

Genetic Algorithm based Automated Calibration Tool for Numerical Selective Catalytic Reduction (SCR) Models

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ABSTRACT

An automated process was developed for the calibration of numerical aftertreatment models. The chemical kinetic mechanism examined in this case was part of a simplified SCR model. The process adopted for calibrating the SCR model was based on a micro-population multi-objective genetic algorithm. The algorithm developed was used to calibrate the SCR model using data derived from another, more detailed model to ensure that the evaluation focused only on the effectiveness of the calibration process and was not affected by issues of experimental inaccuracies or details of the model chemistry involved.

INTRODUCTION

Increasingly stringent emission regulations for both light duty and heavy duty diesel engines are driving the need for deployment of NO_x aftertreatment to provide the best customer value in terms of brake specific fuel consumption. One popular option for the control of NO_x in lean exhaust streams is urea SCR and is currently under evaluation or development in the industry and academia [1-5]. Evaluation of the performance of this technology as a potential NO_x reduction solution involves the development of numerical models to simulate the SCR performance. The use of numerical models allows for efficiency in the development process in terms of cost and effort and also enables for more accurate performance evaluations.

These numerical models require the calibration of certain chemical kinetic constants as well as other model constants for the accurate prediction of experimental results. This calibration is typically specific to the catalyst

formulation used in the generation of the calibration data. Accurate application of the model to other catalyst formulations requires the recalibration of the model to data obtained from experimental testing of the new catalyst formulation. Historically, the calibration process has been conducted through a combination of manual estimation on the part of the analyst/model developer in combination with other techniques such as regression analysis and gradient search techniques [6]. Such an approach is not very desirable due to the large time and effort required on the part of an analyst who is fairly intimate with the SCR chemistry as well as the model structure.

The importance of an automated calibration procedure is further highlighted when attempting to evaluate different catalysts. Additionally, as models continue to get more detailed in their chemistry [6] as a response to the more detailed reaction mechanisms proposed in the literature [6-9] the number of model constants requiring to be calibrated increases rapidly leading to increasing difficulties in a predominantly manual calibration process. Thus, an automated calibration process should not only assist in quicker evaluation and implementation of catalyst formulations, but also assist in the development of more detailed and accurate aftertreatment models.

Genetic algorithms are well-established global search techniques loosely based on the phenomenon of biological evolution for function optimization in a variety of engineering problems. Some applications of these algorithms relating more closely to the field of diesel engine technology include reduction of emissions and fuel consumption [10], optimization of heavy duty diesel engines [11], development of combustion reaction

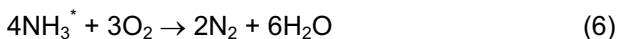
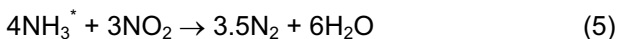
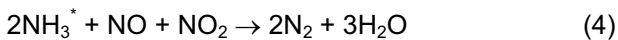
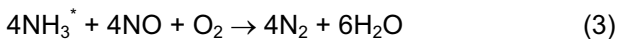
mechanisms [12] and [13]. The application of genetic algorithms to the calibration of numerical models of aftertreatment devices has been limited. The current work outlines some of the issues that need to be addressed in the successful implementation of a genetic algorithm based calibration program for model calibration.

The genetic algorithm implemented in this work is based on the micro-genetic algorithm described by Krishnakumar [14]. This variant of the genetic algorithm utilizes relatively smaller population sizes to allow for a quicker approach to the near optimal solution. Additional changes were incorporated into the algorithm to adapt it to the specific problem of calibrating an SCR model.

SCR MODEL

The SCR reaction mechanism is fairly complex and not very well understood [15]. Also, a model sufficiently detailed to capture the fundamental reactions occurring within the catalyst is likely to be very demanding in terms of computational requirements. For the purposes of this study, therefore, a simplified one-dimensional SCR model, similar to previously outlined models [16, 17], with additional simplifying assumptions to decouple the various reactions was chosen. This decision was motivated by the fact that the simplified model would be significantly quicker than a more detailed model – an important consideration when evaluating various calibration algorithms based on evolutionary strategies.

The simplified SCR model used in this work consisted of six global reactions to approximate the SCR chemistry as outlined previously in the literature [16-18].



This simplified numerical model requires fourteen constants, including pre-exponential terms, activation energies and ammonia storage capacity, to be calibrated to reproduce the results for a given SCR catalyst.

SCR MODEL CALIBRATION TOOL DEVELOPMENT

The SCR model calibration tool is essentially an optimizer working to minimize the differences between the provided experimental data and the model predictions by searching for the optimal set of model constants in the stipulated search space.

While gradient search techniques would be a simpler solution to an optimization problem, the nature of this optimization problem prevents an effective implementation of a gradient search technique based optimizer. This is due to the fact that in addition to various local extrema, the different calibration variables are also strongly coupled to each other due to the nature of their physical origin. For example, changing a calibration constant to change the activation energy of a given reaction would yield a very poor overall solution unless this change is coincident with the corresponding change required in the pre-exponential (frequency) factor for the same reaction.

Based on this knowledge of the problem, a genetic algorithm, or more specifically, a micro-population genetic algorithm based approach to developing the calibration tool was adopted. For reference and added clarity, some of the terms used in the description of the genetic algorithm are defined in a subsequent section.

The genetic algorithm selected as an optimizer for the calibration problem was a micro-population genetic algorithm, which was then tweaked through a number of studies to improve the calibration performance of the tool in terms of speed as well as prediction accuracy.

The formulation of the chemical kinetic rates in the SCR model was changed to “pin” the reaction rates at 600 K, similar to the approach adopted by Chatterjee et al [19]. This was done to reduce the effect of the strong non-linear coupling between the activation energy and pre-exponential term for a given reaction. A modified expression for the reaction rate was thus obtained as

$$r = k \exp\left(-\frac{E}{R}\left(\frac{1}{T} - \frac{1}{600}\right)\right) \quad (7)$$

“Pinning” the reaction rate of a given reaction in this form allowed the calibration tool to change the pre-exponential terms and activation energies somewhat independently of each other. A more detailed explanation of this modification and its consequences is included in the appendix.

As mentioned previously, the model required the calibration of fourteen constants to reproduce the experimental data accurately. The calibration tool was allowed to change these fourteen constants through a set of fourteen multiplicative variables or calibration factors (CF's). The search space for the calibration tool was then defined by the range of values over which it was allowed to change the calibration factors. These variables were defined using a log scale to allow the calibration constant equal access to chemical kinetic constants that were greater and lesser than the baseline value.

$$\text{CF}' = \text{CF} \log V \quad (8)$$



Thus, setting a search space limit of -1 to 1 for a variable allows the calibration tool to select chemical constant values that range from 0.1 to 10 times the original baseline value. This approach was adopted since the optimal chemical constant rates are as likely to be greater than the baseline value as they are to be lesser than the baseline value.

Also, in addition to the fourteen calibration variables that arose due to the structure of the model, another calibration variable was introduced. This calibration variable was introduced as a multiplicative term in the ammonia adsorption and ammonia desorption rates simultaneously. This was done because initial runs of the calibration tool indicated that while the calibration tool was able to match the required trends fairly well, it was struggling to achieve adequate fits for the ammonia adsorption and desorption curves due to the fact that the adsorption and desorption rates are very closely coupled to each other.

This set of fifteen calibration variables comprises the "chromosome" of a given citizen. In the implementation of this calibration tool, the information in the chromosome is retained in base 10 format and operations performed directly on this array of fifteen numbers. The population size for the genetic algorithm was selected to be fifteen based on a series of runs conducted to evaluate the effect of the population size on the final solution. It was found that a population size of fifteen led to relatively quicker optimization times, while still achieving the required level of model prediction accuracy.

The model prediction accuracy (fitness) is determined for each of the individual proposed solutions (citizens) by using the model to predict the emissions out of the SCR over a given calibration cycle. The model prediction accuracy for a given set of calibration variables is quantified based on the differences between the predicted molar flow rate and the experimental molar flow rate for the various chemical species of interest.

$$\text{Fitness} = \frac{100}{\text{NH}_{3\text{Error}} + \text{NO}_{\text{Error}} + \text{NO}_{2\text{Error}}} \quad (9)$$

$$\text{NH}_{3\text{Error}} = \sum_{t=0}^{t=\text{tend}} |\dot{n}_{\text{NH}_3-\text{experimental}} - \dot{n}_{\text{NH}_3-\text{predicted}}| \Delta t \quad (10)$$

$$\text{NO}_{\text{Error}} = \sum_{t=0}^{t=\text{tend}} |\dot{n}_{\text{NO}-\text{experimental}} - \dot{n}_{\text{NO}-\text{predicted}}| \Delta t \quad (11)$$

$$\text{NO}_{2\text{Error}} = \sum_{t=0}^{t=\text{tend}} |\dot{n}_{\text{NO}_2-\text{experimental}} - \dot{n}_{\text{NO}_2-\text{predicted}}| \Delta t \quad (12)$$

Based on this evaluation of the fitness of the calibration constants as determined by each citizen, four citizens are identified from the overall population of citizens – the

overall best prediction, the best NH_3 prediction, the best NO prediction and the best NO_2 prediction. This procedure is in contrast to that employed in typical implementations of micro-population genetic algorithms where only the best solution is identified and preserved. This procedure was adopted in the current implementation of the micro-population genetic algorithm because it was found that the information present in a good individual chemical species prediction ($\text{NH}_3/\text{NO}/\text{NO}_2$) could help improve the overall prediction. By preserving the information related to the best individual species prediction, the overall solution was found to converge much quicker than without such an option. The implemented technique is therefore a multi-objective, multi-elitist version of a micro-population genetic algorithm.

The recombination of the calibration constants (mating) in the individual citizens of the population is based on a roulette based strategy where the probability of a given citizen getting picked to be a parent is directly proportional to the fitness value associated with that individual selection. After two parents are selected for each new "offspring" citizen, the calibration constant information contained in the chromosomes of the parent citizens is recombined to form the chromosome for the new offspring. The probability of a given calibration constant for an offspring coming from either parent was equal. Figure 1 shows a graphical representation of the recombination strategy. Additionally, random changes are made in the new offspring chromosome based on a specified mutation rate – typically set to 5% in this study. A mutation rate of 5% implies that a random calibration variable value would be inserted into the chromosome information for the offspring in 5% of the recombination

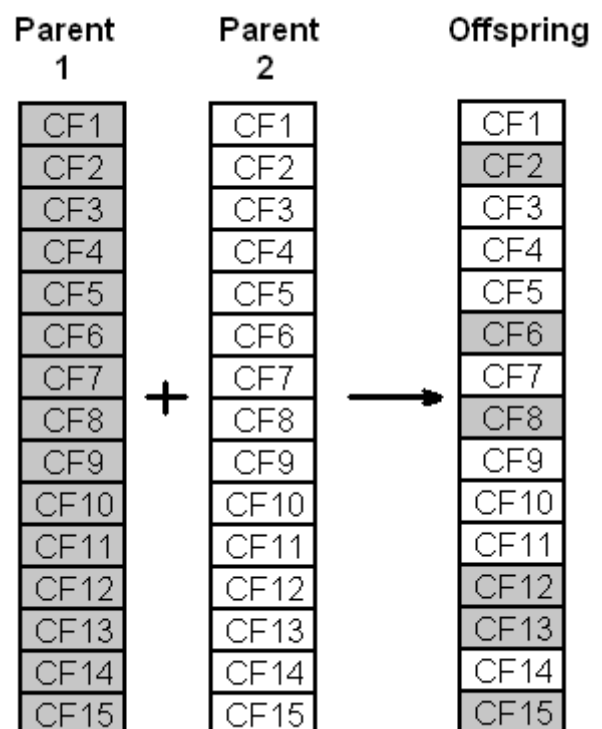


Figure 1: Recombination of calibration constants from current proposed solutions