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ANALYTICAL ESTIMATION OF CHEMICAL KINETICS FOR MODELING OF DIESEL OXIDATION CATALYSTS

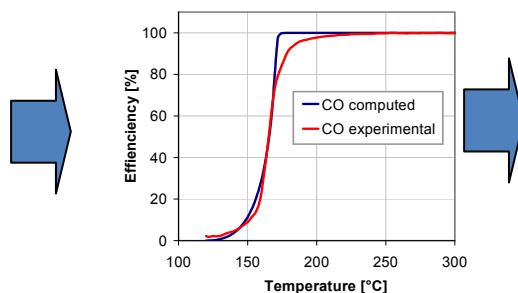
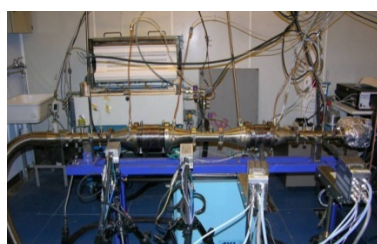
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ABSTRACT: The target of the present work is the development of analytical expressions for chemical kinetics estimation with respect to the widely accepted mathematical models for Diesel Oxidation Catalysts (DOC). The mathematical analysis is applied under ideal conditions using sufficiently simplified reaction schemes in order to identify the minimal input data and extract practical analytical relationships. These simplifications include temperature uniformity, dominant or insignificant inhibition terms and kinetically controlled conditions. In parallel to the mathematical analysis, an experimental procedure is proposed to generate suitable input data having in mind the assumptions used in the analytical expressions. The combined methodology is then tested using numerical experiments conducted with an advanced commercial simulation code. In order to establish confidence in the method, a sensitivity analysis is performed for each kinetic parameter. As a result, it is shown that the reaction kinetics can be estimated with good accuracy in a wide range of values, whereas inhibition kinetics can also be estimated satisfactorily but only for narrow ranges. Summing up, the proposed methodology can serve as a useful tool for fast and repeatable derivation of chemical kinetics in DOC formulations that conform to specific conditions.

KEYWORDS: diesel oxidation catalyst, kinetics estimation, mass transport modeling

INTRODUCTION

Due to increasing environmental concern and the continuously more stringent emission standards, new catalytic formulations for diesel exhaust after-treatment are continuously developed. This includes the Diesel Oxidation Catalyst (DOC), a technology used in vehicles for over three decades. The current development practice involves experimental testing using protocols developed empirically and manual tuning of the chemical kinetics using theoretical models, as shown in Figure 1. This procedure constitutes a substantial “bottleneck” in the development process of more efficient exhaust after-treatment devices since significant experience and extensive investment of effort and time are required.



$$R = \frac{A_1 \cdot e^{-E_1/RT} \cdot c_{CO} \cdot c_{O_2}}{G_2}$$

Figure 1. Workflow of kinetics estimation procedure

The characterization workflow consists of an experimental phase on synthetic gas or engine bench and a kinetics estimation phase involving theoretical models. Regarding the first phase, the current practice, is that a series of simplified experiments, either steady state or transient is conducted with variable inlet exhaust gas conditions (usually temperature and concentration). Typical experimental protocols such as light-off, cool-down, saturation and desorption have been used by almost all researcher, who however use a big variety of inlet conditions and time scenarios. A systematic study of the optimum experimental protocols has yet to be published.

Coming to the second phase of the characterization procedure the disadvantages of the manual calibration technique were identified a long time ago and computer-aided calibration approaches have appeared already since 1973, as published by Buzzi Ferraris and Donati [1]. They examined three variations of a residual sum of squares as an objective function, showing that a weighted approach is more efficient. In 1992 Montreuil et al. [2] presented a calibration procedure for a three-way

catalytic converter model, using also a least square sum as an objective function and minimizing it with the aid of the conjugate gradients method. In 2001 Pontikakis and Stamatelos [3] selected a squared sum of normalized weighted residuals as an objective function, expressed their tuning parameters in a logarithmic form to impose constraints and applied a conjugate gradient method. Later in 2004 [4] they used a sum of absolute conversion efficiency differences as a merit function and a genetic algorithm to find the optimum set of values. Depcik et al. [5] minimized a least square sum of normalized outlet concentrations using built-in MATLAB® optimization subroutines and estimated the kinetics for individual experimental cycles. Sampara et al. [6] elaborated further on the squared sum of residuals, using absolute concentration errors above 50% conversion efficiency and concentration difference errors below the same limit. Their choice for an optimization method was gradient based.

Despite the above mentioned contributions in specific sections, there is still no established solution for the characterization of exhaust after-treatment devices. Furthermore there appears to be scarce references in the literature for usage of analytical expressions. In this context, target of the present study is to develop a kinetics estimation procedure comprising of analytical expressions and appropriate experimental protocols to provide the necessary input.

MATHEMATICAL MODEL AND ANALYTICAL EXPRESSIONS

DOC modeling has been used for decades and it has matured to a common scheme used by the great majority of researchers [6,7]. The species balance in the gas phase along the channel is expressed mathematically with the following equation:

$$\frac{w}{A} \frac{dy_{g,i}}{dz} = -k_{m,i} s (y_{g,i} - y_{s,i}) \quad (1)$$

The right hand-side describes the convection of species from the gas phase to catalytic surface. i corresponds to the species index and k_m is the mass transfer coefficient, which can be calculated from the Sherwood number and the individual species molecular diffusivity:

$$k_{m,i} = \frac{Sh D_{m,i}}{d} \rho M_g \quad (2)$$

The entrance effect at the channel is taken into account with the Hawthorn correlation [7].

$$\overline{Sh} = 2.976 \left(1 + \frac{0.095}{Gr_z} \right)^{0.45} \quad (3)$$

In the absence of any storage phenomena, all convected molecules take part in reactions that lead to formation of products, hence:

$$k_{m,i} s (x_{g,i} - y_{s,i}) = \sum_{j=1} a_{ij} R_j \quad (4)$$

The zero storage assumption mentioned above should be used with extra caution, as it is common for DOC to include storage components (zeolite) in the catalytic formulation. Additionally hysteresis has been reported for NO oxidation on Pt and has been attributed to oxidation of Pt surface [9]. In the transient case additional equations are necessary for sufficient modeling of storage and hysteresis. As the emphasis of this paper is on steady state conditions, these transient phenomena are ignored. More details about these phenomena are available in the literature [10].

The reaction rates proposed by Voltz et al. [11] are widely accepted for platinum catalysts:

$$R_i = \frac{k_{R,i} y_{s,O_2} y_{s,i}}{G} \quad (5)$$

where G the inhibition expression is composed of several terms:

$$G = T G_1 G_2 G_3 \quad (6)$$

$$G_1 = \left(1 + k_{G,CO} y_{CO} + k_{G,C_3H_6} y_{C_3H_6} \right)^2$$

$$G_2 = 1 + k_{G,CO} y_{CO}^2 + k_{G,C_3H_6} y_{C_3H_6}^2$$

$$G_3 = 1 + k_{G,NO} y_{NO}^{0.7}$$

G_1 accounts for the inhibition effects due to chemisorption of CO and C₃H₆. G_2 is required to fit the experimental data at higher concentrations of both CO and C₃H₆ and G_3 accounts for the inhibition of NO.

The above equations constitute a system of differential algebraic equations (DAE), which is typically solved for the species concentrations using numerical methods implemented in commercial software applications, such as axisuite [12] which is employed in this study. The heat balance equations are not included, as a uniform temperature profile in gas and solid will be assumed for the kinetics estimation procedure. The main difficulty in the analytical solution of the DAE system stems

from the non-linear nature of the reaction rate even in the case of a single reactant. Figure 2 shows the reaction rate dependence on molar fraction for the case of CO and C₃H₆. Despite the complexity of this shape, simpler mathematical expressions appear in the two extremes, which are shown here with two asymptotes.

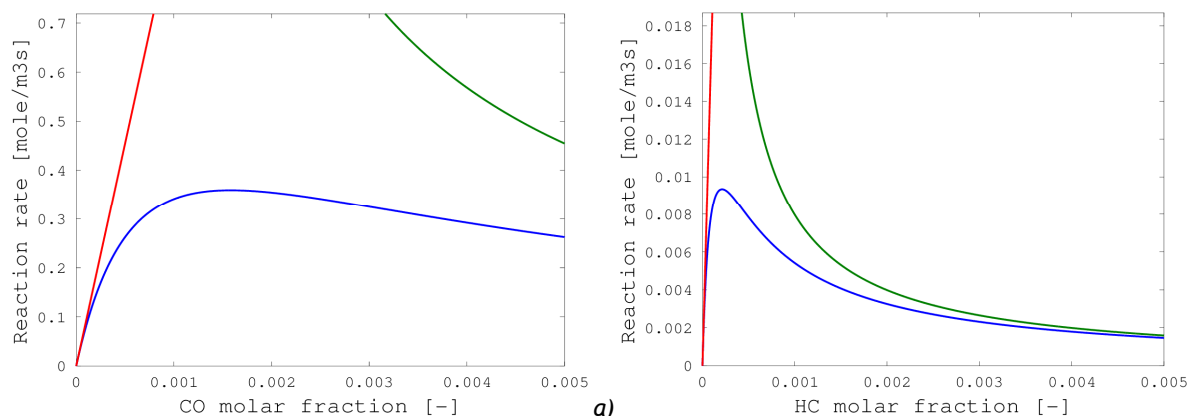


Figure 2. (a) CO oxidation rate as a function of CO molar fraction and (b) HC oxidation rate as a function of HC molar fraction for 10% O₂ and temperature 150°C. Two asymptotes are shown with dashed lines.

The approximation of asymptotes has been used in the past for calculation of non-linear kinetics in modeling of Flow-Through Monoliths [13,1]. At very low concentrations inhibition term G_1 tends to unit. Furthermore G_2 becomes significant only in the presence of both CO and C₃H₆ at high concentrations and at rather low temperatures. For this reason it will be ignored below. G_3 is significant, when NO is part of the mixture. Although, G_3 is important in practice, it will be ignored here as it is practically decoupled from the other equations and can theoretically be determined fairly easily with one experiment containing NO. Having in mind simple compositions of only one pollutant at low concentrations, possible only with synthetic gas testing, these inhibitions can be eliminated and the reaction rate can be simplified to a linear form:

$$R = \frac{k_R y_{O_2} y_s}{T} \quad (7)$$

The maximum rate is obtained at

$$y_{R_{max}} = \frac{I}{k_G} \quad (8)$$

At the temperature of 150°C, $y_{R_{max}}$ is about 1580 ppm for the case of CO oxidation compared to a much lower value of 210 ppm C₃H₆. These values correspond to the inhibition kinetics proposed by Voltz et al. Further assumptions are necessary in order to simplify the DAE sufficiently to derive analytical solution:

- Temperature uniformity
- Zero storage
- Constant concentrations of all species, except the reactant

This way Eq.(4) is solved for the surface molar fraction y_s

$$y_s = \frac{I}{I + Da} y_g \quad (9)$$

where the Damköhler number Da is defined as

$$Da = \frac{k_R / T y_{O_2}}{k_v s} \quad (10)$$

Integration of Eq. (1) across the monolith length yields the conversion efficiency which in the linear regime is expressed as:

$$\eta = 1 - e^{-\frac{k_R / T y_{O_2} L}{1 + Da} \frac{L}{w/A}} \quad (11)$$

With some mathematical transformations, the Arrhenius term is calculated as:

$$k_R = \frac{T}{L} \frac{y_{O_2}}{\frac{\ln\left(\frac{1}{1-\eta}\right) w/A}{k_v s} - \frac{1}{k_v s}} \quad (12)$$

At slightly higher concentrations but still keeping a safety margin from the maximum rate point, the reaction rate can be linearized as:

$$R = R_{y_{s,in}} \frac{y_s}{y_{s,in}} = \frac{k_R^* y_{O_2} y_s}{T} \tag{13}$$

where k_R^* is an equivalent Arrhenius term for the linearized expression. Applying Eq (12) in this regime yields k_R^* , which in turn can be used to calculate the inhibition Arrhenius term k_G with a known k_R , or vice versa:

$$k_G = \frac{\sqrt{\frac{k_R}{k_R^*} - 1}}{y_{s,in}} \tag{14}$$

This expression can also be used to calculate k_G from a different species under the assumption of uniform concentration, e.g the C_3H_6 inhibition of CO. Finally given the Arrhenius terms k_R or k_G at two different temperatures the pre-exponential factor A and activation energy E are determined as:

$$E = \frac{\Re \ln\left(\frac{k_1}{k_2}\right)}{\frac{1}{T_1} - \frac{1}{T_2}} \tag{15}$$

$$A = \frac{k_1}{e^{-\frac{E}{\Re T_1}}} \tag{16}$$

KINETICS ESTIMATION PROCEDURE

As a starting point, a set of reaction kinetics from Pontikakis and Stamatelos [14] were selected to use in numerical experiments. Their reaction kinetics were calibrated to experimental data using a Genetic Algorithm Approach and an in-house simulation code for the above DAE, while the inhibition kinetics were adopted from Voltz et al. It is noted, that the proposed kinetics referred to a 3-way catalyst and consequently showed very high effectiveness when compared to a DOC in preliminary simulations. For this reason the pre-exponential factors of the reactions had to be reduced by three orders of magnitude in order to obtain an efficiency of 50% a little above 150°C. This is not crucial for results of the study, due to its theoretical nature. Finally all parameters were rounded to the values summarized in Table 1.

Table 1: Reaction scheme

	Reaction	A	E
$k_{R,CO}$	$CO + \frac{1}{2}O_2 \rightarrow CO_2$	5.0e+17	90000
k_{R,C_3H_6}	$C_3H_6 + \frac{9}{2}O_2 \rightarrow 3CO_2 + 3H_2O$	4.0e+17	95000
	Inhibition		
$k_{G,CO}$	$G_1 = (1 + k_{G,CO} y_{CO} + k_{G,C_3H_6} y_{C_3H_6})^2$	65	-8000
k_{G,C_3H_6}		2.0e+03	-3000
$k_{G,CO-C_3H_6}$	$G_2 = 1 + k_{G,CO-C_3H_6} y_{CO}^2 y_{C_3H_6}^2$	4	-97000
$k_{G,NO}$	$G_3 = 1 + k_{G,NO} y_{NO}^{0.7}$	4.8e05	31000

Table 2: (a) Experimental conditions and (b) Catalytic converter specifications

Experimental conditions	Value	Catalytic converter specifications	Value
O ₂ concentration [%]	10%	Catalyst length [m]	0.076
Mass flow rate [kg/s]	0.030	Catalyst diameter [m]	0.144
GSHV [1/h]	67700	Cell density [cpsi]	400
Temperature range [°C]	60-250	Wall thickness [mil]	600
Temperature step [°C]	5	Substrate density [kg/m3]	1630
Step duration [s]	30		

The experimental conditions and the specifications of the exhaust are summarized in Table 2. Special care was given to the temperature uniformity assumption. A stepwise scenario was chosen, as shown in Figure 3, which leads to very small non-uniformities at the end of each step. Using

preliminary simulations, it was established that temperature variation in the substrate does not exceed 0.5 °C at the end of each time step. It is important to mention that the same temperature ramp without steps would lead to a temperature difference in the catalyst of about 3 °C, which would nullify the assumption of uniformity.

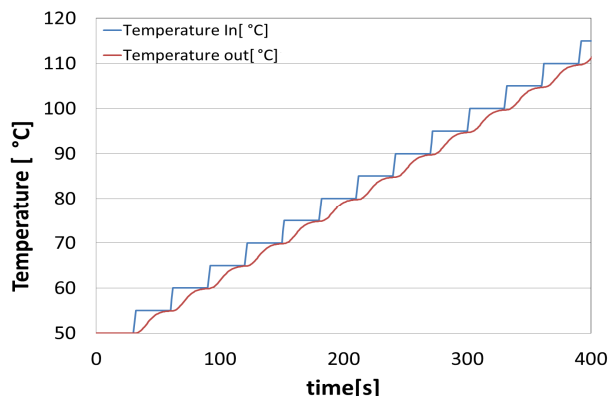


Figure 3. Prescribed inlet exhaust gas temperature and calculated outlet temperature

Based on the analysis presented in the previous section, four virtual experiments (Table 3) were selected for kinetics estimation. Their experimental protocols require special conditions usually available on synthetic gas test benches, as opposed to engine test benches. The first experiment includes only a small amount of CO and is representative of the linear regime of CO oxidation. The second experiment requires a sufficiently high concentration of CO to estimate CO inhibition. The rationale here is to remain close to the linear regime, while approaching to $y_{R_{max}}$, so that the effect of the inhibition

appears even at low concentrations. Thus a different approach is employed, which quantifies first the inhibition of the hydrocarbon on CO oxidation. Experiment 3 includes both species, which could be a problem when trying to study a single reaction. That's why only the initial part of the light-off, where practically no hydrocarbon oxidation takes place, can be used. Finally experiment 4 is used to study the reaction kinetics of C_3H_6 oxidation at conditions slightly below $y_{R_{max}}$. The concentrations are summarized in Table 3, while all other conditions remain constant as described previously.

Table 3: Set of experiments used for kinetics estimation

Experiment	CO [ppm]	C3H6 [ppm C3]	Condition	Conversion efficiency points [-]		Calculated parameter
1	100	0	$y_s < 0.25 y_{R_{max}}$	5%	10%	$k_{R,CO}$
2	1000	0	$0.4 y_{R_{max}} < y_s < 0.8 y_{R_{max}}$	10%	20%	$k_{G,CO}$
3	100	1000	$y_s < 0.25 y_{R_{max}}$	14%	16%	k_{G,C_3H_6}
4	0	30	$0.15 y_{R_{max}} < y_s < 0.5 y_{R_{max}}$	5%	10%	k_{R,C_3H_6}

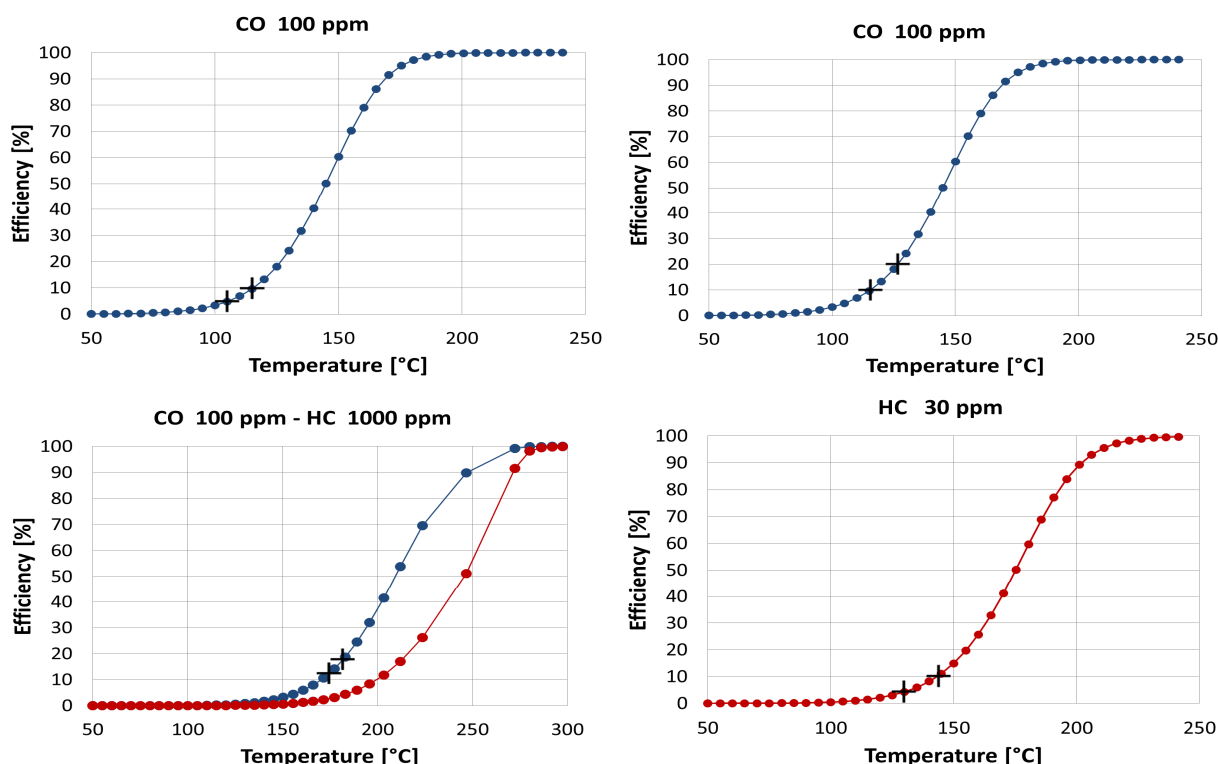


Figure 4. Light-off curves from prescribed experimental procedure. Blue lines correspond to CO and red to C_3H_6 .

In our case the prescribed experimental procedure is conducted virtually. Figure 4 depicts the obtained data and the two points, which were chosen for analysis. Generally low efficiency points are selected to avoid any effects from exotherms and other reactions, trying at the same time to maintain a sufficient level of resolution. It is important to note that the third experiment includes both species. In accordance to literature the oxidation of CO initiates at lower temperatures than C_3H_6 . At CO conversion efficiencies below 20%, the hydrocarbon oxidation is practically insignificant, thus the assumption of uniform C_3H_6 remains valid for the points of interest.

Next the presented mathematical analysis is employed to estimate the actual kinetics. Regarding experiment 1, Eq (12) is applied at both points and two Arrhenius terms k_R are calculated. Subsequently the activation energy and pre-exponential factor are determined using Eq.(15) and (16). Coming to experiments 2 and 3, Eq (12) is used again but this time it yields k_R^* . Combining this and the already known reaction kinetics in Eq. (14) yields the Arrhenius term of the inhibition k_G . The k_G parameters are determined with Eq.(15) and (16). Finally experiment 4 is used to determine the hydrocarbon reaction kinetics from k_R^* and k_G using Eq.(14).

Table 4 presents the analytically estimated kinetics from numerical experiments compared to the original. The obtained pre-exponential factors are within one order of magnitude of the original, while the deviation in activation energies is about 2000 J/mole in the worst case. In order to understand better the error of the estimated kinetics, Figure 5 depicts the light-off curves calculated with the original and estimated kinetics. The light-off temperature is predicted with an accuracy difference of 5°C which is considered very good.

Table 4: Analytically estimated kinetics from numerical experiments compared to the original

	Reaction	$A_{orig} \left[\frac{mole}{m^3 s} \right]$	$A_{est} \left[\frac{mole}{m^3 s} \right]$	$E_{orig} \left[\frac{J}{mol K} \right]$	$E_{est} \left[\frac{J}{mol K} \right]$
$k_{r,CO}$	$CO + \frac{1}{2}O_2 \rightarrow CO_2$	5.0e+17	7.47e+17	90000	91765
k_{r,C_3H_6}	$C_3H_6 + \frac{9}{2}O_2 \rightarrow 3CO_2 + 3H_2O$	4.0e+17	5.28e+17	95000	95749
	Inhibition				
$k_{g,CO}$	$G = T \left(1 + k_{g,CO} y_{CO} + k_{g,C_3H_6} y_{C_3H_6} \right)^2$	65.0	38.7	-8000	-9025
$k_{g,HC}$		2.0e+03	2.306e+03	-3000	-3110

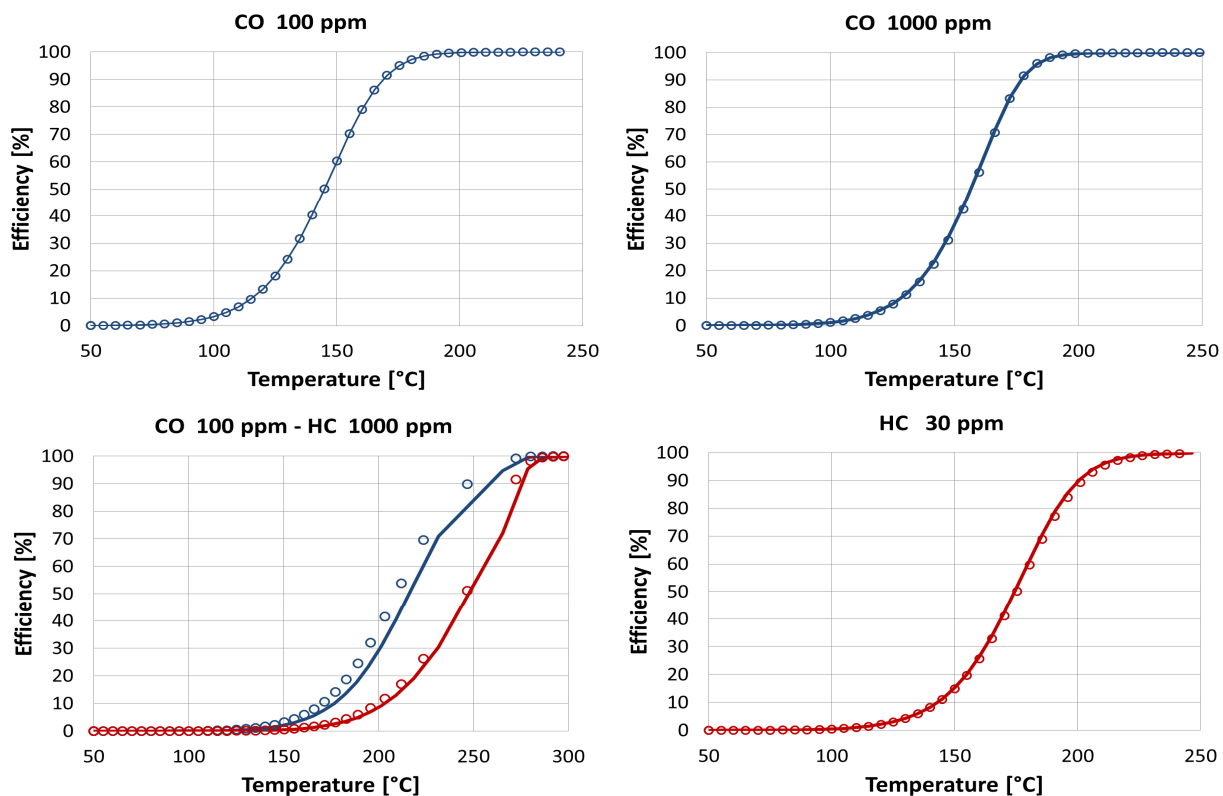


Figure 5. Light-off curves calculated with the original (points) and estimated kinetics (lines). Blue lines correspond to CO and red to C_3H_6 .

SENSITIVITY ANALYSIS

The proposed estimation procedure produces sufficiently accurate estimates for the initial case. In order to establish confidence in the method, a wide range of catalytic applications has to be tested. Here we focus only on the activity of catalytic formulation and not the conditions or design of the converter which can be more easily controlled experimentally or accounted for in the calculations. Thus for each kinetic parameter, two additional levels, shown in Table 5, were selected in order to check its effect on the estimation error and the estimation procedure was repeated. All the other parameters remained constant. Combined effects of two or more parameter changes were not included in this study, except for the reaction activation energies.

Table 5: Levels of kinetics for the complete set of numerical experiments

$A_{r,CO}$	$E_{r,CO}$	A_{r,C_3H_6}	$E_{r,C_3H_6} - E_{r,CO}$	$A_{g,CO}$	$E_{g,CO}$	A_{g,C_3H_6}	E_{g,C_3H_6}
$\left[\frac{mole}{m^3 s} \right]$	$\left[\frac{J}{mol K} \right]$	$\left[\frac{mole}{m^3 s} \right]$	$\left[\frac{J}{mol K} \right]$	$\left[\frac{mole}{m^3 s} \right]$	$\left[\frac{J}{mol K} \right]$	$\left[\frac{mole}{m^3 s} \right]$	$\left[\frac{J}{mol K} \right]$
5.0e+16	80000	4.0e+16	2500	6.5	-13000	2.0e+02	-8000
5.0e+17	90000	4.0e+17	5000	65	-8000	2.0e+03	-3000
5.0e+18	100000	4.0e+18	10000	650	-3000	2.0e+04	2000

The absolute error of activation energies was used as a measure of estimation quality. The reason was that the estimation errors in the pre-exponential factors stem largely from the deviations in the activation energies and do not offer further insight on their own. Regarding the absolute vs relative error, a relative activation energy error would tend to hide estimation problems at high activation energies and overemphasize estimation problems at activation energies close to zero. In this study, estimation with absolute errors below 2500 J/mole is characterized as good. Greater errors up to 5000 J/mole are still considered satisfactory, having in mind that this is more or less the level of accuracy targeted during manual calibrations.

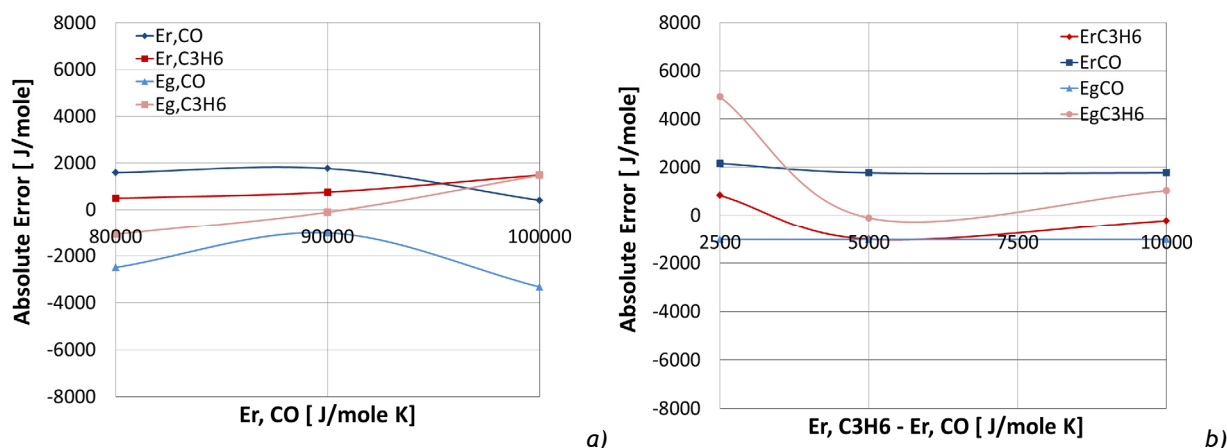


Figure 6. Estimation error as a function of reaction activation energies

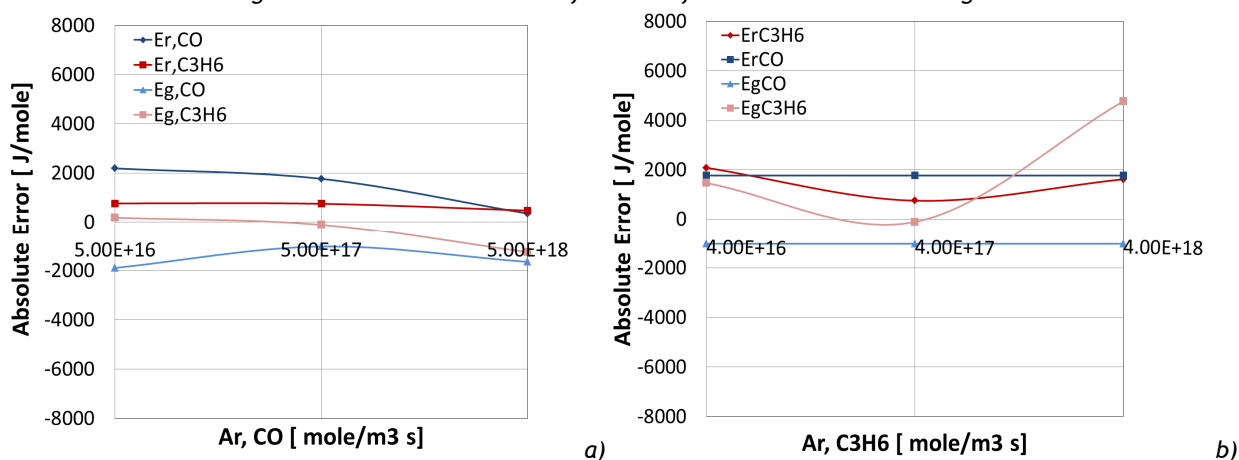


Figure 7. Estimation error as a function of reaction pre-exponential factors

The activation energies of both reactions were studied as a set. In the first case both values were varied together keeping a constant difference and in the second, the difference was altered keeping a fixed level for CO oxidation. Figure 6(a) depicts the effect of $E_{r,CO}$ level on the absolute error of all activation energies (both reactions and inhibitions), while the hydrocarbon value is

adjusted to maintain the original difference. The errors remain in the range of ± 2500 J/mole. Figure 6(b) presents the effect of activation energy difference. Again a very good result is obtained with absolute errors below 2500 J/mole. The lowest studied difference ΔE_r was 2500 J/mole which ensured the faster light-off of CO compared to C_3H_6 as expected in real-life applications. Since this assumption was used in the development of the methodology, any lower value leads to increased estimation error.

Next the effect of reaction pre-exponential factors is examined for both reactants in Figure 7. The induced errors remain within satisfactory limits and there appear to be small effects for a range of three orders of magnitude. Slightly higher effects arise for C_3H_6 inhibition, when the pre-exponential factor of C_3H_6 is increased by one order of magnitude.

Figure 8 depicts the sensitivity of estimation error on the CO inhibition parameters. Focusing on Figure 8(a) it is evident that the pre-exponential factor $A_{g,CO}$ has a considerable impact on almost all estimated parameters at high values, leading to increased errors. These errors can be explained by induced change in the maximum rate concentration $y_{R_{max}}$. Any change in $y_{R_{max}}$ means the conditions defined in Table 3, might not be met. This is the case for the points in the right of the graph, that don't satisfy our quality criteria. In order to overcome this problem, a redesign of the experimental protocols would be necessary with new concentrations. Similar problems appear when the $E_{g,CO}$ takes very small values. To obtain better resolution of this sensitivity, intermediate points have been calculated for all inhibition parameters. In order to ensure the accuracy of procedure with the proposed concentrations, the inhibition activation energy must remain in a range of ± 2500 J/mole and the pre-exponential factor in a range of one third to the triple of the original value. Of course this not known a priori, so a try and error approach might be necessary.

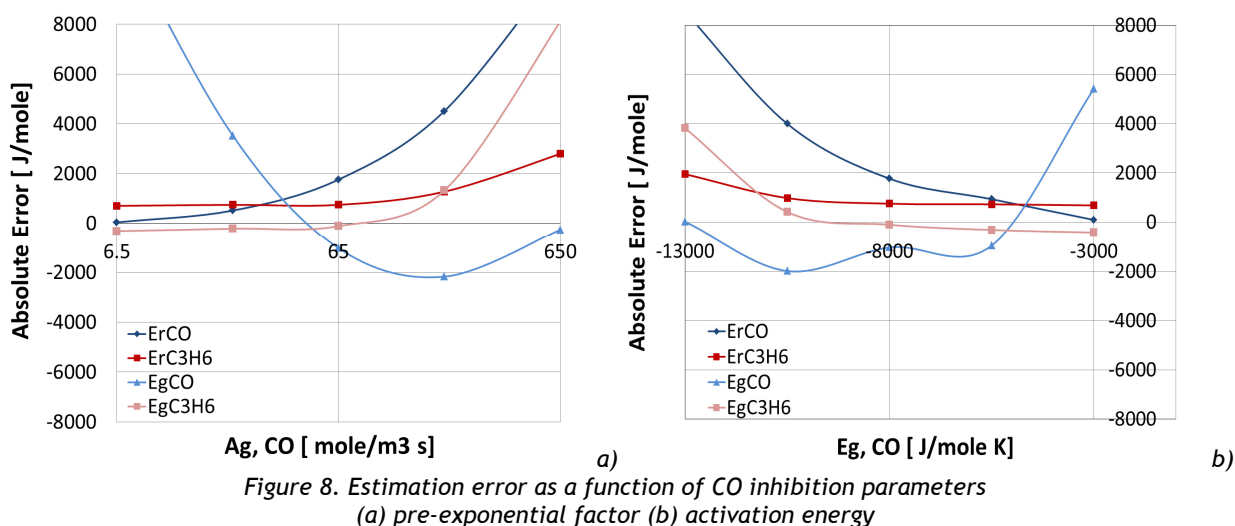


Figure 8. Estimation error as a function of CO inhibition parameters
(a) pre-exponential factor (b) activation energy

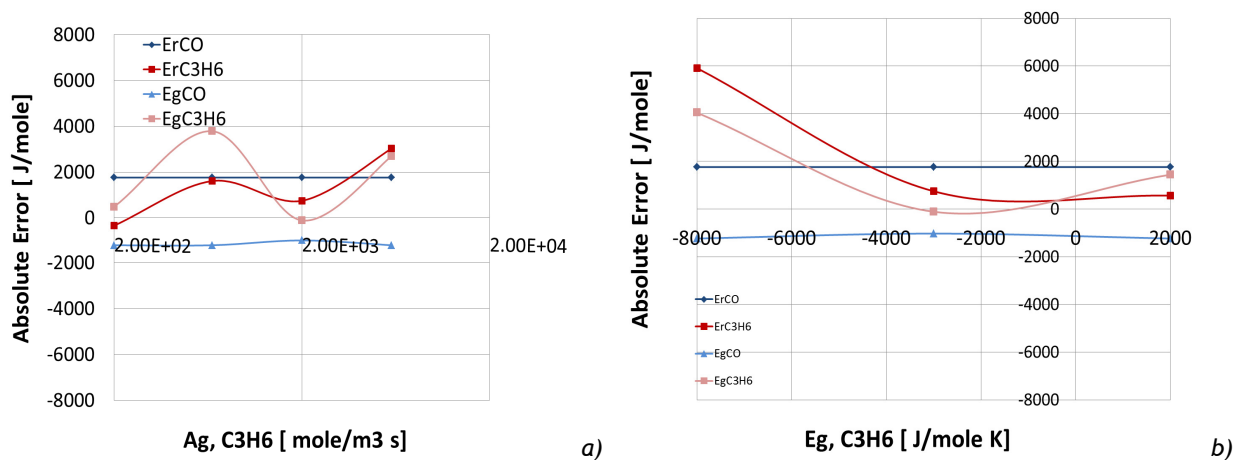


Figure 9. Estimation error as a function of C_3H_6 inhibition parameters
(a) pre-exponential factor (b) activation energy

Variation of C_3H_6 inhibition parameters can also affect the quality of the estimation, as shown in Figure 9. In this case the errors are acceptable; however there might be some cases such as the largest point of A_{g,C_3H_6} where analytical calculation is not possible. For this reason a variation similar to CO inhibition parameters is advised for the application of the procedure.

CONCLUSIONS

A kinetics estimation procedure was developed, comprising of an experimental protocol and analytical calculation methodology. This was achieved by identifying the minimal input data necessary for kinetics estimation and the extraction of practical analytical relationships that took advantage of simplified conditions in the linear reaction regime. Having this in mind, the experimental protocol was designed with four light-off experiments at various concentrations and the analytical calculation procedure was adjusted to the prescribed input.

A sensitivity analysis using numerical experiments was conducted to evaluate the accuracy of the procedure. The sensitivity for each individual kinetic parameter was quantified, thus establishing a confidence for a wide range of kinetics values. With regards to reaction kinetics, the activation energy error was usually below 2500 J/mole and almost always below 5000 J/mole. Furthermore the error showed small sensitivity to the variation of reaction kinetics. The picture is slightly different for inhibition kinetics. The estimation procedure showed small errors for values relatively close to the reference; however greater variation led significant estimation errors in some cases. In order to overcome this problem the experimental concentrations have to be adjusted accordingly to meet all the necessary conditions.

Considering the above, the developed methodology can serve as a useful tool for fast and repeatable derivation of chemical kinetics in the simple DOC formulations that conform to the conditions described above. Depending on the desired level of accuracy, it can replace completely manual calibration or serve as an initial solution for manual/automatic calibration. Further improvements would be useful in the direction of covering an expanded range of possible kinetics, more complex phenomena in the DOC and other modern catalytic reactor types.

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