THE USE OF PLASMA AND NEURAL MODELLING TO OPTIMISE THE APPLICATION OF A REPELLENT COATING TO DISPOSABLE SURGICAL GARMENTS

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Abstract

The modification of the surface properties of and the application of coatings to textile materials by means of exposure to plasma has attracted much attention in recent years. The advantages of using excited gases include low process cost and duration, and the avoidance of effluents such as solvents or chlorine. Low-pressure plasma treatment with hexafluoroethane has been shown to create a hydrophobic surface on cotton, which would normally be hydrophilic. Cotton is a popular material for surgical garments and drapes because of its comfort and low cost. The acquisition of hydrophobic behaviour will provide haemo-repellancy and the prevention of bacterial attachment.

This paper describes a series of designed experiments to vary three parameters for the plasma process, gas concentration, power and duration, and to measure the resulting degrees of hydrophobic behaviour at the cotton surface by means of observing water droplets. Neural networks can provide rapid development of simulation models of processes by adaptation to observed conditions as inputs and the results as outputs. The data from the plasma trials has been used to develop a neural model to predict surface hydrophobic behaviour. The model is itself optimised for interpolative ability, and allows a search to be made through the data space to find the best possible combination of the process parameters to encourage optimal surface treatment, and thus make the cotton most hydrophobic.

The work indicates how the environmentally-friendly approach of plasma treatment can be used to provide garments and drapes for surgery which are comfortable but also protective.

Introduction

Plasma treatment of textile materials

A plasma is a partially-ionised gas normally generated by an electrical discharge at near-ambient temperatures and reduced pressures. Details of the process are presented in the preface of [1]. The components present will include ions, free electrons, photons, neutral atoms and molecules in ground and excited states, and there is a high likelihood of surface interaction with organic substrates. This interaction may be physical, for example in the cleaning of organic contaminants from the surface; or the effect may be chemical, for example in the bonding of hydroxyl groups to the surface. In the treatment of textile substrates, the cleaning effect can modify wettability and dye uptake, and the free radicals can incorporate atoms which also change the surface, for example making a hydrophilic material into a hydrophobic one.

The main attraction of plasma in industrial processing is the avoidance of chemical effluents. Other advantages include: low cost, rapid reaction times, high cleaning efficiency, low consumption of gas due to physical effects, and the enclosed and dry nature of the process. Fluorocarbons have been used to reduce the wettability of synthetic polymers such as polyethylene [1,2]; this paper describes the plasma fluorination of cotton fabric with the objective of making this high-comfort, low-cost, cellulosic polymer water-repellent. Because of the complex nature of the plasma as a chemical and physical modifier, the effects of the plasma under varying conditions of the process were modelled by neural networks, adaptive systems which are based on observed behaviour rather than recognised rules or explicit functions. It was considered that rapid modelling would help to ensure efficient investigation of the data space, as well as clarification of the conditions required to provide the optimal degree of repellency.
Neural networks

The building of models or simulations of industrial processes offers many benefits. These include: forecasting the outputs from untried combinations of parameters values, unlimited experimentation and searching at no cost, process improvements through studying the model, minimised downtime for trials, training for operatives, and investigation of hazardous events. In recent years the availability of fast personal computers has provided software tools which can enable researchers to build computer simulations of the relationships observed in sets of observations by adaptation to the data. The internal functions which result from ‘training’ neural networks may well be too complex to capture by mathematical models or express as rules; nevertheless, if neural networks are trained on examples which are a good statistical representation of the parameter space and are also optimised in their own design, the resulting models of processes are likely to be able to provide all the model features which are presented above.

Experimental method

Data collection

The material to be treated consisted of pieces of natural cotton woven fabric, each 6 cm square and kept under controlled conditions of humidity. The fluorinating gas was hexafluoroethane C₂F₆. The plasma system used was the CD600 PC by Europlasma nv [6]. The equipment has six main parts: the vacuum chamber where the samples are exposed to the plasma, the vacuum pump, high frequency generator, power distribution rack, PC (computer) rack, and measuring equipment required to set up and maintain the required conditions and gas state in the chamber. The mode of operation used was as follows: the operator set the power level, time of treatment and flow rate of the gas feed, and the system automatically controlled the pressure in the chamber to maintain the plasma state. The treatment process for each sample was as follows. The sample was placed at a standard location on the multilayer sample frame. This is an aluminium electrode of alternating positive and ground-connected layers between which the gas discharges. Preliminary experiments were conducted to find a suitable sample position, which was where the surface effect on the cotton (see below for the repellency testing) appeared to be greatest for a standard (median) set of treatment conditions. The power level (watts), treatment time (seconds), and flow rate (SLM or standard litres per minute) were entered by the operator, and the process was started to evacuate the chamber to 100 mTorr, introduce the gas and initiate the plasma. On completion, the sample was quickly removed to controlled conditions of temperature and humidity to await repellency testing. The repellency of the cotton was quantified from the spread of droplets. This approach was considered preferable to that using the contact angle, because variations in the weave structure appeared to affect the time taken for each drop to spread to its maximum size.

Image analysis was used to provide objectivity and image quality, since the woven nature (that is, with capillary actions in the warp and weft dimensions) of the material encouraged irregularity of the final drop areas. The process for each sample was as follows. First, 20 µl of an aqueous solution of the dye Direct Red 81 was pipetted from 3 cm onto the surface at several separate locations on the fabric, and allowed to evaporate to dryness under controlled conditions of temperature and humidity. The drying took up to 60 minutes, allowing the droplet to spread out into the fabric according to the surface encountered. A CCD camera and image analysis software (Semper 6+) was used to capture square-pixel images of each of the red areas on the cotton. Each image was refined by thresholding and particle analysis, which provided objective values for perimeter, circularity, and area. The area value was selected as the most appropriate for irregular shapes, and the mean final drop area was recorded for each treated fabric. To provide a baseline of non-repellency, a sample was treated for 2 minutes with oxygen plasma at 100 watts power and SLM 0.17 to clean off any spin finish and other contaminants but provide no hydrophobic layer, then treated as in the process above. An index of repellency (Final Area Index or FAI) was calculated for all the treated samples:

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\text{FAI} = \frac{\text{Final drop area of oxygen-cleaned sample}}{\text{Final drop area of this sample}}
\]
Neural modelling

The experimental approach regarding the neural modelling involved three improvement stages. In the first, the data from 52 trials was used to train an MLP model. The weights adjustment process was implemented in the NeuFrame neural software tool [7]. Correlation analysis suggested that all three experimental parameters (power, time, and SLM) were positively linked to the FAI results, although power and time appeared to have the most effect on repellency. Accordingly, the training set of trials varied all three parameters within reasonable ranges available with the CD600 PC, in a pseudo-random distribution to provide a comprehensive but concise view of the process. Once these experiments had been conducted, their FAI values constituted the targets set for supervised training of the MLP neural network. The measured final drop areas ranged from 37,646 pixels to 1,708 pixels, corresponding to FAI values of 1.07 to 23.66 respectively. It was found that an MLP with three nodes in the hidden layer, that is, with topology \( \{3,3,1\} \) would train down to a mean error or distance from the targets of 2.82 FAI, but no further. An adaptive model should be trained only to the stage where it fits the trend of the data. Beyond this stage the model may overfit the data, and become a poor predictor for points which do not correspond exactly to those included in the training sample. In general, the number of weights in the MLP should be no more than 0.1 of the number of training examples, which should be large enough to allow partitioning into a training set, a validation set, and a test set. The process of optimising a neural network for generalisation is described in detail in [8]. Although the \( \{3,3,1\} \) with 12 connection weights probably overfit the 52 trial points, a plot of the model outputs against the observed FAI values was useful because it showed that the first stage of data consisted of two clusters: a set of points with very low repellencies, and a smaller set of points with much higher repellencies. It was decided to enrich the data set with more median repellency points, and also more points where the highest repellencies appeared likely. A set of 1,000 random inputs of power, time, and SLM was input to the MLP and the FAI values predicted were sorted, so that parameter sets would be identified to provide the required improvements to the training data.

In the second stage of improvement, an MLP trained on the now enriched data set of 67 trials and results was optimised for generalisation and harnessed in software developed in-house to find the parameters values which would optimise repellency. Single random holdouts (trials excluded from the training to provide tests) were used to find the optimal training error and optimal hidden layer size for this MLP model. It was found that a \( \{3,6,1\} \) network trained to a mean error of 1.2 FAI performed best on predicting the repellencies for the holdout tests, and this model was ‘run’ 160,000 times to predict the experimental parameters which would provide the highest repellency. The FAI optimum from repeated 160K batches was 29.6. The settings of power, time, and SLM to provide this, along with additional points of expected high repellency, were added to the 67 trials set. It was found that the observed FAI for the model's best prediction was 39.93, suggesting that the neural model offered a very conservative forecast.

The new expanded training data included the 67 trials plus the additional ‘good’ points. It was also decided to clarify the process logic and help learning by incorporating the baseline experiment (zero values for the three \( C_2F_6 \) treatment parameters and a target FAI of unity) into the data. In this third phase of improvement, 80 sets of plasma treatment parameters and FAI results were used to develop and optimise an MLP model. This was found to be quite small, \( \{3,2,1\} \) with only 8 connection weights (see Figure 1 below), and the best error state for generalisation was a mean error of 3.27 FAI in predicting the observed repellency indices.

![Figure 1: The final neural network model for predicting repellency](image-url)
At this distance from the training points, $R^2$ was equal to 0.79 for the regression line relating the predicted FAI values and the observed FAI values. Using this improved version of the simulation model, the 160,000 trial search engine arrived at a new prediction of optimal repellency: an FAI of 36.29 using a power of 300 watts, treatment time of 300 seconds, and SLM of 0.1. Considering the tendency (noting the results for the first two stages of improvement above) for the models to be conservative in predictions for high repellency points, it might be expected that the observed FAI should exceed 50 for these settings, which were the maxima for the respective parameter ranges, and not included in the 80 trials.

Because the number of input parameters was small, it was possible to visualise the responses of the plasma treatment process to varying conditions. The final simulation model provided curves for repellency against treatment time which reflected the observed behaviour, except for the conservative tendency which tended to underestimate the best results by about one-third. This was probably because the training data as a population was skewed towards low-repellency trials. Examples of these response curves are shown below in Figures 2 to 4:

**Figure 2:** Effect of time and litres per minute at 200 watts power

**Figure 3:** Effect of time and litres per minute at 300 watts power

**Figure 4:** Effect of time and litres per minute at 400 watts power
At low power, a small effect on surface repellency was noted, but with the superiority of using a high SLM gas concentration being more evident after longer treatments. Using 300 watts, a marked surface effect over time was observed for both levels of SLM, with the benefit of high SLM still evident with longer treatment times. The best repellencies were achieved at the highest power, 400 watts; however, the responses suggested less benefit from high SLM and diminishing returns from the application of high power for longer durations.

**Barrier behaviour**

The FAI results indicated (as a continuous dependant variable) the reluctance of the fluorinated cotton to absorb the aqueous solution, but the essential requirement for a protective surgical garment would be that the droplets should not be allowed to pass through the fabric to contact the wearer. On examination of the samples, it was found that those of final drop area approximating 1000 pixels or less (FAI 39 or more) allowed no passage of the dye through the fabric. This suggested that the plasma treatment would provide an effective barrier to aqueous contamination as long as a threshold of surface fluorination was reached; from the responses of the model, this would correspond to any FAI of at least 39, much less than the predicted best of FAI 50 described above. Allowing for the conservatism of the model, the above responses (in the charts Figures 3, 4, 5) suggested that the barrier would be achieved by conditions such as 300 watts at 300 seconds with 0.1 SLM (the predicted FAI of 33 would be expected to over 39 in observable behaviour), 400 watts for 180 seconds at 0.1 SLM, or 400 watts for 270 seconds and 0.05 SLM. Considering input energy as an important commercial constraint, the second of these three might be preferred.

**Conclusions**

Although plasma processes involve complex chemical and physical reactions, it was found that the fluorination of cotton fabric could be controlled and optimised using commercial plasma equipment and adaptive modelling. The use of neural networks can provide models to accelerate progress toward optimal solutions and minimise the volume of experiments without reliance on simplifying assumptions and mathematical analysis of such complex systems. This work has shown that a low-cost, environmentally-friendly process is available to allow the comfort of a natural material to be utilised by nurses and theatre staff whose safety depends on the hydrophobic nature of their clothing.

**References**

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