Study of Response Surface Methodology in Predicting Optimum Conditions of Biodiesel Production

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Abstract— The optimum input parameters can be predicted by applying response surface methodology. The various studies show RSM, an effective technique for enhancing the output by creating design of experiments. Applications of RSM technique include manufacturing engineering production engineering, renewable energy etc.

Key words: Optimization, RSM, Design of Experiments

I. Introduction

Optimization is defined as the evaluation of minimum or maximum value of function at particular conditions, where the function represents the desired benefit or effort required. A mathematical model created by each optimization technique is considered an efficient if it predicts the response variable accurately. Optimization of trans-esterification process parameters is one of the most widely studied problems in biodiesel production and is important in terms of producing high biodiesel yield in minimum time. Optimization methods for biodiesel production include trans-esterification process parameters relationship with required objective (biodiesel yield) and predicting of optimum or near optimum conditions of trans-esterification process [Dhingra et al., 2013a; Dhingra et al., 2013b; Dhingra et al., 2014a; Dhingra et al., 2014b; Dhingra et al., 2014c; Dhingra et al., 2014d; Dhingra et al., 2016a; Dhingra et al., 2016b]. The trans-esterification process is affected by numerous controllable and uncontrollable input variables as discussed in the previous chapter.

II. Response Surface Methodology

RSM is a combination of mathematical and statistical techniques in building the empirical model. The experiments are carefully designed, with the main objective of optimizing the response (output parameter) which is affected by independent parameters (input parameters). RSM was developed by Box and Wilson in 1951 while working on a chemical investigation based on the pioneer works of R. A. Fisher (1931) in connection with agricultural experimentation [Box and Hunter, 1957; Box and Benkhen, 1960]. A series of experiments (runs) are performed, where changes in the input parameters are made in order to investigate the reasons for changes in response (output parameter). Initially, RSM was developed only for model responses of experiments (Box and Hunter, 1957) which further migrated into the numerical experiments modelling. The random errors are often produced in RSM.

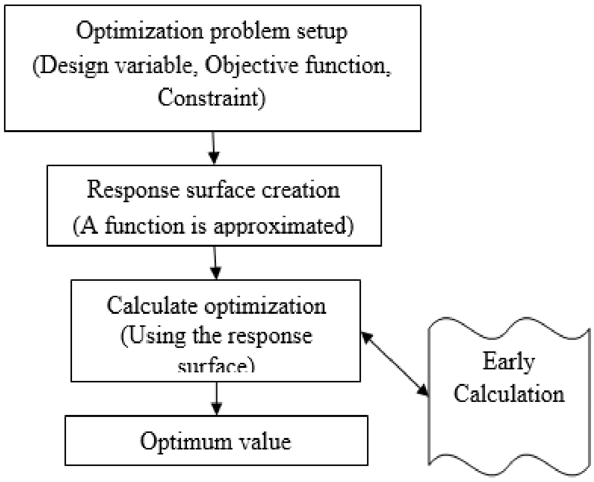

Fig. 1: Steps of applying response surface methodology in achieving the optimization

The response surface function gives a complete outline of the experiments performed and enables to predict the response of the experiments with regards to controllable input parameters that are not tested actually [Palanikumar, 2008]. It also predicts the relationship between response surfaces and controllable input parameters. Furthermore, it is having an ability to develop the predictive model. The methodology has been successfully applied in chemical field, production engineering works, renewable energy fields (such as biodiesel development, biodiesel fuelled engine tests, solar energy) etc. The procedure of applying RSM is as follows [Gunaraj and Murugan, 1999]:

- Design of experiments for reliable and adequate measurement of required response.
- Development of non-linear mathematical response surfaces with best fittings.
- Prediction of optimum combination sets of experimentation parameters that give maximum or minimum value of response.
- Representation of direct and interaction effects of input parameters from two and three dimensional plots.

The complete methodology of RSM is shown in figure 1.

III. Design of Experiments (DoE)

Experiments are designed on the basis of selected input parameters for evaluation of response and are originally applied to only physical experiments but it can applied to numerical experiments also. The main objective of DoE is to select the points at which the response is evaluated.

The criteria for optimum design of experiments are allied with mathematical model of the process and these models are polynomial with different structures which are unknown [Montgomery et al., 2001; Myers and Montgomery, 2002]. Hence, for every particular problem corresponding experiments are designed and have large effect on accuracy of approximation and cost of building response surface [Antony, 2003; Adler et al., 1975; Peterson, 1985; Jivani et al., 2011].

In traditional DoE, preliminary investigation of process parameters are carried out by applying one factor a time (OFAT) approach [Roy, 2001]. By this method, significant parameters are found by changing one parameter keeping others at midlevel of ranges selected and corresponding response parameters are measured. Those parameters which affect more to the response are considered in design of experiments [Ferreira et al., 2007]. Design Expert 6.0.8® software has been considered in the present work for design of experiments using central composite rotatable design (CCRD) of RSM.

IV. Central Composite Rotatable Design (CCRD) and Development of Regression Model

A non-linear mathematic model can be constructed efficiently with central composite rotatable design (CCRD) [Gunawan et al., 2005]. CCRD is a first order (2N) design which is having a centre point, factorial and axial points to allow evaluation of tuning parameters of non-linear model [Montgomery, 2002].

The tuning parameters are the regression coefficients included in the approximation model and are evaluated by minimizing predicted residual sum of squares. For three design parameters, there are 2N (= 8) factorial points, 2N (= 6) axial points and 1 centre point. One of the important advantages for applying CCRD is the reduction of experiments by choosing full, half and small fraction in Design Expert 6.0.8® software. Also it uses the five levels of the input parameters and is surrounded in the design by means of factorial, axial and centre points. In the present research work, ‘22’ experiments with one replication were performed using CCRD for production of each biodiesel. The number of experiments suggested by CCRD (22) was much smaller than suggested by full factorial design (243). In addition ‘15’ experiments with one replication were performed for each biodiesel using CCRD for evaluation of biodiesel performance in a single cylinder direct injection diesel engine.

To check the significance of a model, ‘p’ test is performed in the analysis of variance (ANOVA). It is the probability test of all the coefficient terms in the predicted regression equations. If p-value is less than 0.05, the model is significant at 95 % confidence level. Also the formation of quadratic equations for the response parameters show that there exist an optimum value at particular input parameters. The response plots are drawn by considering input parameters that affect the output. The values of R2, adjusted R2 and predicted R2 close to ‘1’ indicate that error between actual and predicted responses is less. Adequate precision measures the signal to noise ratio. A ratio greater than 4 is desirable. So, the model can be used to navigate the design space. Moreover small predicted residual sum of square (PRESS) values of predicted models shows that model predictions are closer to the experimental values.

A regression equation of second order is generated by using Design Expert 6.0.8® software and initially the response is fitted to the parameters via multiple regressions. The excellence to the fit of the model is evaluated using the ANOVA and coefficients of determination [Gunaraj and Murugan, 1999]. The generalized equation of the quadratic response model is:

$$Y = \beta_0 + \sum \beta_i x_i + \sum \beta_{ii} x_i^{\,2} + \sum \beta_{jj} x_i x_j \qquad \text{..... (1)}$$

Where ‘Y’ is predicted response parameter, i and j are the linear and quadratic coefficients respectively, β is the regression coefficient of the model and xi, xj (i=1, 5; j=1, 5) indicate the independent parameters (reaction conditions). The predictive ability and accuracy of this polynomial model can be checked by the coefficient of determination (R2).

V. Desirability Approach

Desirability describes the multiple response method. D (X) (known as desirability function) transforms the response into d (X) (a free value called desirability) [Hameed et al., 2009]. A desirable value is assigned to each response (objective) which may vary from 0 to 1 (least to most desirable). If the response parameter value is beyond acceptable limits, the desirability is assumed to be zero. If it reaches the target, the value of desirability becomes one. The overall desirability function is created by accumulating desirability of individual objectives [Hajar et al., 2009]. The creation of mathematical model of overall desirability is the common trend which is a function of input parameters. The optimum solutions are used to predict parameter combinations in achieving maximum desirability. The confirmation tests are performed at optimum combination of input parameters (having maximum desirability). These are also mandatory tests for authentication of the predicted results.

VI. Conclusion

Following points are highlighted when Response surface methodology based on central composite design is applied in the problem:

- An effective tool to design the experiments
- To ease in predicting regression equation by the use of statistical tool like design expert 6.0.8
- To enhance the biodiesel production from various oils (edible/non-edible) at optimum conditions of input process parameters

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