C.F.O	0.72	0.36	0.16	0.04	-0.01	0.07	0.06	0.05
FUEL OIL	0.58	0.47	0.24	0.23	-0.37	0.02	0.20	0.10
C7-C9	0.61	0.47	0.18	0.21	-0.32	-0.04	0.17	-0.06
***Min.**	0.01	0.01	0.01	0.03	0.01	0.01	0.00	0.02
****Max.**	0.89	0.77	0.24	0.57	0.59	0.24	0.30	0.33
*****Mean**	0.33	0.27	0.09	0.19	0.26	0.12	0.09	0.13
Dependent variable	Regression Residual Coefficients							
POLYETHYLENE	0.1973	0.1054	0.0006	0.0030	0.0506	0.0001	0.0026	0.1012
HIPS	0.0035	0.0100	0.0376	0.0165	0.0521	0.0025	0.0148	0.0154
GPPS	0.0100	0.0586	0.0000	0.0065	0.0296	0.0379	0.0873	0.0972
EPS	0.0002	0.0209	0.0020	0.0010	0.0551	0.0524	0.0005	0.0101
ABS	0.0416	0.0158	0.0024	0.2257	0.3453	0.0213	0.0008	0.0237
TOLUENE	0.1268	0.0034	0.0000	0.3324	0.1563	0.0320	0.0013	0.0025
BD	0.0002	0.0040	0.0029	0.0132	0.0023	0.0013	0.0000	0.0018
PENTANE	0.0138	0.0335	0.0067	0.0107	0.0617	0.0208	0.0002	0.0044
PROPYLENE	0.8054	0.5753	0.0030	0.0735	0.2343	0.0233	0.0154	0.0425
C4 RAFFINATE	0.0061	0.0066	0.0025	0.0312	0.0137	0.0069	0.0030	0.0096
C.F.O	0.5245	0.1337	0.0218	0.0032	0.0019	0.0053	0.0060	0.0046
FUEL OIL	0.3359	0.2275	0.0702	0.0697	0.1335	0.0001	0.0556	0.0092
C7-C9	0.3640	0.2366	0.0495	0.0379	0.0957	0.0066	0.0428	0.0065
***Min.**	0.0002	0.0034	0.0000	0.0010	0.0019	0.0001	0.0000	0.0018
****Max.**	0.8054	0.5753	0.0702	0.3324	0.3453	0.0524	0.0873	0.1012
*****Mean**	0.1869	0.1101	0.0153	0.0634	0.0948	0.0162	0.0177	0.0253

* Min=min(abs(xi))
** Max=max(abs(xi))
*** Mean=mean(abs(xi))

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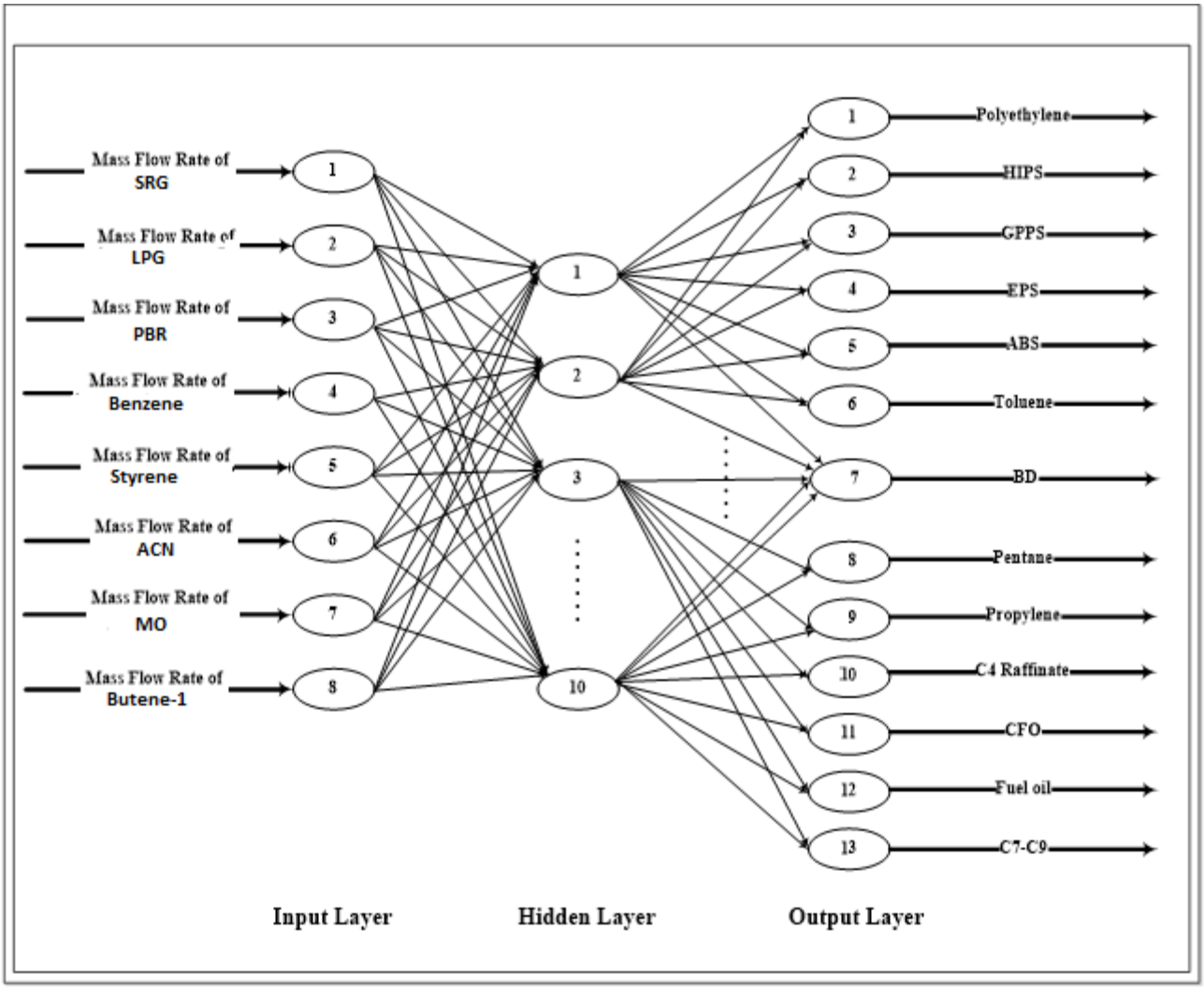


Fig. 4. Basic BPN model architecture.

hidden layer are considered: 5, 10, 15, 20, and 100. Changing the number of neurons does not have a considerable effect on *R* for all data records, which varies from 0.968-0.978. All-*R* refers to the weighted average for the *R* values for the training, validation, and testing subsets. However, the MSE values for the independent testing subset are revealing, as MSE increases for BPN with greater than 10 neurons (i.e., >740 tons/day). This suggests that the BPN models with one hidden layer and greater than 10 neurons have a tendency to overfit this dataset.

The less than perfect prediction accuracy achieved by the BPN model is likely due to several influencing factors. These include:

Unrealistic data distribution values

Measurement errors in some variables in certain data records

Substantial operational changes during daily product production

Inappropriate hidden relationships established within the neural network

Low influence of some input variables on output variable values

Careful consideration of the data distributions led to some outlying data records being discarded from the dataset. The most important reason for rejecting some of the compiled actual data records is that they incorporate some outlying extreme values of the input variables. For the data records selected the distribution statistics are presented in Table 5. Variable values outside of the distribution ranges defined in Table 5 are not considered by the model, as to do so would reduce its efficiency.

5- 3- Hybrid BPN and PSO model

The maximum correlation coefficient achieved between predicted and actual output values by the basic BPN model is 0.978 (Table 7). Various factors contribute to this less than

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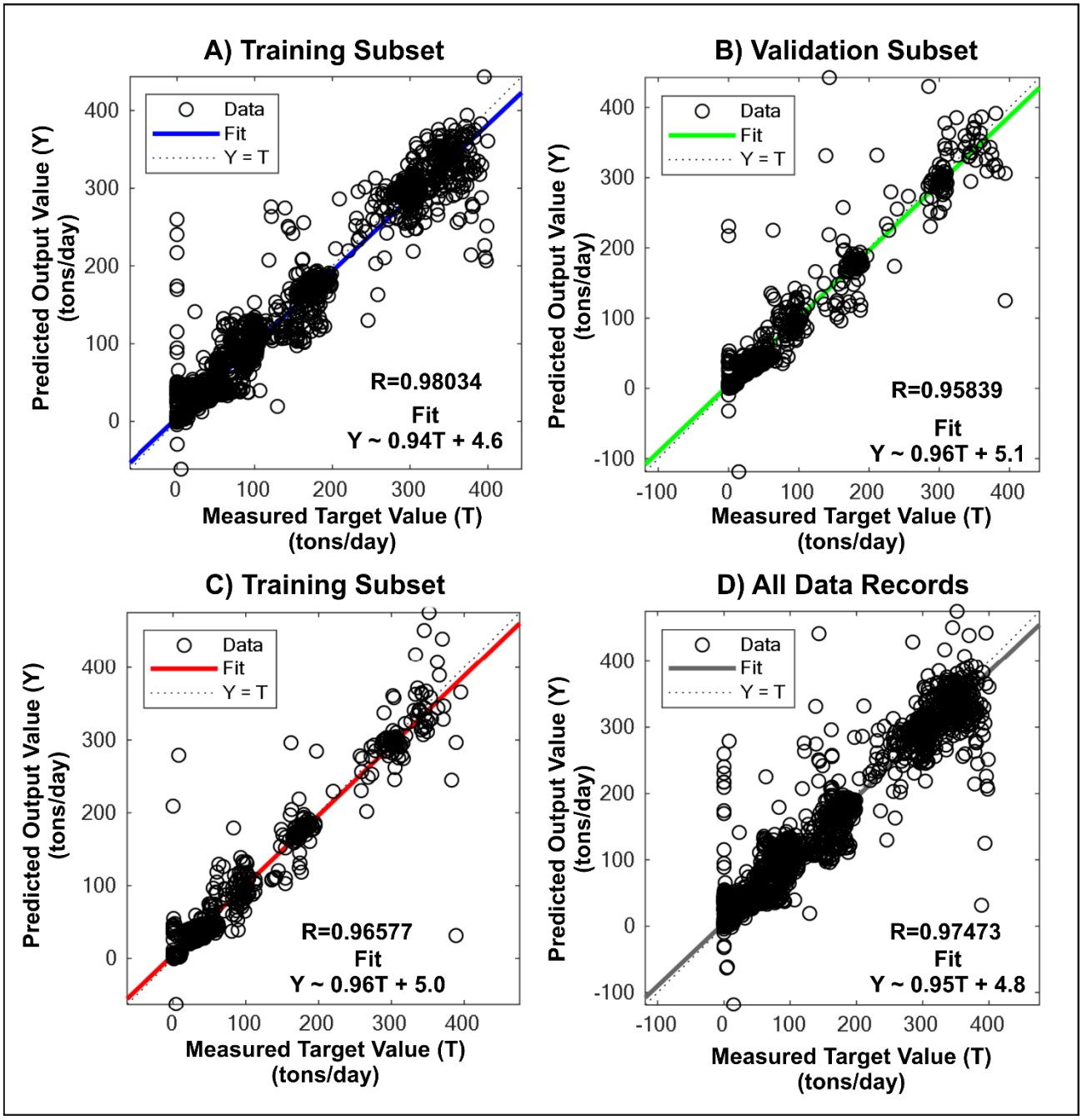


Fig. 5. Results of the BPN model comparing predicted with measured target plant output values. Note that each data point displayed represents the outcome for an individual output variable not the output of the entire petrochemical plant.

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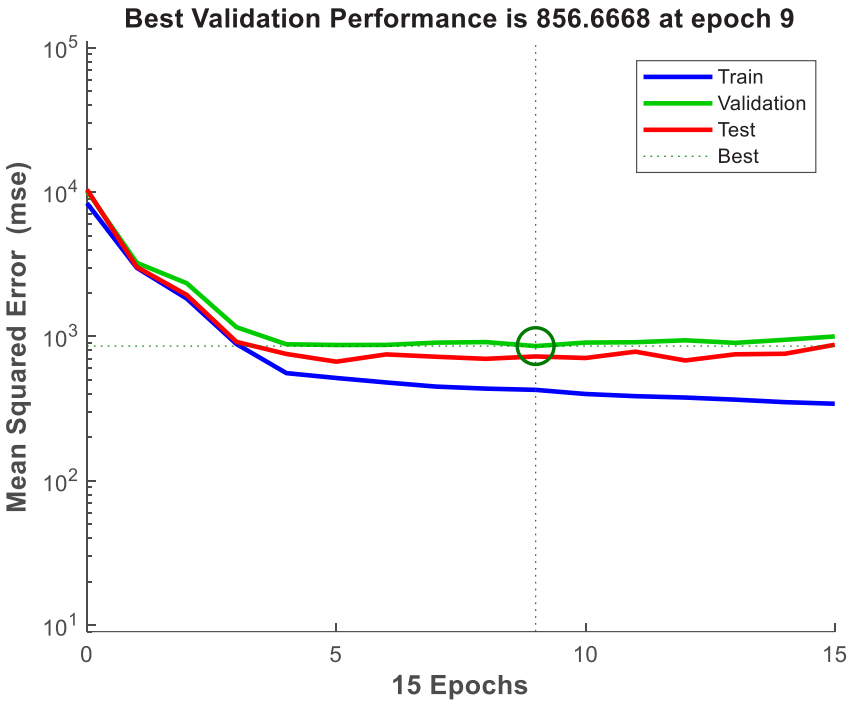


Fig. 6. BPN performance for the 10 neurons in the hidden layer.

Table 7. BPN prediction performance for different numbers of neurons in the hidden layer.

Number of neurons in the hidden layer	5	10	15	20	100
Training subset data records	256	256	256	256	256
Validation subset data records	55	55	55	55	55
Testing subset data records	55	55	55	55	55
Training MSE	627	426	356	430	227
Validation MSE	794	856	539	936	961
Testing MSE	733	726	926	747	1394
Training *R*	0.97	0.98	0.983	0.98	0.99
Validation *R*	0.962	0.958	0.975	0.955	0.956
Testing *R*	0.965	0.965	0.956	0.966	0.932
All *R*	0.968	0.974	0.978	0.974	0.976

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Table 8. Index matrix of variables

Independent variable	SRG	LPG	PBR	BEN	STYRENE	ACN	MO	BUTENE-1	**Sum**	
Dependent variable	Index values									
PE	1	1	0	1	0	0	1	1	**5**	
HIPS	0	1	1	0	0	0	1	0	**3**	**Min.**
GPPS	0	1	1	0	0	0	0	1	**3**	**Min.**
EPS	1	1	1	1	1	0	1	1	**7**	**Max.**
ABS	1	1	1	0	1	1	1	0	**6**	
TOL	1	1	1	1	0	1	1	1	**7**	**Max.**
BD	1	1	1	0	1	0	1	0	**5**	
PEN	1	1	1	1	1	1	0	0	**6**	
PROP	1	1	1	0	0	1	0	1	**5**	
C4 R	1	1	1	0	1	1	1	0	**6**	
CFO	1	1	1	1	0	1	1	1	**7**	**Max.**
FO	1	1	0	0	0	1	1	0	**4**	
C7-C9	1	1	0	0	0	1	1	0	**4**	
Sum	**11**	**13**	**10**	**5**	**5**	**8**	**10**	**6**		
		Max.		**Min.**	**Min.**					

perfect accuracy. These factors include:

Inappropriate distribution of data variable values

Measurement errors in the recorded data

Severe short-term changes in plant operating conditions

Inadequate mathematical model

The ineffectiveness of some input variables in influencing specific output variable values

Some of these factors can be corrected, by further filtering the data records and refining the mathematical model. By depicting minimum, maximum, and average values, some data record outliers were discarded. The hybrid PSO and BPN model was then applied to identify the main influencing variables, the model was configured to generate an index matrix, based on a feed-forward BPN optimized by PSO. This optimization algorithm was employed to identify the key variables influencing each specific output variable on the overall training performance of the BPN. In this matrix, the number 1 means that an input variable is influential and a zero value means that the variable has no effect on the target function (Table 8). Lists of the control parameter values used in the configured hybrid BPN-PSO model have been illustrated below:

PSO input data
Particle size: 10
Number of parameters: 8
Epoch: 5
c1: learning factor: 1.4047
c2: learning factor: 1.494
w_{max}: maximum inertia weight: 0.9
w_{min}: minimum inertia weight: 0.4
ANN input data
ANN type: generalized regression neural network (GRNN)
Spread: 0.01
Number of neurons per hidden layer: 10
Number of hidden layers: 2
Transfer function of the first layer: radial basis
Transfer function of the second layer: purelin

The PSO algorithm requires tuning parameters to be assigned. These include inertia weight *w*, the total number of

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Table 9. Final regression coefficient (R) results using the hybrid BPN-PSO model.

Dependent variable	Regression coefficient
POLYETHYLENE	0.994
HIPS	0.996
GPPS	0.99
EPS	0.982
ABS	0.983
TOLUENE	0.978
BD	0.966
PENTANE	0.963
PROPYLENE	0.997
C4 RAFFINATE	0.995
C.F.O	0.988
FUEL OIL	0.971
C7-C9	0.984
Max.	**0.997**
Min.	**0.963**
Mean	**0.984**

particles m, acceleration constants $c1$ and $c2$, maximum limit to velocity v_{max}, the maximum number of iterations T_{max}, and computed precision ε. Of them, w, m, $c1$, $c1$, and v_{max} represent algorithm control parameters that are dataset-specific. On the other hand, T_{max} and ε are used to determine algorithm-stopping conditions and to influence progressive changes in w as the algorithm progresses through its iterations, as shown in Eq. (3).

$$w = w_{\max} - \frac{w_{\max} - w_{\min}}{T_{\max}} \times t \tag{3}$$

Where w_{max} is the maximum inertia weight, and w_{min} is the minimum inertia weight (typically, $w_{max} \sim 0.9$ and $w_{max} \sim 0.4$); t is current iteration number; T_{max} is the maximum iteration number.

The reason that in some cases there is no relationship between independent and dependent variables is that in the production of some products (the dependent variables), some of the input feeds (independent variables) are not involved.

In Table 8, the index values displayed reflect the degree of influence the independent variables exert on the dependent variables. For no output products (specific dependent variables) do all the independent variables exert an influence. The LPG variable did though exert an influence on all thirteen output variables. Of the dependent variables, EPS and CFO had the highest number of influential independent variables (i.e., 7 out of the 8 input variables involved). By exploiting these identified influences, the PSO-BPN model improves the prediction accuracy of the basic BPN model for the studied petrochemical plant.

In the first iteration of the hybrid BPN-PSO model, the index and g_{best} matrix are allocated the same values in all matrix elements equal to 2 and 1 as initial assumptions, respectively. After 5 iterations, each striving to optimize MSE between target and predicted values and calculating R for each step, the prediction performance of the BPN-PSO model is assessed (Table 9). The mean R value achieved 0.984 after 5 iterations, i.e., an improvement on the BPN model. Pentane achieves the lowest R value (0.963) and propylene has the highest R value (0.997).

The primary objective of the BPN-PSO algorithm is to identify the independent variables that exert a specific influence on each dependent variable. It effectively achieves that (Table 8) and the information it provides can be used in feature selection for a customized BPN model, as described in section 5.3. Finally, according to Table 9, the regression coefficients are calculated and reported in Table 9 at the end of the 5th iteration of the modified BPN.

5- 4- Modified BPN model exploiting feature selection suggested by the BPN-PSO model

After filtration of all data by using a hybrid BPN-PSO algorithm and deletion of previous outlying data records, a modified ANN structure was configured and evaluated with training, validation, and testing subsets. As described in Section 4.2, the generalized regression neural network method was used for the modified BPN utilizing the newgrnn MATLAB function, configured as follows:

Net. =newgrnn (P, Spread) takes three inputs,

P: R-by-Q matrix of Q input vectors

T: S-by-Q matrix of Q target class vectors

Spread: Spread of radial basis functions (default = 1.0)

Generalized regression neural networks (grnns) utilize a Radial Basis Function (RBF) to train their predictions. This enables them to be designed and converges very quickly. In this study, the newgrnn function was applied using its MATLAB software default setting. After 5 iterations for each dependent variable separately, the MSE objective function reached a minimum value.

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Table 9. Final regression coefficient (R) results using the hybrid BPN-PSO model.

Relative errors (*RE*) for example data records from the testing subset evaluated by the modified BPN model							
Data No.	PE	HIPS	GPPS	EPS	ABS	TOL.	BD
3	3.27%	0.67%	14.63%	14.71%	23.30%	7.74%	12.34%
9	21.41%	0.98%	2.44%	3.12%	5.91%	31.25%	3.85%
12	1.52%	1.35%	3.70%	0.00%	0.00%	20.00%	9.52%
16	1.27%	1.63%	1.11%	17.50%	35.88%	25.00%	5.18%
20	11.48%	0.00%	5.06%	15.38%	34.86%	28.57%	8.45%
24	3.81%	3.55%	2.38%	28.57%	0.76%	27.63%	7.77%
29	1.29%	0.97%	10.77%	2.78%	9.44%	21.36%	24.30%
33	5.29%	7.56%	3.12%	8.33%	31.60%	1.64%	7.11%
36	0.48%	12.78%	5.52%	10.53%	2.57%	1.33%	6.03%

Relative errors (*RE*)…						
3	PEN.	PROP.	C4 R	CFO	FO	C7-C9
9	17.50%	0.92%	9.30%	3.47%	11.36%	6.17%
12	14.75%	4.70%	10.00%	16.01%	15.08%	10.37%
16	12.53%	5.40%	0.19%	0.37%	22.53%	0.72%
20	3.80%	0.13%	8.70%	9.71%	10.00%	5.68%
24	0.36%	6.19%	7.53%	10.84%	5.09%	14.01%
29	22.04%	1.29%	1.12%	7.09%	11.56%	1.41%
33	31.00%	3.93%	5.99%	10.78%	6.17%	2.00%
36	4.91%	2.72%	0.25%	12.23%	9.52%	1.88%

The best indicator of the modified BPN model performance is the prediction accuracy it achieves when applied to the testing subset, which consists of 55 filtered data records. Predictions are in close agreement with the observed output variable values (Table 10). Maximum, minimum, and average Relative Error (RE) values are 59.1%, 0.0%, and 9.9%, respectively. This level of accuracy is considered acceptable for a nonlinear production planning model applied to a large scale petrochemical plant. The influence matrix established by the hybrid BPN-PSO model is used for feature selection to enable the modified BPN model to generate acceptable Relative Error (RE) accuracies when applied to the testing subset data records, as displayed in Table 10. In this table, *RE* is defined as Eq. (4).

$$\mathrm{Re}\,lative\ Error\,(RE)(\%) = \frac{\left|DCS\ datavalue - ANN\ datavalue\right|}{DCS\ datavalue}\times 100 \tag{4}$$

In summary, the study models and optimizes the throughputs of the considered petrochemical plant in four stages:

1- basic BPN

2- PSO algorithm to optimize feature selection

3- hybrid BPN-PSO algorithm

4- modified BPN

The basic BPN delivered sub-optimal relationships between the input and output variables in predicting the performance of the overall plant. There are two reasons for this outcome: 1) the inclusion of some unrepresentative data records; and, 2) some input variables may have little impact on specific output variables. To solve the first problem, the statistical distributions of the variables were used to identify and remove outlying data records. To resolve the second problem, the PSO algorithm was used to identify the influential input variables (features) for each specific output variable (Table 8). By eliminating outlying data records and using only the effective features as input variables, the output variable values were predicted using a modified BPN tuned with an RBF function. The modified BPN yielded substantially more accurate plant output predictions. Clearly, the elimination of outlying data records and concentration on the most influential input features are more efficient for creating an accurate model for predicting outputs for the production planning of complex petrochemical plants. The regression coefficients achieved between predicted and measured values for specific output products applying the hybrid PSO-BPN model vary between 0.963 and 0.997 (Table 10). These values indicate the ability of the developed hybrid model to accurately predict product output values.

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6- Conclusion

There are many factors that may result in uncertainty in a manufacturing plant that can lead to poor productivity and diminished profitability. The most common uncertainties are associated with processing time, process set-up time, and transportation time. Production planning models are therefore essential in optimizing the performances of large scale production plants such as those required in the petrochemical and refining sectors.

In this study, three neural networks are evaluated associated with a large complex petrochemical plant with the objective of optimizing its production outputs in terms of production volumes. These models are:

a basic back-propagating network (BPN).

a hybrid basic network combined with a particle swarm optimizer (BPN-PSO) model.

a generalized regression neural network (GRNN) utilizing features selected by the BPN-PSO model

All models consider eight input variables in their efforts to predict the outputs of 13 products (dependent variables) as accurately as possible. The basic BPN model could only achieve a correlation coefficient between actual versus predicted product production volumes of about 0.984 (mean of correlation coefficients). This prediction accuracy although good is considered to be insufficient for a plant of this type. The main limitation of the basic BPN model is that it considers all input features when predicting each output product. Applying the hybrid BPN-PSO model identified which of the input variables were influential in predicting the production volumes of each output product individually. The BPN-PSO model revealed that three of the output products are influenced by seven of the input variables, whereas the remaining output products are influenced by less than seven of the input variables. Indeed, two of the output products are only influenced by three of the input variables.

Applying the features selected for each output prediction identified by the BNP-PSO model to a modified BNP employing the newgrnn function (MATLAB) with default settings leads to improved predictions of the dependent variables as a whole. Applied to the testing subset the modified BNP achieved maximum, minimum, and average relative errors (*RE*) of 59.1%, 0.0%, and 9.9%, respectively. Prediction errors in that range are considered acceptable for the collective production processes of a large scale petrochemical complex evaluated with a nonlinear planning program.

Nomenclature

Abbreviations

ABS	Acrylo-Butyl-Styrene
ANNs	Artificial Neural Networks
BD	Butadiene
BEN	Benzene
BPN	Back Propagation Artificial Neural Network
C4R	C4 Raffinate
CAN	Acrylonitrile
CHP	Combined Heat And Power
DCS	Distributed Computer System
DEA	Data Envelopment Analysis
FEPS	Expanded Poly Styrene
FO	Fuel Oil
GPPS	General Purpose Poly Styrene
GRNN	Generalized Regression Neural Networks
HIPS	High Impact Polystyrene
MF	Mass Flow
MLP	Multi-Layer Perceptron
MO	Mineral Oil
MSE	Mean Squared Error
NN	Neural Network
PBR	Poly Butadiene Rubber
PE	Polyethylene
PEN	Pentane
PEN	Pentane
Prop.	Propylene
R	Pearson's Correlation Coefficients
R.E.	Relative Error
SRG	Of Source Reagent Gas
TOL	Toluene

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