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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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**Abstract**

Hydrocarbon fuels appear as good candidates for cooling purpose within aerospace applications. Fuel flows through permeable structures. Thus, internal convection cooling is reinforced by chemical kinetics (endothermic effect of fuel pyrolysis). Perfectly tuned conditions may thus rapidly change due to unexpected coke formation that will clogged the pores of the material and thus strongly affect the cooling efficiency. The pressure drop is one of the indicator to monitor the modification of the through-flow and thus of the cooling. Having a tool to predict these variations is of practical and theoretical interest for a better management of the complex chemical and physical phenomena. This paper presents a model based on artificial neural networks (ANN) for estimating the transient changes of the pressure drop of a reactive fluid (n-dodecane) under pyrolysis conditions passing through porous

metal material. The ANN is developed using experimental data obtained from an experimental bench, which assures the monitoring of fluid mass flow rate, pressure and temperature in stationary and transient conditions. For each case, the fluid pressure which crosses the metallic porous material is measured as a function of test time, inlet operating pressure, temperature and fuel mass flow rate. The optimal ANN architecture with error backpropagation (BPNN) was determined by the cross validation method. The ANN architecture having 9 hidden neurons gives the best choice. Comparing the simulated values by ANN with the experimental data indicates that the ANN model give correct results. The performance of the ANN model is compared with the multiple linear regression model. This work is expected to be used for later prediction of pressure drop under a wide range of clogging conditions.

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

## 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

85 substitution of the complex simulation model by an approximation of the input-output

86 relationship. ANN has the advantage over regression that the form of the model needs not to

87 be pre-determined [30]. In addition, ANN can theoretically approximate any function to any

88 level of accuracy, which is very interesting when the governing physical mechanisms are

89 non-linear like in high velocity fluid flow in porous materials. The database was built with

90 four input parameters (experiment time, inlet fuel mass flow rate, inlet operating pressure and

91 the uniform temperature) and with the outlet fuel pressure as the output parameter. The

92 results obtained experimentally are used to construct, to optimize and to validate the model.

93 This artificial neural network has been trained and tested on this database using the error

94 backpropagation algorithm and cross validation. The performance of the ANN model is

95 compared with a multilinear regression approximation method.

## 2. Material

96

97 2.1 Experimental permeation bench

98 The COMPARER pyrolysis test bench (Fig. (1)) is used to pressurize and to heat the fuel

99 under flow conditions [4]. Its main characteristics are the following:

100 • Maximum operating conditions: 1800K, 8MPa, 0.0006 $kg.s^{-1}$ for liquid fuel and

101 0.006 $kg.s^{-1}$ for gas.

102 • Sensors: 5 pressure transducers, 5 mass flow rates, over 10 K-type and R-type

103 thermocouples with data acquisition system (16 bits, 48 channels, 0.1 Hz).

104 A permeation test cell contains the porous sample (Fig. 1). This cell is inserted inside the

105 furnace of the COMPARER bench and it is connected to the fluid supply system and to the

106 suitable sensors. The permeable material bounds the cell in two high and low pressure

107 chambers (upstream and downstream to the porous material respectively). An inlet pipe

108 provides the fuel into the system. This cell is connected to a dynamic sampling system to get

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 μm and a pore diameter of 4.1 μm. Further geometrical

115 information can be found in Gascoin *et al.* [4].

<p align="center">***Figure 1 should be placed here***</p>

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=725K, 765K and 810K. 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).

### 3. Experimental results

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

*Figure 2 should be placed here*

### 4. Construction of ANN models

4.1 Construction of the database

ANN models learn the relationship between the input and the output parameters as a result of training with previously recorded data. The database was built using experimental data which are obtained from the developed experimental bench with input parameters: test time ($t$), operating inlet pressure ($P_{in}$), inlet fuel mass flow rate ($q_{in}$) and temperature ($T$) varying in a range of representative values: between 0 and 858s for $t$; between 3.3MPa and 3.8MPa for $P_{in}$; between 0.000033 kg/s and 0.0001 kg/s for $q_{in}$ and 725K, 765K and 810K for $T$. Totally, the database contains an appreciable size of 979 experimental test points.

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.

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

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*

177

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:

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

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.

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

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:

$$ASE = \frac{1}{p} \times \frac{1}{s} \times \sum_{q=1}^{s} \sum_{k=1}^{p} \left( t_{qk} - O_{qk} \right)^2 \tag{4}$$

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).

205

*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 $\{X_1, X_2, ..., X_n\}$ to outputs $\{O_1, O_2,$

215 $..., O_p\}$ and containing one hidden layer with m hidden nodes will be noted:

$$\{O_1, O_2, ..., O_p\} = \text{ANN}_{n\square m\square p} \{X_1, X_2, ..., X_n\} \tag{5}$$

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.

$$\{P_{out}\} = ANN_{4\text{-}9\text{-}1} \ \{t, P_{in}, q_{in}, T\} \tag{6}$$

228       The ASE values for the training, testing and validation phases for the optimal artificial

229 neural network model ($ANN_{4\text{-}9\text{-}1}$) are respectively 0.000114, 0.000101 and 0.000132.

230                        ***Figure 5 should be placed here***

231 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):

$$R^2 = 1 - \frac{\dfrac{1}{N}\displaystyle\sum_{i=1}^{N}\left(Y_i - \hat{Y_i}\right)^2}{\dfrac{1}{N-1}\displaystyle\sum_{i=1}^{N}\left(Y_i - \overline{Y_i}\right)^2} \tag{7}$$

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 $\overline{Y_i}$ is the mean of the $N$ target values. $R^2$ coefficients close to unity indicate a high degree

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

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

***Figure 6 should be placed here***

***Table 1 should be placed here***

An application of ANN is now proposed in the following part. Considering a constant inlet pressure at 3.6 MPa, it is now possible to investigate the chemical effect within the range of 725K-810K. It should be noticed that fixing arbitrarily the inlet pressure imposes the outlet pressure to decrease, which simulate the pressure drop increase. The evolution of the predicted outlet pressure ($P_{out}$) using BPNN as a function of time and temperature inside the

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.

277 ***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

291 pressure should remain constant.

## 6. Conclusion

293 In this article, an artificial neural networks tool has been used to simulate the transient

294 pressure drop of n-dodecane under pyrolysis conditions and crossing a metallic porous

295 material (Stainless steel). Based on experimental data, the optimum architecture of artificial

296 neural network was trained and validated, in order to generalise the prediction of the pressure

297 drop under clogging configurations not included in the database for difficult access reasons.

298 The validation showed excellent performance of this ANN model for the prediction of

299 dodecane transfer in the porous material ($R^2 > 0.983$). An example of application was

300 presented to detect the temperature at which chemistry starts to strongly impact the fluid flow

301 within the porous medium. It was found that a turning point around 760 K-770K has to be

302 expected in terms of clogging when using n-dodecane at 3.6 MPa in stainless steel medium.

303 This study is a contribution to the growing evidence of the benefits of ANN models in

304 Aeronautical engineering. This important result may be applied to automate pressure drop

305 estimations, which are used in space flight applications, without prior knowledge of material

306 parameters and particularly for materials with transient changing properties.

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393

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

395

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

397 **Fig. 2** Measured pressure drop variations with the measured fuel mass flow rate and

398 experiment time for T=725K.

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

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

401 **Fig. 5** Average squared error (ASE) variations with the number of hidden nodes for the

402 testing data subset.

403 **Fig. 6** Comparison between target and predicted values for $P_{out}$ using BPNN (model 1) and

404 multi-linear regression (model 2) for all data subset.

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

406 $P_{in} = 3.6$MPa.

407

**Table 1**

**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 2**
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Figure 3

**Figure 4**
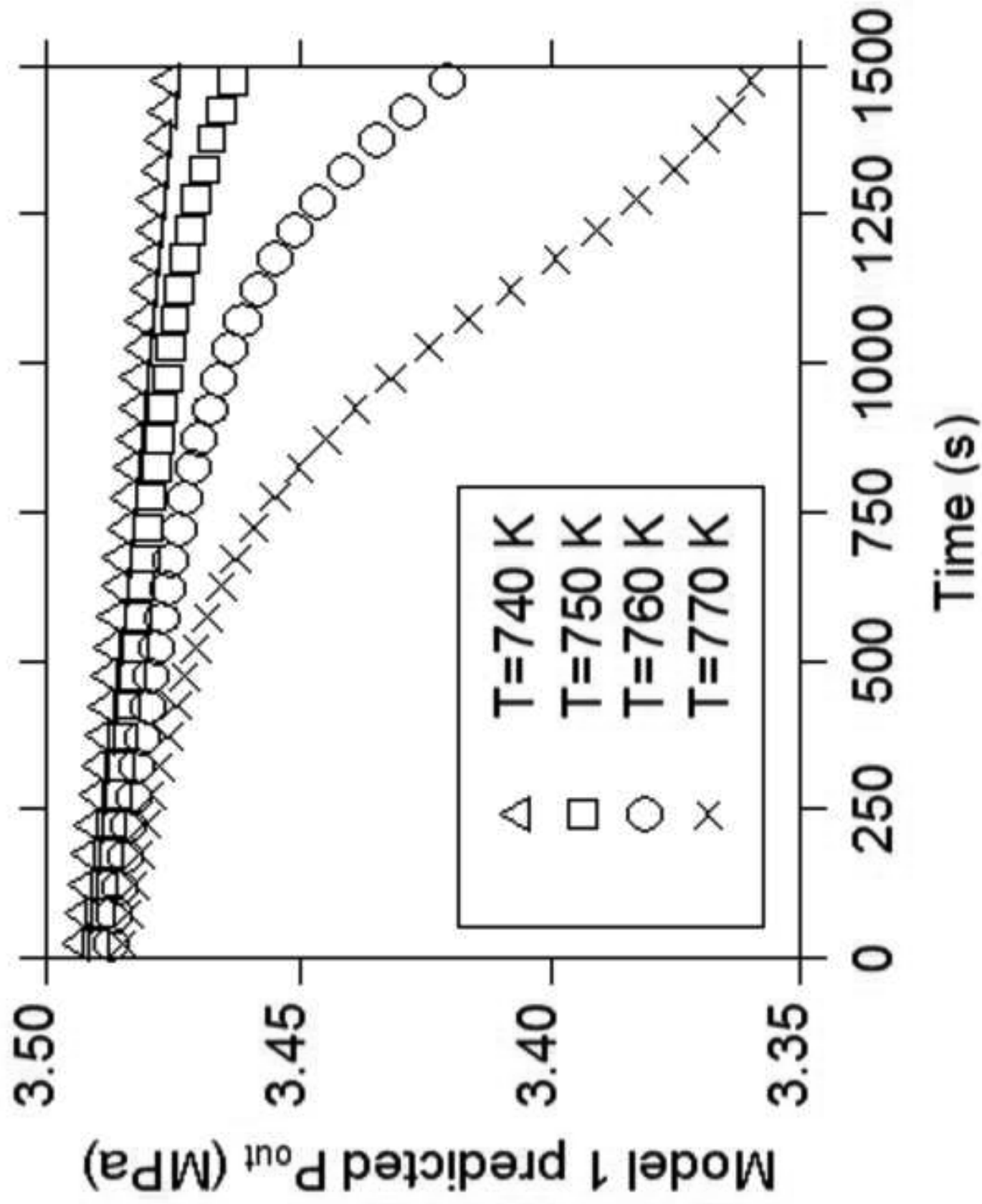
**<u>Highlights</u> :**

- 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.