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# **Prediction of transient chemistry effect during fuel pyrolysis on the pressure drop through porous material using artificial neural networks**

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HAL Authorization

1     **Prediction of transient chemistry effect during fuel pyrolysis on**  
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4     **the pressure drop through porous material using artificial neural**  
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31  
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33     **Abstract**  
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35     Hydrocarbon fuels appear as good candidates for cooling purpose within aerospace  
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37     applications. Fuel flows through permeable structures. Thus, internal convection cooling is  
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39     reinforced by chemical kinetics (endothermic effect of fuel pyrolysis). Perfectly tuned  
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41     conditions may thus rapidly change due to unexpected coke formation that will clogged the  
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43     pores of the material and thus strongly affect the cooling efficiency. The pressure drop is one  
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45     of the indicator to monitor the modification of the through-flow and thus of the cooling.  
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48     Having a tool to predict these variations is of practical and theoretical interest for a better  
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50     management of the complex chemical and physical phenomena. This paper presents a model  
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52     based on artificial neural networks (ANN) for estimating the transient changes of the pressure  
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54     drop of a reactive fluid (n-dodecane) under pyrolysis conditions passing through porous  
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22 metal material. The ANN is developed using experimental data obtained from an  
23 experimental bench, which assures the monitoring of fluid mass flow rate, pressure and  
24 temperature in stationary and transient conditions. For each case, the fluid pressure which  
25 crosses the metallic porous material is measured as a function of test time, inlet operating  
26 pressure, temperature and fuel mass flow rate. The optimal ANN architecture with error  
27 backpropagation (BPNN) was determined by the cross validation method. The ANN  
28 architecture having 9 hidden neurons gives the best choice. Comparing the simulated values  
29 by ANN with the experimental data indicates that the ANN model give correct results. The  
30 performance of the ANN model is compared with the multiple linear regression model. This  
31 work is expected to be used for later prediction of pressure drop under a wide range of  
32 clogging conditions.

33 **KEYWORDS:** Pyrolysis; Artificial neural networks; Modelling; Permeation; Coke; Porous  
34 medium.

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## 1. Introduction

The development of hypersonic vehicles for future access to space or civil transport applications leads to an important heating of the engine and air frame. At flight speeds near Mach 4 and above, the air taken on board these vehicles will be too hot to cool the engines and airframe. Therefore, using fuel within regenerative cooling technique may be applicable [1]. To do so, it will be necessary to study and develop adapted light weight and high-temperature materials whose characteristics in terms of permeability and porosity are well defined. Among the materials the composite ones made of Ceramic Matrix (e.g. silicon based matrix) with carbon fibers are particularly interesting. For the lowest speed regime, metallic materials may also be used [2]. The aero-thermal loads must be thus addressed to quantify permeability/porosity fluctuations of materials as a function of operating conditions.

In the literature, different studies are found in relationship with this need, experimentally [3-5] or numerically [6,7]; even mathematically [8]. Such studies are not only dedicated to the flow description but also to the heat transfers [9-11]. The flows in porous materials are widely studied under common operating conditions.

The problem becomes more difficult when the coolant can react with the materials or within the material (local coking) [2]. In case of chemical reaction, the formation of carbon deposit on the surface and inside the porosities can impact the physical properties of the material (lowering the permeability and the porosity) and thus the cooling efficiency. These reactions can be due to the thermal fluid decomposition and to the degradation of the material itself. The degree of decomposition is highly dependent on the operating conditions (temperature, pressure, type of flow, nature of reactor) [10,12-15]. Thermal cracking of hydrocarbons have been widely studied in petrochemical industry [16-20] and in the context of chemical vapor infiltration for the preparation of carbon/carbon composites [21-25]. It

60 appears than the bigger the molecule, the higher the number of reactions which occur.  
61 Considering dodecane pyrolysis, the number of reactions largely overpasses 1000 [11]. This  
62 implies very complex phenomena (heat and mass transfers with chemistry).

63 A lot of studies, often under high pressure (up to 2MPa) are available for ambient to  
64 average temperature conditions (under 800K) [3] or for low pressure and high temperatures  
65 [1]. But only few are dedicated to both high temperature and high pressure conditions in case  
66 of reactive fluid. Numerous equations (derived from Brinkman's equation) which relate the  
67 pressure drop ( $\Delta P = P_{in} - P_{out}$ ) through the porous material to the through-flow velocity have  
68 been published [4,6]. They are based on coefficients, whose physical meaning is not evident  
69 [4]. One of the complexities of such configuration is due to the fact that along the chemical  
70 reactor (cooling channel of the hot vehicle), the fluid is supercritical [2]. Multi-species flow  
71 is found due to fuel degradation during which heavy compounds (coke particles) are formed  
72 and produce solid particles that can block the pore within the porous medium where they are  
73 flowing [10,26]. Due to these large and open difficulties, CFD calculations may not be  
74 relevant and experimental tests are costly and they cannot cover the entire range of test  
75 conditions/material variety, fluid nature.

76 As a consequence in this paper, we have used an approach based on the artificial neural  
77 networks (ANN) for simulating the transient changes of the pressure drop of n-dodecane  
78 (reactive fluid) passing through the porous material (Stainless Steel) by taking into account  
79 both high temperature and high pressure conditions. This work intends to indirectly predict  
80 the chemical effect of fuel pyrolysis, of coking and of clogging on the permeation process  
81 which directly controls the cooling efficiency. The description of the same numerical  
82 approach applied to another set of gas mixture (inert) and flow conditions can be found in a  
83 previous study [7]. Over the last two decades, ANN have been successfully used by many  
84 researchers for a wide range of engineering applications [27-29]. ANN is based on the

1 85 substitution of the complex simulation model by an approximation of the input-output  
2 86 relationship. ANN has the advantage over regression that the form of the model needs not to  
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4 87 be pre-determined [30]. In addition, ANN can theoretically approximate any function to any  
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7 88 level of accuracy, which is very interesting when the governing physical mechanisms are  
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10 89 non-linear like in high velocity fluid flow in porous materials. The database was built with  
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12 90 four input parameters (experiment time, inlet fuel mass flow rate, inlet operating pressure and  
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14 91 the uniform temperature) and with the outlet fuel pressure as the output parameter. The  
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17 92 results obtained experimentally are used to construct, to optimize and to validate the model.  
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19 93 This artificial neural network has been trained and tested on this database using the error  
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22 94 backpropagation algorithm and cross validation. The performance of the ANN model is  
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24 95 compared with a multilinear regression approximation method.

## 27 96 **2. Material**

### 28 97 2.1 Experimental permeation bench

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30 98 The COMPARER pyrolysis test bench (Fig. (1)) is used to pressurize and to heat the fuel  
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33 99 under flow conditions [4]. Its main characteristics are the following:  
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- 37 100 • Maximum operating conditions: 1800K, 8MPa, 0.0006 kg.s<sup>-1</sup> for liquid fuel and  
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39 101 0.006 kg.s<sup>-1</sup> for gas.
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42 102 • Sensors: 5 pressure transducers, 5 mass flow rates, over 10 K-type and R-type  
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44 103 thermocouples with data acquisition system (16 bits, 48 channels, 0.1 Hz).

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47 104 A permeation test cell contains the porous sample (Fig. 1). This cell is inserted inside the  
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50 105 furnace of the COMPARER bench and it is connected to the fluid supply system and to the  
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52 106 suitable sensors. The permeable material bounds the cell in two high and low pressure  
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55 107 chambers (upstream and downstream to the porous material respectively). An inlet pipe  
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57 108 provides the fuel into the system. This cell is connected to a dynamic sampling system to get  
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109 hot pressurized samples at three location points in the cell. Despite its small size (external  
110 diameter of 40mm), it enables measuring the temperature, pressure and mass flow rate on  
111 each side of the porous sample.

112 In the present work, an isotropic stainless steel material is preferred to composite one to  
113 avoid considering complex microstructure (fibres, layers). It is characterized by a porosity  
114 around 30 %, a grain diameter of 14.1  $\mu\text{m}$  and a pore diameter of 4.1  $\mu\text{m}$ . Further geometrical  
115 information can be found in Gascoin *et al.* [4].

*Figure 1 should be placed here*

## 117 2.2 Experimental test condition

118 The different test conditions which were considered for the present work are the  
119 following:

- 120 • Temperature set-up: 3 different experimental test have been done for thermal plateau  
121 at  $T=725\text{K}$ ,  $765\text{K}$  and  $810\text{K}$ . Each plateau last for about 30 min to one hour  
122 depending on the time requested by the system to reach steady-state conditions.  
123 Monitoring the entire test length enables getting transient evolution of all parameters.
- 124 • Absolute inlet pressure: in the range of [3.4 MPa ; 3.8 MPa].
- 125 • The experimental protocol is achieved with constant mass flow rate and given  
126 downstream pressure ( $P_{out}$ ). The upstream pressure ( $P_{in}$ ) increases due to coking and  
127 clogging of the porous medium; which makes the pressure drop to increase as a  
128 function of the test time.
- 129 • Monitoring of the chemical species: transiently thanks to a FTIR spectrometer for 5  
130 gaseous species (methane, ethane, ethylene, propane, propylene) and during the three  
131 thermal plateaus by using a dedicated sampling system [10] coupled with a  
132 GC/TCD/FID/MS apparatus (more than 40 species analysed).

### 133 3. Experimental results

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2 134 We present in this section an experimental test result obtained for  $T=725\text{K}$ . As shown in  
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5 135 Fig. 2, the measured pressure drop (Measured  $P_{in} - P_{out}$ ) varies as a function of experimental  
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7 136 time ( $t$ ) and the measured fuel mass flow rate ( $q_{in}$ ) when the fuel (dodecane) temperature is  
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10 137 kept constant ( $T=725\text{K}$ ). Other obtained experimental results [10] showed that the  
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12 138 temperature has a major effect on the measured pressure drop. Further details on the  
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14 139 experimental results can be found in previous work [10]. Globally, based on the overall  
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17 140 obtained experimental results, we can conclude that there are three parameters ( $t$ ,  $q_{in}$  and  $T$ )  
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19 141 that have a great influence on the measurements of the pressure drop. These experimental  
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22 142 results are necessary to construct, to optimize and to validate a model based on ANN for  
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24 143 predicting the transient changes of the pressure drop of a reactive fluid (n-dodecane) passing  
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27 144 through porous metal material (stainless steel). The construction of the developed ANN  
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29 145 model is discussed in the following section.

30  
31 146 *Figure 2 should be placed here*

### 32 33 34 35 147 4. Construction of ANN models

#### 36 37 38 148 4.1 Construction of the database

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41 149 ANN models learn the relationship between the input and the output parameters as a  
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43 150 result of training with previously recorded data. The database was built using experimental  
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46 151 data which are obtained from the developed experimental bench with input parameters: test  
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48 152 time ( $t$ ), operating inlet pressure ( $P_{in}$ ), inlet fuel mass flow rate ( $q_{in}$ ) and temperature ( $T$ )  
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51 153 varying in a range of representative values: between 0 and 858s for  $t$ ; between 3.3MPa and  
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53 154 3.8MPa for  $P_{in}$ ; between 0.000033 kg/s and 0.0001 kg/s for  $q_{in}$  and 725K, 765K and 810K for  
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55 155  $T$ . Totally, the database contains an appreciable size of 979 experimental test points.  
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156 The present database was subdivided in three subsets. A first subset (490 experimental  
157 tests) is used to train the networks. A second one (245 experimental tests) is used to test the  
158 ANN models to determine when to stop the training stage. The third subset (244 experimental  
159 tests) is used to validate the performance of the selected model on unseen cases.

160 Each input or output parameter has been normalized relative to its minimum and  
161 maximum values observed in the data (according to Eq. (1)) to make the training procedure  
162 more efficient.

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

164 where  $X$  is an arbitrary parameter,  $X_{norm}$  is the normalized value, and  $X_{max}$  and  $X_{min}$  are the  
165 maximum and minimum values of  $X$ .

#### 166 4.2 Architecture and learning process of ANN models

167 An artificial neural network model is composed of interconnected group of artificial  
168 neurons or nodes. The most frequently utilized network is the multilayer backpropagation  
169 neural network (BPNN) which is used in the present study. The BPNN structure consists of  
170 three layers, an input layer which receive data; an output layer which sends computed  
171 information; and one or more hidden layers to link input and output layer. All the neurons  
172 (nodes) in a layer are connected with all the neurons of the previous and the next layer. In  
173 general, the number of the nodes in the input and output layer are determined by the nature of  
174 the problem. The architecture of a typical 3-layer backpropagation neural network is shown  
175 in Fig. 3.

176 *Figure 3 should be placed here*

178 Mathematically, a 3-layer BPNN with  $n$ ,  $m$ , and  $p$  the number of input, hidden and output  
 179 neurons respectively, can be formulated as in the following:

$$O_k = f \left( b_k + \sum_{j=1}^m f \left( b_j + \sum_{i=1}^n W_{ij} X_i \right) \times W_{jk} \right) \quad (2)$$

181 where  $X_i$  the input values of the network and  $O_k$  are the output values;  $b_j$ , the hidden unit  
 182 biases;  $b_k$ , output nodes biases;  $W_{ij}$ , the connection weights between the input layer and the  
 183 hidden layer;  $W_{jk}$ , the connection weights between the hidden layer and the output layer;  $f$  is a  
 184 transfer function. The sigmoid transfer function (Eq. (3)) was used in the present study.

$$f(x) = \frac{1}{1 + e^{-x}} \quad (3)$$

186 Where  $x$  is the excitation.

187 The learning process of BPNN is based on a series of connection weight adjustments in  
 188 order to minimize the gap (global error) between the outputs of the BPNN and the target  
 189 values [31]. Initially, all biases and connection weights are initialized to random values in the  
 190 range of  $[-1, +1]$ . Inputs are first propagated forward through each layer of the ANN. Errors  
 191 between outputs and target values are then propagated backwards and the connection weights  
 192 are modified according to a specific learning algorithm (delta rule) to reduce the overall error.  
 193 This process (forward-backward) is repeated until predicted outputs and target answers  
 194 coincide within a given tolerance [32].

195 The commonest convergence criterion is the average squared error (ASE) defined as:

$$ASE = \frac{1}{P} \times \frac{1}{S} \times \sum_{q=1}^S \sum_{k=1}^P (t_{qk} - O_{qk})^2 \quad (4)$$

197 where  $t_{qk}$  and  $O_{qk}$  are respectively the target and predicted value of the output node k for the  
 198 pattern  $q$ ,  $p$  is the number of output nodes, and  $s$  is the number of patterns. It should be noted  
 199 that any level of agreement between predicted and target vectors can be achieved by  
 200 providing a sufficient number of training cycles to be carried out. Such an *overtraining* is  
 201 however detrimental to the capacity of the network to generalize from unseen data (a network  
 202 that can accurately predict the output of the testing patterns is said to have generalized). It is  
 203 thus preferable to calculate the ASE both on training and testing patterns during training  
 204 cycles for optimum convergence: this process is called cross-validation (Fig. 4).

*Figure 4 should be placed here*

## 5. Results and Discussion

### 5.1 Optimum artificial neural network architecture

209 The determination of the ANN architecture constitutes one of the major tasks in the use of  
 210 the ANN. The overall performance of an ANN is dependent on the numbers of hidden layers  
 211 and hidden nodes. In the usual case of a 3-layer BPNN, the optimum number of hidden nodes  
 212 can be determined by cross-validation in the same way as the optimum number of training  
 213 cycles (Fig. 4).

214 In the present article, a neural network relating inputs  $\{X_1, X_2, \dots, X_n\}$  to outputs  $\{O_1, O_2,$   
 215  $\dots, O_p\}$  and containing one hidden layer with  $m$  hidden nodes will be noted:

$$\{O_1, O_2, \dots, O_p\} = \text{ANN}_{n \times m \times p} \{X_1, X_2, \dots, X_n\} \quad (5)$$

217 In our case, the outlet operating pressure ( $P_{out}$ ) is sought as a function of  $t$ ,  $P_{in}$ ,  $q_{in}$  and  $T$ . So,  
 218 it is possible to compute  $P_{out}$  by using a BPNN model with one node in the output layer (Eq.  
 219 (6)). It could be noticed that usually the pressure drop through the porous medium is  
 220 investigated as a function of the through-flow rate.

221 In this present study, the choice of the outlet pressure is preferred to limit the impact of  
 222 experimental uncertainties due to the two pressure transducers (which are generally  
 223 multiplied if compared to a single transducer). In addition, since the upstream pressure is an  
 224 inlet parameter, looking at the pressure drop or at the pressure outlet is equivalent when  
 225 focusing on the behaviour of the ANN model. As can be observed in Fig. 5, the optimal value  
 226 of ASE was calculated while using 9 nodes in the hidden layer for our model.

$$\{P_{out}\} = ANN_{4-9-1} \{t, P_{in}, q_{in}, T\} \quad (6)$$

228 The ASE values for the training, testing and validation phases for the optimal artificial  
 229 neural network model (ANN<sub>4-9-1</sub>) are respectively 0.000114, 0.000101 and 0.000132.

*Figure 5 should be placed here*

## 5.2 Discussion of the performance of the models

232 The performance of the ANN model is evaluated by comparing target ( $Y_i$ ) and predicted  
 233 ( $\hat{Y}_i$ ) values. Fig. 6 shows the comparison between the BPNN predicted values and the target  
 234 values for  $P_{out}$  on training, testing and validation data. Despite the pressure drop is the  
 235 parameter of interest for engineering application, the present model focuses on the outlet  
 236 pressure to clearly estimate the validity of the model. On the same graphs the best fit line  
 237 through the origin is also plotted and the coefficient of determination  $R^2$  for this line is  
 238 computed according to Eq. (7):

$$R^2 = 1 - \frac{\frac{1}{N} \sum_{i=1}^N (Y_i - \hat{Y}_i)^2}{\frac{1}{N-1} \sum_{i=1}^N (Y_i - \bar{Y}_i)^2} \quad (7)$$

240 where  $N$  is the number of data,  $Y_i$  is the target value,  $\hat{Y}_i$  is the value predicted by the model  
 241 and  $\bar{Y}_i$  is the mean of the  $N$  target values.  $R^2$  coefficients close to unity indicate a high degree

242 of linearity between predicted and target values. Associated with a best fit line slope close to  
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2 243 unity, it indicates a high model prediction accuracy.

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4 244 A basis of comparison for BPNN performance is usually sought in multiple linear  
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7 245 regression [33], a more ubiquitous prediction tool in fluid flow through porous material  
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10 246 research. Least square parameter fitting for a linear model expressing  $P_{out}$  as a function of  $t$ ,  
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12 247  $P_{in}$ ,  $q_{in}$ , and  $T$  (model 2) is performed on the same training database subset as for BPNN  
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14 248 model. This model is tested to predict the never-seen data from the BPNN validation database  
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17 249 subset. The lowest  $R^2$  value is obtained for multiple linear regression model. It is also noted  
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19 250 that the trend line deviates somewhat from the 1:1 line in the case of model 2. The  
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22 251 coefficients of determination ( $R^2$ ) for model 1 and model 2 are given in Table 1. The model 2  
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24 252 seems to be less efficient than model 1 for predicting the variations of  $P_{out}$ . This result is  
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27 253 expected: the physical phenomena captured in the database are complex and non-linear. In  
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29 254 ANN non-linearity is accounted for by the use of transfer functions (Eq. (3)), while  
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31 255 complexity can be controlled by varying the number of hidden nodes. In the present case, the  
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34 256 artificial neural networks provide good and realistic predictions.

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40 258 *Figure 6 should be placed here*

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45 260 *Table 1 should be placed here*

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48 262 An application of ANN is now proposed in the following part. Considering a constant  
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51 263 inlet pressure at 3.6 MPa, it is now possible to investigate the chemical effect within the  
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53 264 range of 725K-810K. It should be noticed that fixing arbitrarily the inlet pressure imposes the  
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56 265 outlet pressure to decrease, which simulate the pressure drop increase. The evolution of the  
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58 266 predicted outlet pressure ( $P_{out}$ ) using BPNN as a function of time and temperature inside the  
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267 porous medium is given in Fig. 7. It is found with model 1 that the predicted outlet pressure  
268 decreases as a function of time. This expected result is due to the formation of carbon deposit  
269 (coke) on the surface and inside the porosities of the studied material. We can observe also  
270 that the model 1 predicted outlet pressure decreases when the temperature inside the porous  
271 medium increases. The density decreases due to the thermal rise and since the mass flow rate  
272 inside the medium is kept constant, the mean reactive fluid velocity increases. Thus, the  
273 outlet pressure decreases; which means that the pressure drop increases. This is clearly  
274 understandable when paying attention to the Brinkman equation. It is thus very important to  
275 note that the BPNN approach is able to reproduce physical variations. In particular, it is clear  
276 that the chemical effect strongly increases at 760 K and is clear at 770K.

*Figure 7 should be placed here*

278 The result of Fig. 7 can be not only related to thermal effect on density and velocity but  
279 also to the chemical effect. Indeed, the reactive fluid outlet pressure decreases as a function  
280 of time due to the formation of the coke on the surface and inside the studied material. The  
281 thermal effect may increase the fluid velocity within the porous material by enhancing coke  
282 formation and pore clogging (the lower the cross-section area, the higher the fluid velocity  
283 and the higher the pressure in case of constant mass flowrate configuration).

284 Measuring the pressure drop through porous material could be a way to get information  
285 of phenomena within the porous material where no direct microscopic measure seems to be  
286 possible for the fluid properties. In addition, these results should drive the engineering study  
287 of material cooling because ensuring constant cooling efficiency, thus constant fluid flow  
288 through the porous medium, clearly requires compensating higher pressure drop depending  
289 on the temperature seen by the solid materials. As a consequence, performance of pumping

290 system should be designed to furnish this increasing need for upstream pressure if outlet  
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2 291 pressure should remain constant.  
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## 6 292 **6. Conclusion**

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9 293 In this article, an artificial neural networks tool has been used to simulate the transient  
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11 294 pressure drop of n-dodecane under pyrolysis conditions and crossing a metallic porous  
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13 295 material (Stainless steel). Based on experimental data, the optimum architecture of artificial  
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15 296 neural network was trained and validated, in order to generalise the prediction of the pressure  
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17 297 drop under clogging configurations not included in the database for difficult access reasons.  
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19 298 The validation showed excellent performance of this ANN model for the prediction of  
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21 299 dodecane transfer in the porous material ( $R^2 > 0.983$ ). An example of application was  
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23 300 presented to detect the temperature at which chemistry starts to strongly impact the fluid flow  
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25 301 within the porous medium. It was found that a turning point around 760 K-770K has to be  
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27 302 expected in terms of clogging when using n-dodecane at 3.6 MPa in stainless steel medium.  
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34 303 This study is a contribution to the growing evidence of the benefits of ANN models in  
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36 304 Aeronautical engineering. This important result may be applied to automate pressure drop  
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38 305 estimations, which are used in space flight applications, without prior knowledge of material  
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40 306 parameters and particularly for materials with transient changing properties.  
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394 **Table 1**  $R^2$  values between target and predicted outputs for all models.

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4 396 **Fig. 1** Schematic of the permeation test cell with porous material and associated measures.

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7 397 **Fig. 2** Measured pressure drop variations with the measured fuel mass flow rate and  
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9 398 experiment time for  $T=725K$ .

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12 399 **Fig. 3** Architecture of a typical multilayer BPNN.

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14 400 **Fig. 4** Convergence criterion and optimum network architecture.

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17 401 **Fig. 5** Average squared error (ASE) variations with the number of hidden nodes for the  
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19 402 testing data subset.

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21 403 **Fig. 6** Comparison between target and predicted values for  $P_{out}$  using BPNN (model 1) and  
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23 404 multi-linear regression (model 2) for all data subset.

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27 405 **Fig. 7** Model 1 predicted transient  $P_{out}$  variations with the temperature for  $q_{in} = 0.04g/s$  and  
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29 406  $P_{in} = 3.6MPa$ .

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**Table 1**  $R^2$  values between target and predicted outputs for all models.

$R^2$	Neural network (model 1)	Multiple linear regression (model 2)
Training phase	0.986	0.897
Testing phase	0.986	0.878
Validation phase	0.983	0.891

Figure 1  
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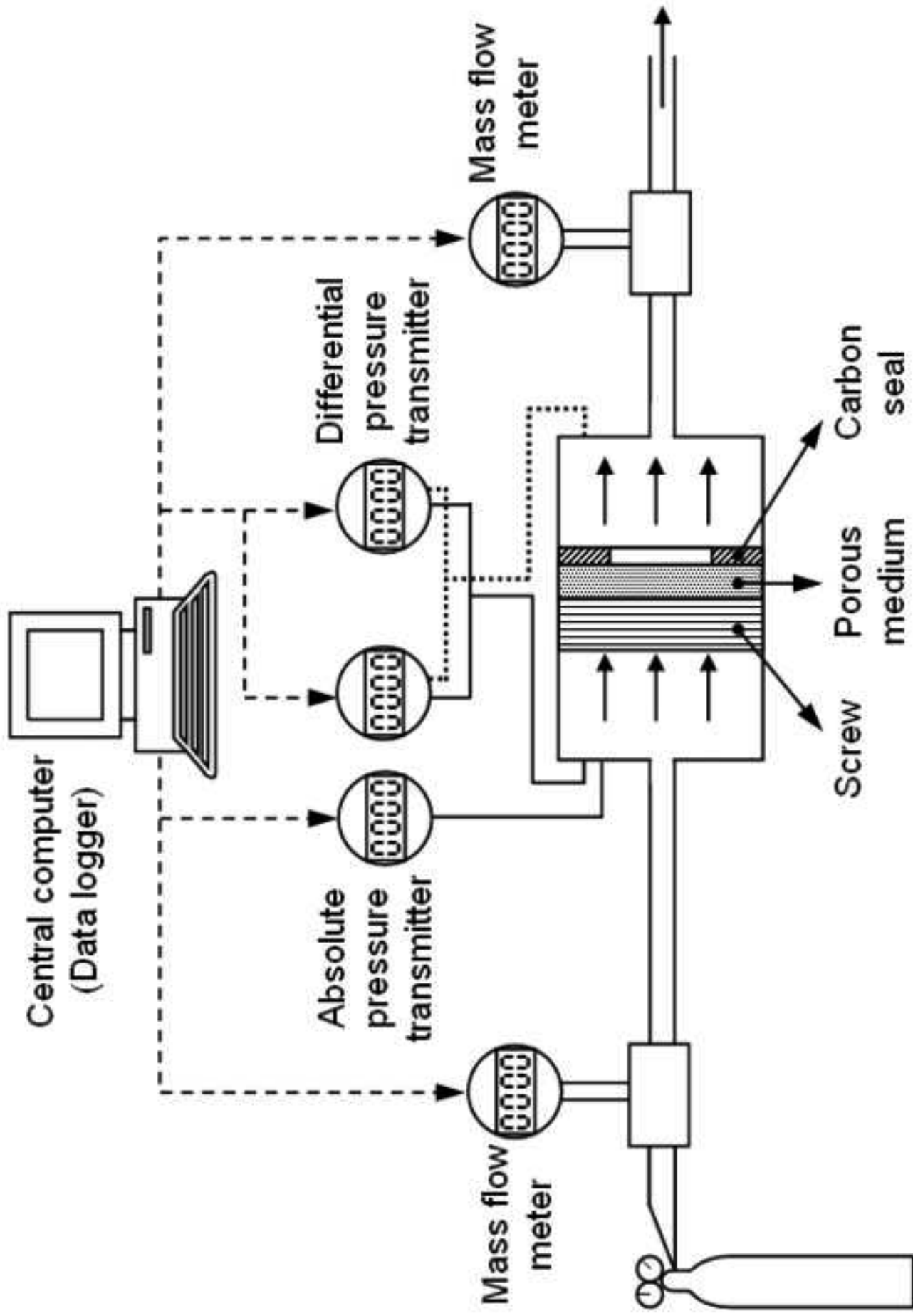


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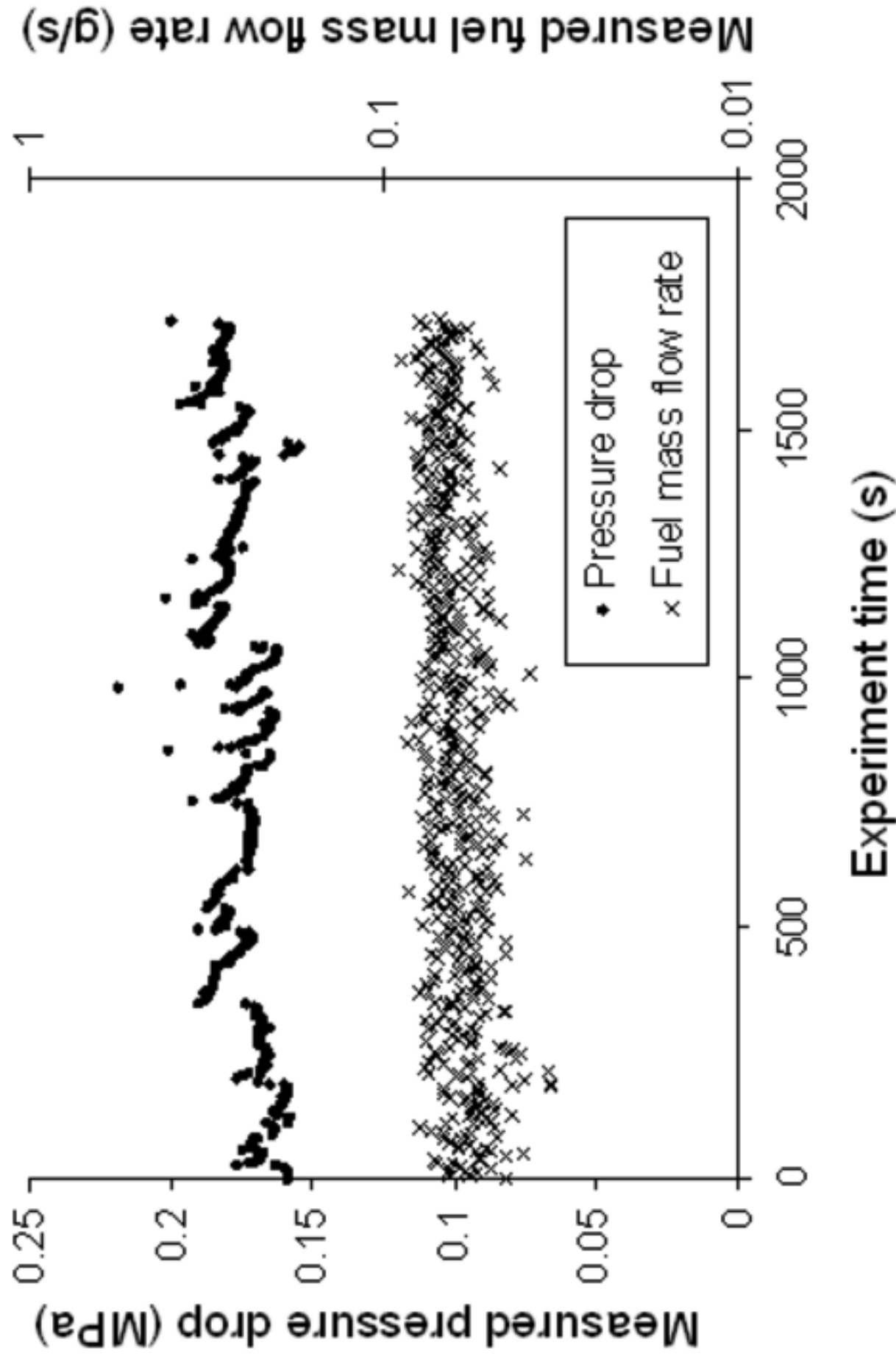


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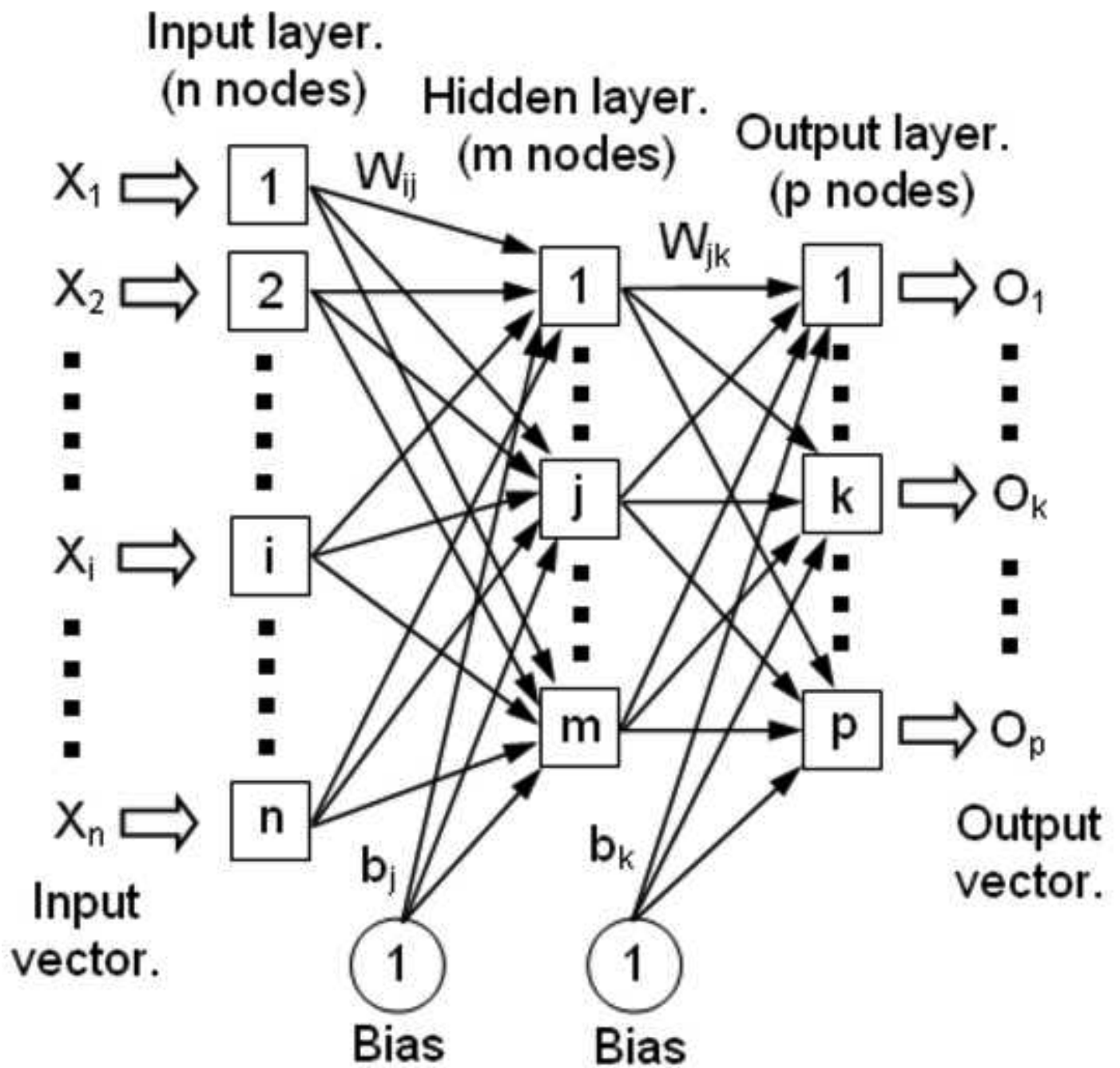


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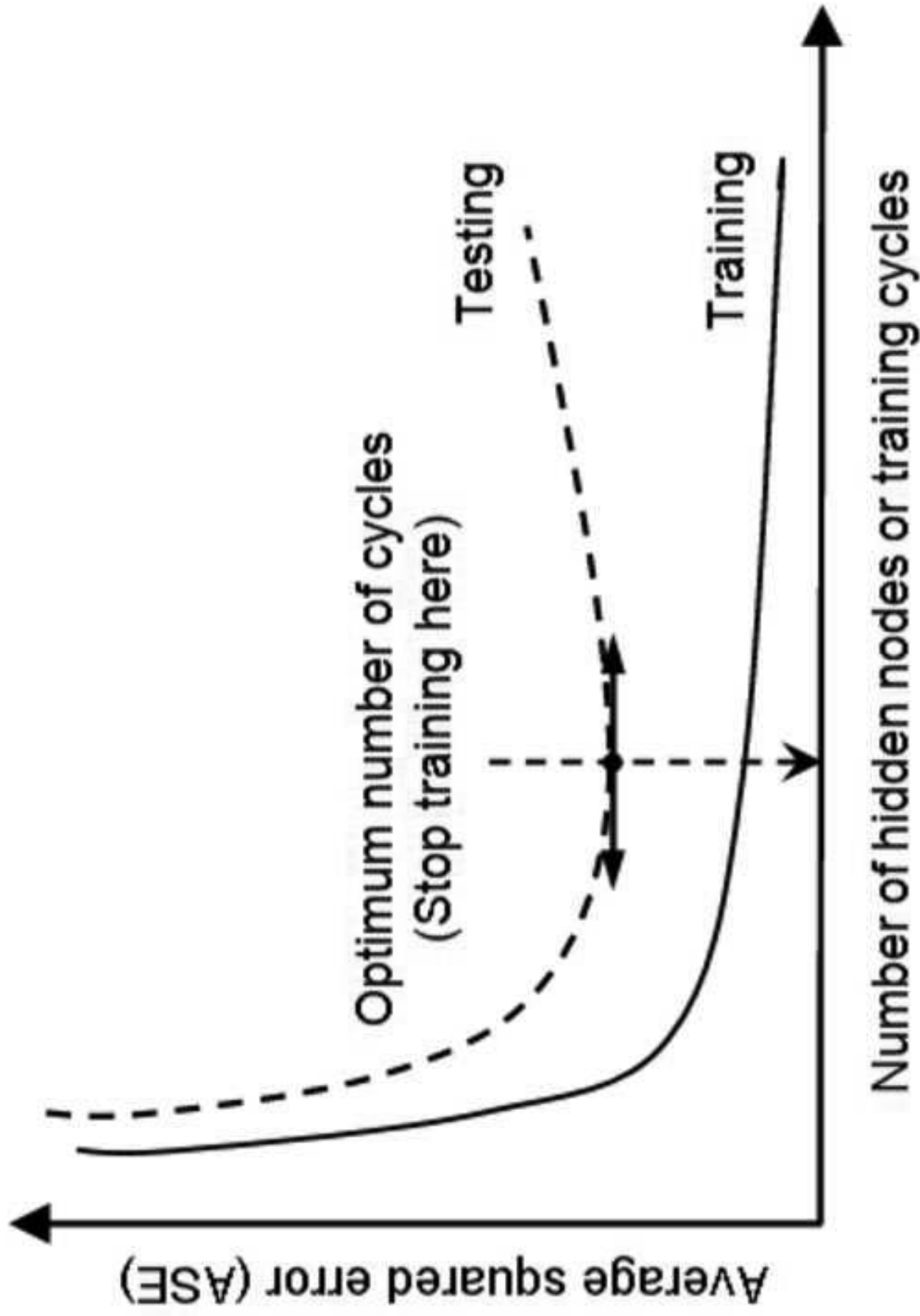


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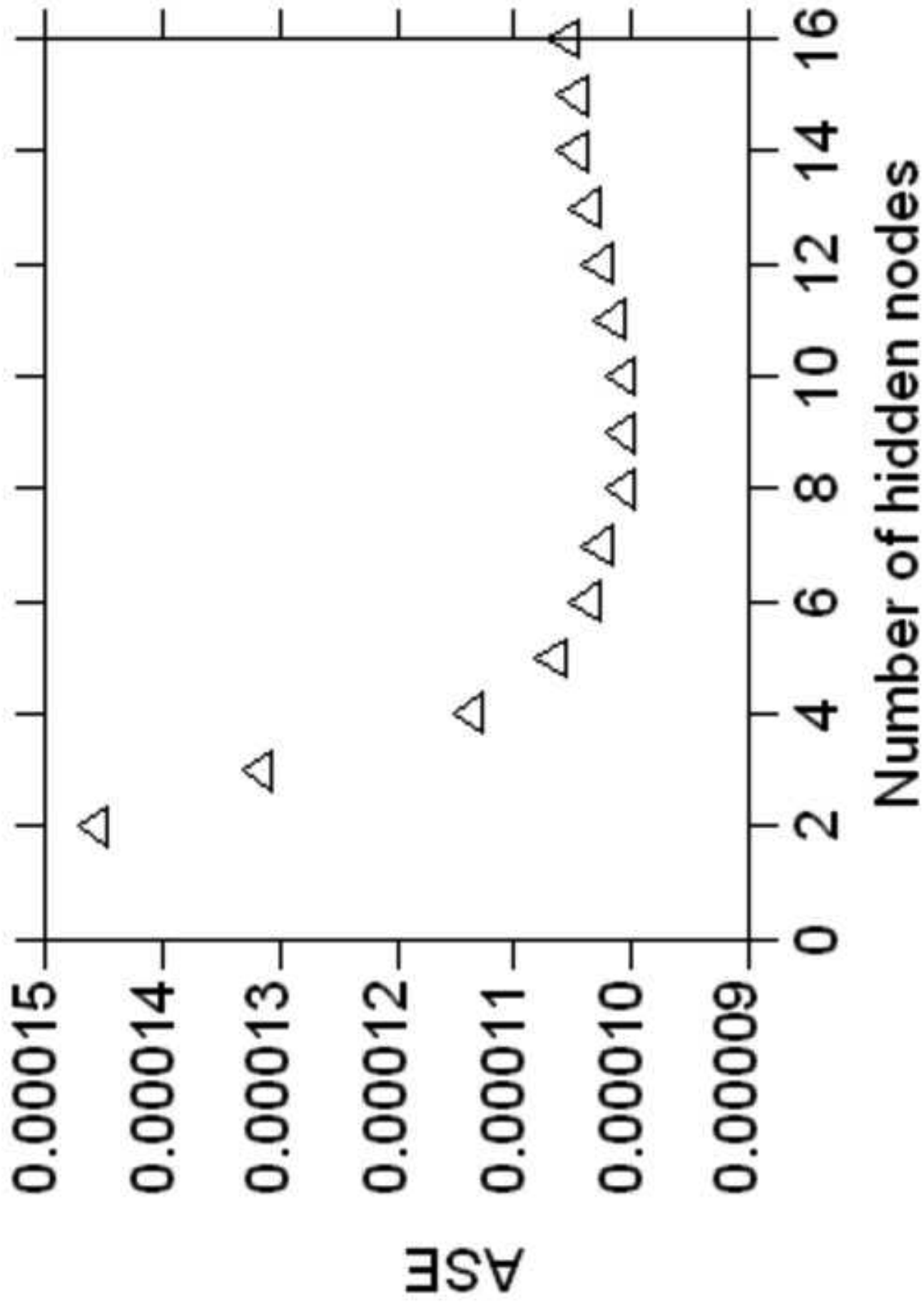


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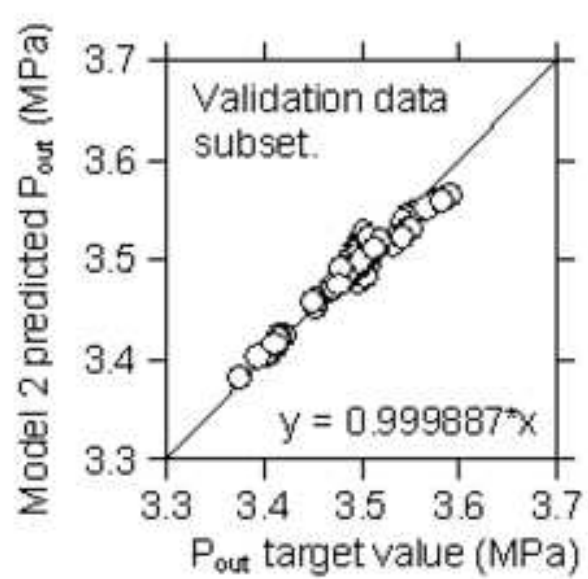
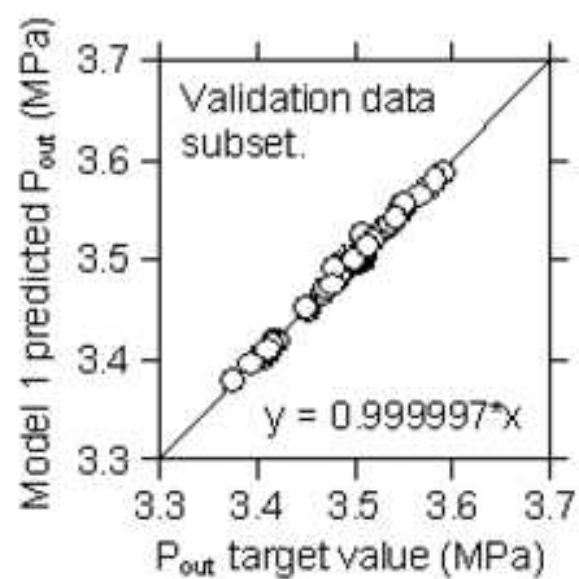
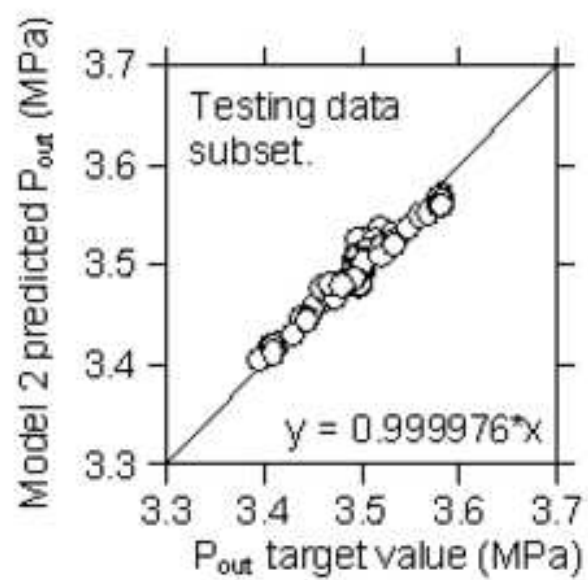
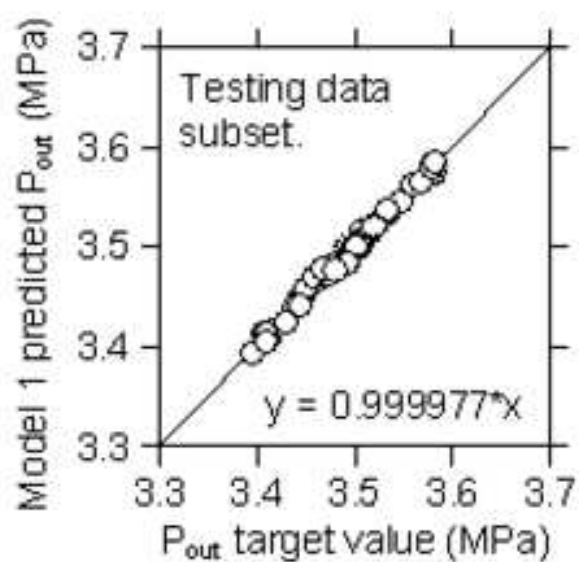
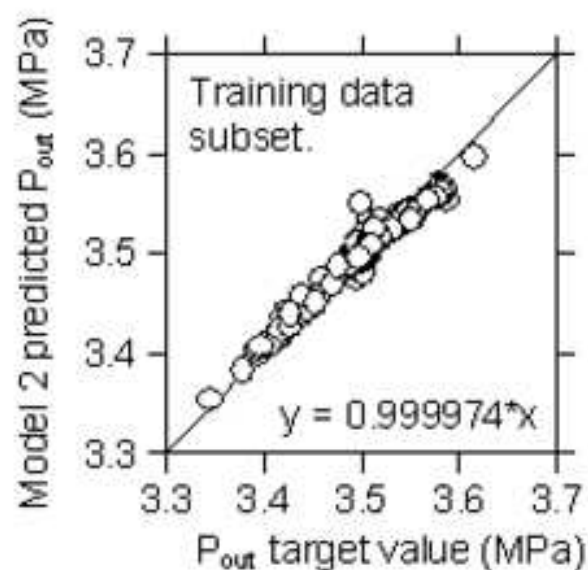
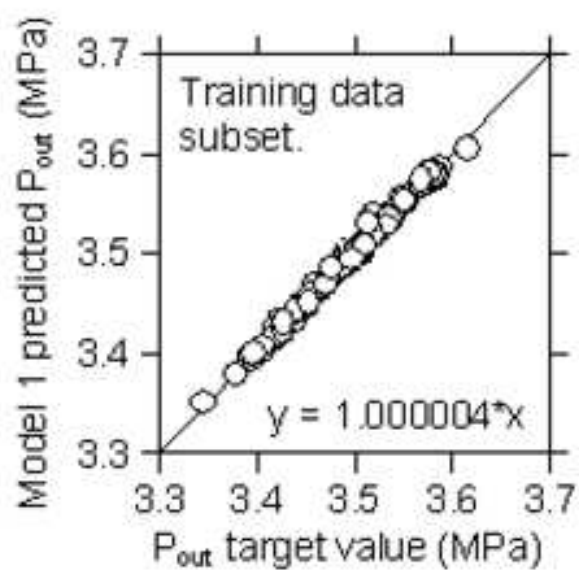
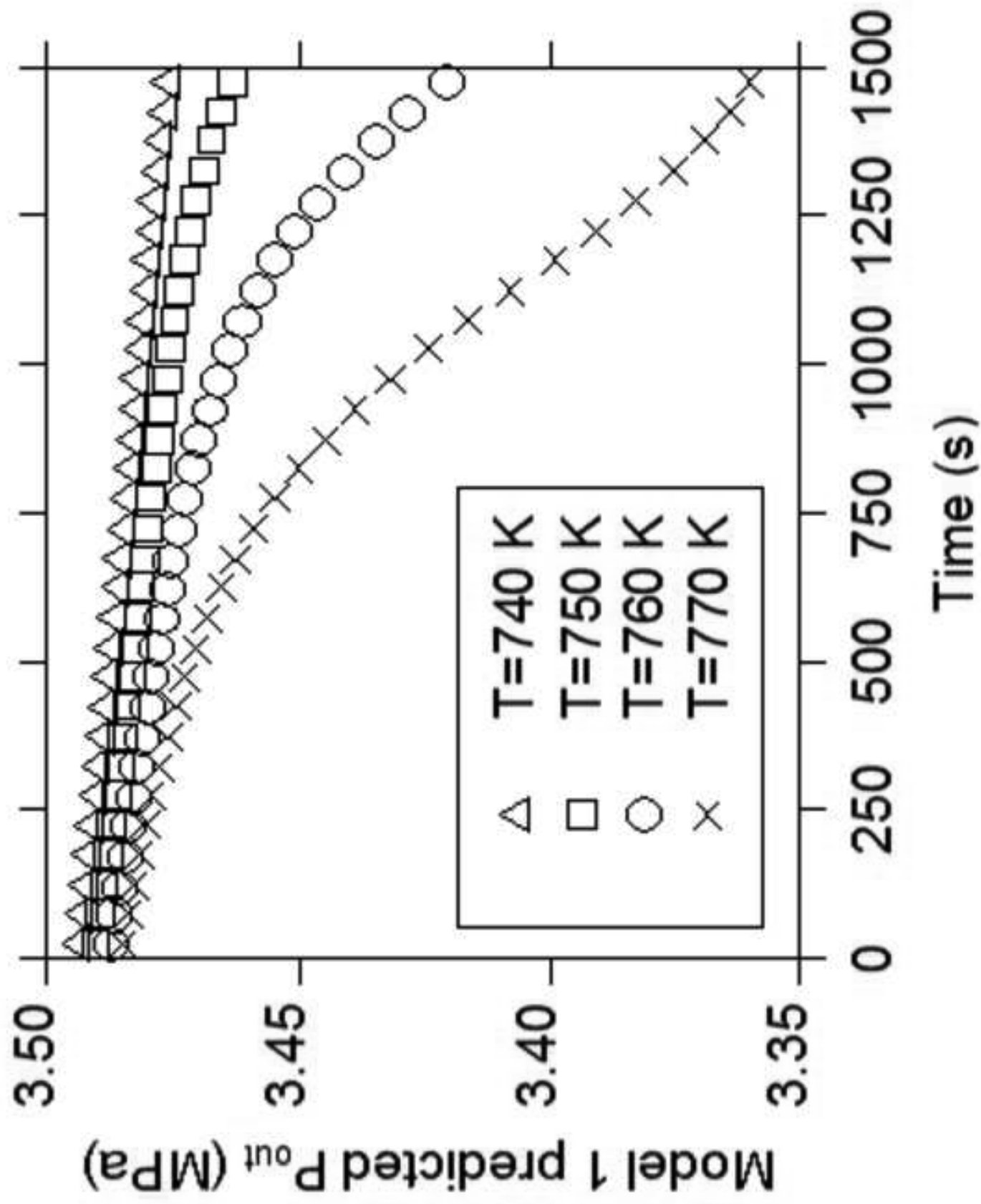


Figure 7  
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**Highlights :**

- We modeled the transient pressure drop of n-dodecane under pyrolysis conditions.
- We found a good agreement between the numerical results and the experimental data.
- We found that the developed model is able to reproduce physical variations.
- The model has been applied successfully on a series of examples.