Computers and Chemical Engineering 74 (2015) 144–157

Contents lists available at ScienceDirect

Computers and Chemical Engineering

journal homepage: www.elsevier.com/locate/compchemeng

Model-based experimental screening for DOC parameter estimation

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ARTICLE INFO

Article history:
Received 4 August 2014
Received in revised form 4 December 2014
Accepted 7 January 2015
Available online 19 January 2015

Keywords:
Parameter estimation
D-optimal design
Diesel Oxidation Catalyst
Multivariate Data Analysis
Engine rig experiments

ABSTRACT

In the current study a parameter estimation method based on data screening by sensitivity analysis is presented. The method applied Multivariate Data Analysis (MVDA) on a large transient data set to select different subsets on which parameters estimation was performed. The subset was continuously updated as the parameter values developed using Principal Component Analysis (PCA) and D-optimal onion design. The measurement data was taken from a Diesel Oxidation Catalyst (DOC) connected to a full scale engine rig and both kinetic and mass transport parameters were estimated. The methodology was compared to a conventional parameter estimation method and it was concluded that the proposed method achieved a 32% lower residual sum of squares but also that it displayed less tendencies to converge to a local minima. The computational time was however significantly longer for the evaluated method.
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1. Introduction

Common kinetic mechanisms involve a large number of parameters. These mechanisms and the complex interaction between different reactions often result in a high correlation between the kinetic parameters (Bernaerts et al., 2000; Franceschini and Macchietto, 2008b). This severely complicates the parameter estimation process and increases the importance of Design of Experiments (DoE) and the parameter estimation algorithm. DoE in reaction kinetics has a long tradition reaching back to the pioneering work by Box and Lucas (1959), Box and Hunter (1965), Draper and Hunter (1966, 1967a,b), Box (1968), Hill et al. (1968), and Hunter et al. (1969). The focus has however been generally more directed toward steady-state systems rather than transient ones (Franceschini and Macchietto, 2008a) even though the need and benefits of transient experiments have been demonstrated (Goodwin, 1977; Berger et al., 2008). The system studied in the current paper is a reactor model of a full scale Diesel Oxidation Catalyst (DOC) connected to a Heavy Duty Diesel engine rig. The system is transient and the model parameters highly correlated; DoE is therefore of highest importance.

A wide range of catalyst models with varying level of detail can be found in literature. Generally, the kinetics are either described by a microkinetic model (Dumesic et al., 1993; Olsson et al., 2002; Crocoll et al., 2005; Salomons et al., 2006), where every reaction is described by elementary steps, or by more empirical global kinetic models (Voltz et al., 1973; Ansell et al., 1996; Lafossas et al., 2011; Watling et al., 2012). However, the catalyst model is not only defined by the kinetics but the influence of heat and mass transport must also be taken into account. The general trend for monolith converters is still to describe heat and mass transfer with simple one-dimensional models (Güthenke et al., 2007), especially for the purpose of parameter estimation, but different levels of complexity up to three-dimensional CFD-based models (Štěpánek et al., 2012) exist. The preference for simple, and thereby fast, catalyst models in parameter estimation tends to make the kinetic parameters case specific, resulting in kinetic models only giving reliable predictions for a catalyst similar to the one used in the experiments from which the model was derived (Wang et al., 2008). This means that efficient methods to tune model parameters from existing models to measurement data from new catalysts are highly desirable.

To tune the catalyst model to measurement data a method of parameter optimization is needed. The methods can broadly be divided into either global or local optimization algorithms where the latter historically have been far more favored in automotive catalysis parameter estimation. The local optimization methods are generally based on an evaluation of the parameter sensitivity to identify the direction of steepest reduction of the residual. The advantage of these algorithms is that they are fast and accurate but the drawback is that they have a tendency to converge to a

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http://dx.doi.org/10.1016/j.compchemeng.2015.01.004
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local minimum close to the initial guess and thereby failing to converge to the global minima (Blockley, 2010). The global methods generally evaluate a larger parameter space which means that they are more likely to find the global optima. The main drawback with the global methods is very high computational cost which means that they often are not realistic to use for complex systems with many parameters. To be successful the global algorithms also are more dependent on robust models since a wide parameter span will be needed to be evaluated. Examples from literature where global optimization algorithms have been applied in catalysis modeling include Glielmo and Santini (1999) who used the Genetic Algorithm (an evolutionary algorithm) and Ramanathan and Sharma (2011) who showed that an improved fit could be achieved if a global algorithm was followed by a local algorithm to increase the accuracy. A method of reducing the tendencies of the local methods to converge to a local minimum close to the initial guess may therefore be the more desirable way of improving parameter optimization for the current application.

In our previous study (Lundberg et al., 2014), an experimental plan that included several different DOC catalyst configurations, was applied to a full scale engine rig system and used for parameter tuning. The best model fit was achieved with a model that included internal transport resistance with the effective diffusivities of the species being tuned in addition to the kinetic parameters. In the current study, the data and catalyst model formulation will be re-used but with a new approach to parameter tuning will be presented and evaluated. The method is based on a study by Sjoblom and Creaser (2008) who developed methods for model-based DoE including transient data. The methodology presented by Sjöblom and Creaser includes Multivariate Data Analysis (MVDA) to reduce the dimensionality of the largely correlated Jacobian and subsequent selection of a D-optimal sub-set of parameters to estimate based on the parameter sensitivity of simulation data. The relatively simple global kinetic model in the current study makes the number of parameters to estimate less of a concern. Instead the method was revised to select a set of time points from the large transient data set with high sensitivity for parameter changes and at the same time retaining a good representation of the entire data set. To achieve these properties the D-optimal onion design, introduced by Olsson et al. (2004), was selected as an algorithm for data point selection. The algorithms combine the D-optimal design, which by itself tends to only select the most extreme points (Pinto et al., 1990; Zullo, 1991), with a space filling approach making the selection more evenly distributed over the entire data set. Parameter estimation was performed based only in the selected time points with the aim of making use of improved statistical properties to improve the overall fit to measurement data. Since the parameter sensitivity, and thereby the data selection, will depend on the parameter values, the parameter estimation was performed in an iterative process where the data point selection was updated as new parameter values were found. This change of data points used for parameter tuning may also help to avoid local optima. As an evaluation, the efficiency and resulting fit to measurement data achieved by the presented method will be compared to the results of a traditional method of parameter estimation.

2. Experimental

The most important characteristics of the reactor model and adjustable parameters are summarized in the current section and for completeness the defining equations are given in Appendix. A thorough description of the experimental set-up, measurements and engine operation design is given in the preceding study (Lundberg et al., 2014).

2.1. Reactor model

A full scale catalyst, connected to an engine with varying inlet properties displays a highly dynamic behavior. This means that the catalyst outlet conditions will not only be influenced by the current inlet conditions but also those at previous time points. To describe this behavior a transient catalytic reactor model is needed. In this work a uniform radial flow and concentration distribution over the catalyst cross section was assumed which makes it sufficient to model only one channel. The single channel model, closely based on the model presented by Ericson et al. (2008), was discretized as tanks in series where the catalyst washcoat was discretized both radially and axially while the gas phase was only discretized axially. This 1D/2D (gas phase/washcoat) structure was chosen since it was considered a good compromise between accuracy and computational speed (Mladenov et al., 2010). A film theory model was used to model the external heat and mass transport between gas bulk and washcoat surface. Axial diffusion and radial temperature gradients in the washcoat were neglected.

The global kinetics of the DOC has been described in literature with several different levels of detail. The simplest kinetic models only describe the oxidation of CO, HC and NO (Voltz et al., 1973; Oh and Cavendish, 1982; Wang et al., 2008) (where HC is represented as one molecular species) but more detailed models with a more complex description of HC (Stamatelos et al., 1999; Lafossas et al., 2011) and other additional reactions (Ansell et al., 1996; Salomons et al., 2006; Pandya et al., 2009) have also been developed. The kinetic model used in this study is of Langmuir–Hinshelwood type and was originally suggested in the classical work by Voltz et al. (1973) and later modified by Oh and Cavendish (1982). The model, which has been widely and frequently used in DOC modeling over the years, only includes three reactions of which one is equilibrium-limited:

$$CO + 0.5O_2 \rightarrow CO_2$$

$$C_3H_6 + 4.5O_2 \rightarrow 3CO_2 + 3H_2O$$

$$NO + 0.5O_2 \leftrightharpoons 2NO_2$$

The reaction rates were calculated according to Eqs. (1)–(5).

$$r_1 = \frac{k_1 y_{CO} y_{O_2}}{G(y_i, T_s)} \quad (1)$$

$$r_2 = \frac{k_2 y_{C_3H_6} y_{O_2}}{G(y_i, T_s)} \quad (2)$$

$$r_3 = \frac{k_3 y_{NO} y_{O_2}}{G(y_i, T_s)} \left(1 - \frac{K'}{K_p}\right) \quad (3)$$

$$K' = \frac{y_{NO_2}}{y_{NO} y_{O_2}^{1/2}} \quad (4)$$

$$G(y_i, T_s) = T_s(1 + K_4 y_{CO} + K_5 y_{C_3H_6})^2 (1 + K_6 y_{CO}^2 y_{C_3H_6}^2)(1 + K_7 y_{NO}^{0.7}) \quad (5)$$

where K_j is the reaction rate coefficient for the inhibition terms in the denominator G and K_p is the equilibrium constant for NO oxidation. At thermodynamic equilibrium, K_p will be equal to K' and reaction rate r_3 will be equal to zero. Both the rate coefficients k_j and the inhibition terms K_j were described by Arrhenius expressions:

$$k_j = A_j e^{-E_{A,j}/RT_s} \quad (6)$$

The start values for estimation of kinetic parameters were taken from the start values in Wang et al. (2008) where results from several studies (Chen et al., 1988; Koltsakis et al., 1997; Dubien

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