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To cite this article: J F Lin *et al* 2018 *J. Phys.: Conf. Ser.* **1039** 012034

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Stepwise Regression Modeling of the Retardance in Dextran-Citrate Coated Ferrofluids

J F Lin¹, J J Sheu² and Y Y Yang¹

¹ Department of Industrial Design, Far East University, No. 49, Zhonghua Rd., Xinshi Dist., Tainan City 74448, Taiwan R.O.C.

² Department of Mechanical Engineering, Southern Taiwan University of Science and Technology, No. 1, Nantai St., Yungkang Dist., Tainan City 71005, Taiwan R.O.C.

E-mail: jacklin@mail.feu.edu.tw

Abstract. Double-layer coating citrate (citric acid, CA) and dextran on Fe₃O₄ ferrofluids (FFs) have been conducted for biomedical application such as hyperthermia. In a previous study, the magneto-optical retardance of dextran-citrate (DC) coated FFs was measured by a Stokes polarimeter. At this work, instead of using the multiple regression (MR) analysis, we adopted the stepwise regression to model the retardance of DC coated FFs in a systematic way. From the results of stepwise regression by MATLAB, the developed model had highly predictable ability owing to F of 667.365 and had a high correlation coefficient R of 0.99989. The average absolute error of predicted retardances to measured retardances was just 0.85%. Using the genetic algorithm (GA) in MATLAB, the optimized parametric combination was determined as [0.075, 75.856, 0.323, 0.65] corresponding to Fe₃O₄ concentration, coating temperature, CA mass, and dextran mass. The maximum retardance was found as 119.653°, close to those of [0.075, 75.794, 0.322, 0.65] and 119.658° obtained by Fmincon function and a relative error of -0.004%. Above all, the second order stepwise regression method was useful to model the retardance of DC coated FFs, and the maximum global retardance was determined by GA.

1. Introduction

Citrate (citric acid, CA) or dextran coated Fe₃O₄ ferrofluids (FFs) have been conducted for biomedical application such as hyperthermia [1, 2]. It has been known that the surface of the magnetic nanoparticles (MNPs) can be stabilized in an aqueous dispersion by the adsorption of CA or dextran. Effect of synthesis conditions on the properties of CA- and dextran-coated iron oxide nanoparticles was discussed [3-5]. The stabilized biocompatible CA coated FF was successfully produced with high retardance and magnetization in the previous study [4]. The retardance values (magneto-optical property as the phase retardation of linearly birefringent medium, such as quartz and certain liquid crystals) of FFs were measured by a developed Stokes polarimeter [4]. In the recent work, the dextran-citrate (DC) coated FFs have been developed, and we investigate not only magnetic retardance but also heating performance of the DC coated FFs for the hyperthermia application [2].

For the modeling and prediction of the retardance in FFs, multiple regression (MR) and optimization of retardance in CA coated FFs were executed by Taguchi method and Microsoft Excel, and the F value of regression model was large enough [6]. However, the modeling of retardance executed by Microsoft Excel was not in a systematic way. Further, the stepwise regression executed by MATLAB was successful for modeling the retardance of CA coated FFs [7]. The regression model had highly predictable ability and had a high correlation coefficient of one. Moreover, genetic



algorithm (GA) solver (in MATLAB® Optimization Toolbox) was used to find the global maximum retardance value efficiently.

In this study, the second order stepwise regression executed by MATLAB was successfully used to model the retardance of DC coated FFs. The regression model had highly predictable ability and had a high correlation coefficient of 0.99989. Above all, two optimization techniques, including Fmincon function and GA solver (both in MATLAB® Optimization Toolbox), were used to find the local and global maximum retardance value, respectively. Then the DC coated FFs could be more useful in practical applications such as hyperthermia.

2. Method

In this study, the methods including uniform design method, stepwise regression method, Fmincon function and genetic algorithm were briefly introduced.

2.1. Uniform design method

Uniform design (UD) method is based on uniform distribution in number theory. It makes experiment points uniformly scattered in the range of experiment parameters for getting more information by less experiment [2]. The optimal synthesis condition of DC coated Fe₃O₄ FFs with high retardance was determined by the UD and the test results of retardance were shown as table 1 [2].

Table 1. Uniform design and test results of retardance.

Test No.	Level of parameter				
	Fe ₃ O ₄ (g/ml)	Temp. (°C)	CA (g)	Dextran (g)	Retardance (deg)
1	1(6/80)	2(50)	4(0.30)	7(0.65)	27.8628
2	2(6/80)	4(60)	8(0.36)	5(0.60)	13.5872
3	3(6/90)	6(70)	3(0.24)	3(0.55)	12.2155
4	4(6/90)	8(80)	7(0.36)	1(0.55)	31.8867
5	5(6/100)	1(45)	2(0.24)	8(0.65)	7.1405
6	6(6/100)	3(55)	6(0.30)	6(0.60)	26.5201
7	7(6/110)	5(65)	1(0.24)	4(0.60)	30.3393
8	8(6/110)	7(75)	5(0.30)	2(0.55)	20.0765
9	9(6/120)	9(85)	9(0.36)	9(0.65)	56.7898

2.2. Stepwise regression

While dealing with large number of independent variables, it is of significant importance to determine the best combination of these variables to predict the dependent variable [8]. Stepwise regression method is a routine statistic technique used for variable selection and is a combination of forward and backward procedures. The method starts with an initial model which includes a subset of all the candidate variables. And then, a so-called stepping procedure which iteratively altering the model established at the previous step by adding or removing variables in accordance with the stepping criteria is used in order to add significant variables or remove insignificant variables.

2.3. Fmincon function and genetic algorithm

The Fmincon function (Find MINimum of CONstraint nonlinear multivariable function, a deterministic gradient-based method) was in-built in MATLAB and used for optimization [9]. It uses sequential quadratic programming (SQP) method for optimization. SQP methods represent the state of the art in nonlinear programming methods. Based on the works of Biggs, Han and Powell; an SQP method mimics Newton's method for constraint optimization. It is an iterative method of starting from some initial point and converging to a constrained local minimum [9]. It was noted that different

algorithms could be chosen, including interior point, active set, and trust region reflective. And this technique has the disadvantage that the solution found could be a local minimum of the function depending on the initial estimates of the parameters. Moreover, the genetic algorithm (GA) technique is based on the natural process of evolution to solve optimization and search problems. There are three main operators in GA which are reproduction, crossover and mutation [10]. GAs were pioneered by Holland in the 1960s and 70s and have emerged as a highly effective technique for solving a wide variety of optimization problems [10]. Above all, the global maximum could be found by GA.

3. Results and discussions

3.1. Results of stepwise regression

Results of the second order stepwise regression by MATLAB are shown in figure 1, the model has highly predictable ability owing to F of 667.365 and has a high correlation coefficient R of 0.99989, which is suggested that this regression model is statistically significant and gives useful information about the response variable. The average absolute error of predicted retardances to measured retardances is less as 0.85%. The regression equation is given as:

$$\text{Retardance} = -415.933 + 1760.06X_3 - 0.176898X_2^2 - 8857.9X_3^2 - 300.709X_4^2 + 25.0825X_1X_2 + 52.1548X_2X_3 + 12.4852X_2X_4 \tag{1}$$

As shown in figure 1 and table 2, we can see the meaningfulness degrees of input variables. This degree of meaningfulness is determined via being value of p -val below 0.05. Thus meaningfulness ranking of input variables is determined as $7(X_3^2)$, $13(X_2X_4)$, $6(X_2^2)$, $12(X_2X_3)$, $9(X_1X_2)$, $3(X_3)$, and $8(X_4^2)$. As shown in figure 1, the RMSE (Root Mean Square Error) value is 0.609. Further, the R^2 value is determined as 0.999786 (close to 1). It is indicated that the ability of prediction in the second order stepwise regression is excellent.

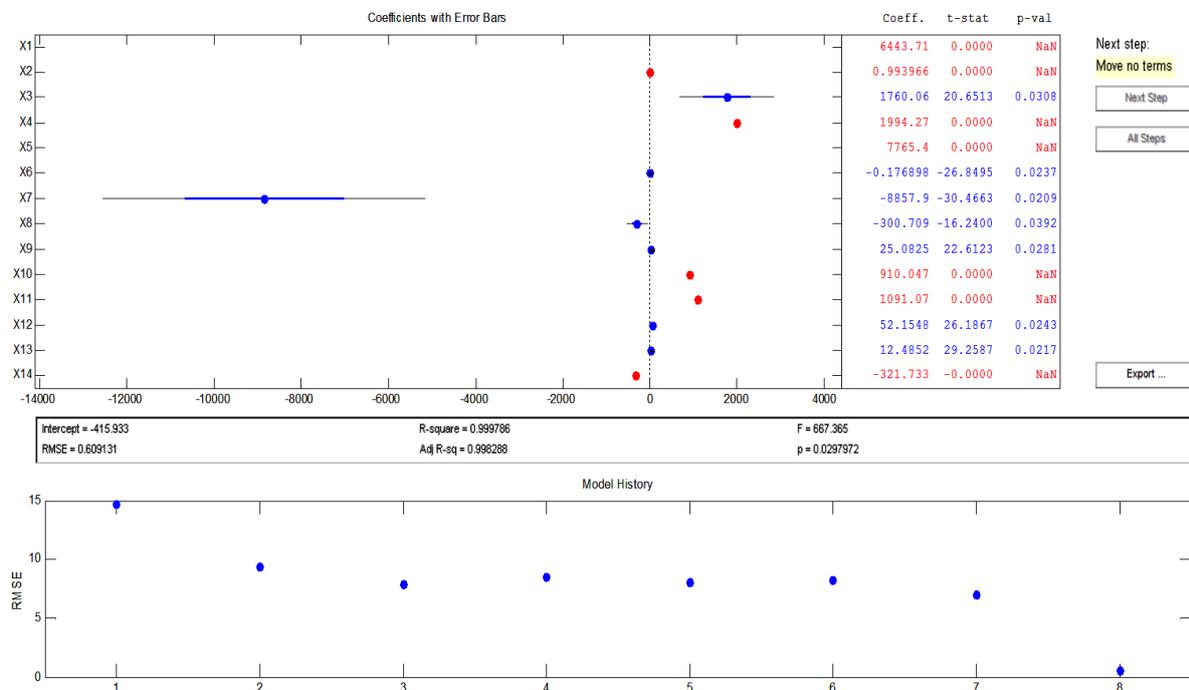


Figure 1. Results of the second order stepwise regression.

The significance t -test of each variable is listed in table 2. It is seen that the significant influence of each term on the retardance of DC coated FFs is given by: $X_3^2 > X_2X_4 > X_2^2 > X_2X_3 > X_1X_2 > X_3 > X_4^2$. This indicates that the effect of CA mass (X_3) on the retardance is of the most significance and followed by dextran mass (X_4), coating temperature (X_2), and Fe_3O_4 concentration (X_1). The relative

influence of cross correlations on the retardance of DC coated FFs (from examining the magnitude of the P value or the significance level of the cross items in t -test) is given by: $X_2X_4 > X_2X_3 > X_1X_2$. The item of coating temperature (X_2) seems significant in the second order stepwise regression; the X_2 plays an important role in the influence of retardance judging from the X_2X_4 , X_2^2 , X_2X_3 , and X_1X_2 .

Table 2. Results of the second order stepwise regression.

	Coefficient	t -test	P value
X_3	1760.06	20.6513	0.0308
$X_2^2 (X_6)$	-0.176898	-26.8495	0.0237
$X_3^2 (X_7)$	-8857.9	-30.4663	0.0209
$X_4^2 (X_8)$	-300.709	-16.2400	0.0392
$X_1X_2 (X_9)$	25.0825	22.6123	0.0281
$X_2X_3 (X_{12})$	52.1548	26.1867	0.0243
$X_2X_4 (X_{13})$	12.4852	29.2587	0.0217

3.2. Results of optimization using Fmincon function and genetic algorithm

In this study, the start points are chosen as [0.05, 45, 0.24 0.55], [0.05625, 55, 0.27, 0.575], [0.0625, 65, 0.30, 0.60], [0.06875, 75, 0.33, 0.625], and [0.075, 85, 0.36, 0.65] are input into the program in MATLAB Optimization Toolbox subsequently. It is noted that @FitFun830 is obtained by changing the sign of equation (1) and is used to find the minimum value. Hence, the maximum retardance for the five different start points is obtained the same as 119.658° for [0.075, 75.794, 0.322, 0.65]. A graph output using Fmincon function is shown as figure 2 for start points are set as [0.0625, 65, 0.30, 0.60]. The Fmincon function method is efficient and solves the problem directly. It is known that the local maximum or minimum could be found by Fmincon function, and the global extreme could be further found by using GA technique or a hybrid of the GA and Fmincon optimization technique.

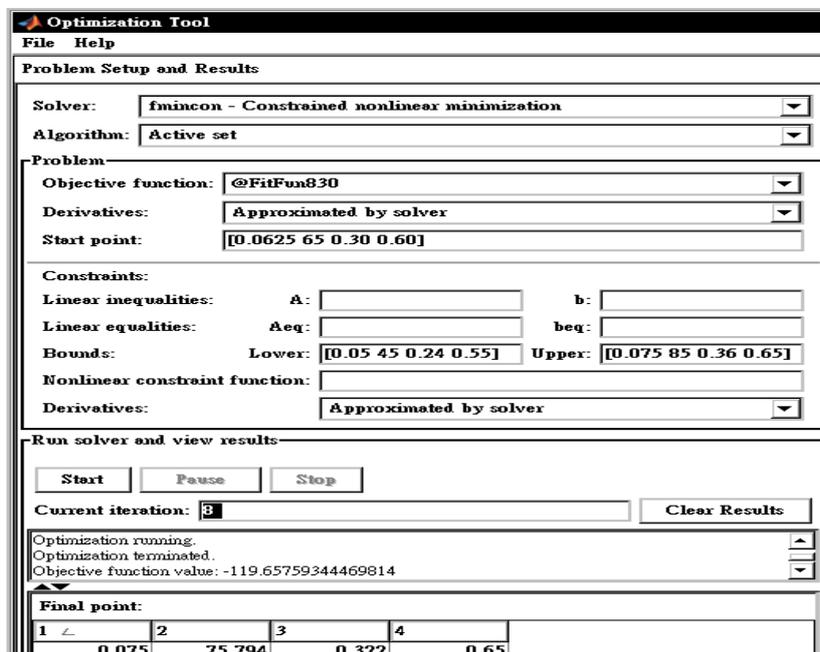


Figure 2. A graph output using the fmincon in MATLAB® Optimization Toolbox.

Further, the optimized parametric combination and maximum retardance of DC coated FFs are determined as [0.075, 75.856, 0.323, 0.65] and 119.653° (the highest retardance in 12 runs of GA and as shown in figure 3), close to that of [0.075, 75.794, 0.322, 0.65] and 119.658° obtained by Fmincon function and a relative error of -0.004% in retardance. The corresponding graph output using GA in

MATLAB® optimization is shown in figure 3. It is noted that the Fitness function as @FitFun830 is obtained by changing the sign of equation (1) and is used to find the minimum value.

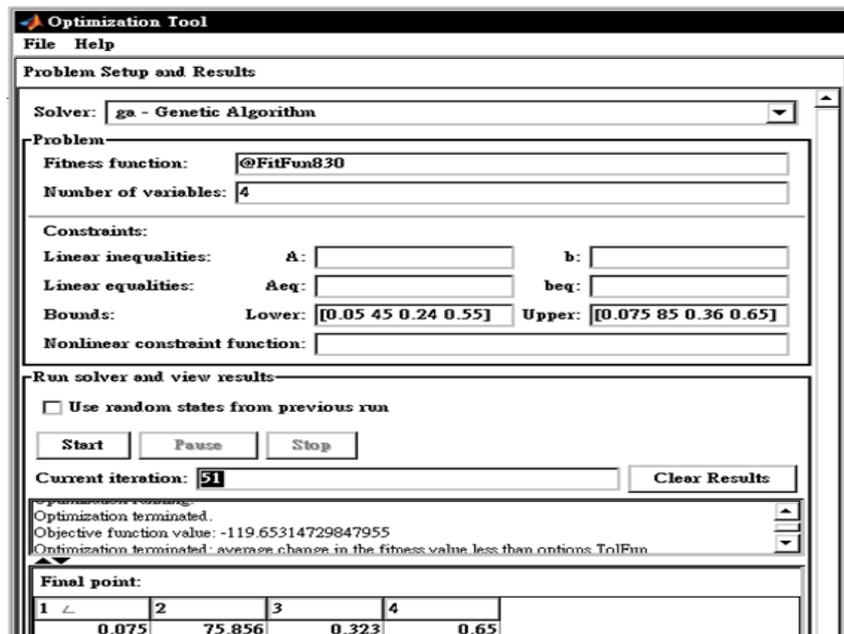


Figure 3. A graph output using the GA in MATLAB® optimization.

4. Conclusions

The second order stepwise regression method was successfully used to model the retardance of DC coated FFs. According to the results of the second order stepwise regression, the F value was obtained as high as 667.365 and had a correlation coefficient of 0.99989; the developed regression model had highly predictable ability. Using the genetic algorithm in MATLAB for 12 runs, the optimized parametric combination with the highest retardance value was determined as [0.075, 75.856, 0.323, 0.65]. The maximum retardance was found as 119.653°, close to those of [0.075, 75.794, 0.322, 0.65] and 119.658° obtained by `fmincon` function in MATLAB and a relative error of -0.004%.

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Acknowledgements

The financial support provided by the Ministry of Science and Technology in Taiwan under MOST 105-2221-E-269-001 and MOST 106-2221-E-269-001 is gratefully acknowledged.