



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 clog the pores of the material and thus strongly affect the cooling efficiency. The pressure drop is one of the indicators 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 metallic material. The ANN is developed using experimental data obtained from an experimental bench, which enables 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 back propagation (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.

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1. Introduction

The development of hypersonic vehicles for future access to space or civil transport applications motivates the study of situations in which occurs an important heating of the engine and air frame. At flight speeds near Mach 4 and above, the air taken on board of these vehicles will be too hot to cool the engines and airframe. Therefore, using fuel as cooling fluid is applicable, in the frame of the regenerative cooling technique [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, composites containing a 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 transfer [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

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

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

As a consequence in this paper, we have used an approach based on the artificial neural networks (ANN) for simulating the transient changes of the pressure drop of n-dodecane (reactive fluid) passing through the porous material (Stainless Steel) by taking into account both high temperature and high pressure conditions. This work intends to indirectly predict the chemical effect of fuel pyrolysis, of coking and of clogging on the permeation process which directly controls the cooling efficiency. The description of the same numerical approach applied to another set of gas mixture (inert) and flow conditions can be found in a previous study [7]. Over the last two decades, ANN have been successfully used by many researchers for a wide range of engineering applications [27–29]. ANN is based on the substitution of the complex simulation model by an approximation of the input-output relationship. ANN has the advantage over regression that the form of the model needs not to be pre-determined [30]. In addition, ANN can theoretically approximate any function to any level of accuracy, which is very interesting when the governing physical mechanisms are non-linear like in high velocity fluid flow in porous materials. The database was built with four input parameters (experiment time, inlet fuel mass flow rate, inlet operating pressure and the uniform temperature) and with the outlet fuel pressure as the output parameter. The results obtained experimentally are used to construct, to optimize and to validate the model. This artificial neural network has been trained and tested on this database using the error backpropagation algorithm and cross validation. The performance of the ANN model is compared with a multilinear regression approximation method.

2. Material

2.1. Experimental permeation bench

The COMPAREER pyrolysis test bench (Fig. 1) is used to pressurize and to heat the fuel under flow conditions [4]. Its main characteristics are the following:

- Maximum operating conditions: 1800 K, 8 MPa, 0.0006 kg s⁻¹ for liquid fuel and 0.006 kg s⁻¹ for gas.

- Sensors: 5 pressure transducers, 5 mass flow rates, over 10 K-type and R-type thermocouples with data acquisition system (16 bits, 48 channels, 0.1 Hz).

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

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

2.2. Experimental test condition

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

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

3. Experimental results

We present in this section an experimental test result obtained for $T = 725$ K. 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 ($T = 725$ K). 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.

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