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Investigation on the solution of nitric oxide emission model for diesel engine using optimization algorithms

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ABSTRACT

Research on reducing the NO emission from internal combustion engine is a challenging work. NO emission prediction model plays a significant role in simulation-based research. According to extended Zeldovich, the determination of equilibrium concentration of combustion products is vital in the prediction of NO formation. Besides the well known STANJAN and Newton-Raphson iteration, Trust-region dogleg, PSO (Particle Swarm Optimization), and GA (Genetic Algorithm) are added to investigate the performance of those methods on the determination of combustion products. Twelve species are considered in the combustion products. STANJAN uses minimizing Gibbs energy to derive the needed nonlinear equations while the others use Equilibrium Constant Method. In terms of the results, it is found that Trust-region dogleg method shows the best performance which achieves the desired accuracy within 0.1 s and the calculated results are comparable to STANJAN. In addition, perturbed PSO also reveals excellent global convergence capability. On the contrary, unmodified Newton-Raphson is unsuitable for this problem and Newton-Raphson downhill shows satisfactory performance neither. According to the results of parameter study, the equilibrium concentrations of combustion products are greatly influenced by equivalence fuel-air ratio and temperature but little affected by pressure. The NO formation process shows good agreement with AVL BOOST. Compared to measured value, the best-predicted emission value reaches −5.45% but the worst drops to −17.72%.

1. Introduction

The nitrogen oxides (NOx) emission control regulations are stringent on marine diesel engines. Reducing emission is a great challenge for manufacturers and researchers. Simulation-based research shows the vital significance for engine design. Therefore, accurate prediction of NOx emission exposes its importance. At present, the in-cylinder combustion control, such as injection strategies[1,2], alternate fuels[3], RCCI (Reactivity Controlled Compression Ignition)[4,5] or their combinations[6,7], show the most promising way for emission reduction. Injection timing had been successfully used in marine diesel engines for complying with Tier II. For Tier III, EGR and LNG based RCCI have been widely investigated and show a good promising[8,9]. The extended Zeldovich mechanism or its variant is widely accepted for predicting NOx formation in diesel engines[10–12], which leads to the determination of equilibrium concentrations and solution of nonlinear equations. The determination of equilibrium concentrations using minimization of Gibbs energy had been studied by Gordon S. and McBride B. J.[13], Reynolds W. C.[14], and Pope S. B.[15] with their carefully designed solver. For the combustion products determination from an internal combustion engine, Equilibrium Constant Method and Newton-Raphson method are widely used[16–21]. In order to investigate and validate the performances, three optimal algorithms have been added besides the Newton-Raphson method and STANJAN.

The nitrogen oxides are considered to be formed by thermal NOx in post flame zone, prompt NOx in the flame, and nitrogen compounds in the fuel. Among these sources, the thermal NOx dominates the NOx formation in the diesel engine. The NO prediction model has varied complexity, accuracy and physical mechanism in terms of different purposes, which can be typically classified into empirical model [22–24], the extended Zeldovich mechanism[25,26], the six-step with eight species mechanism[27,28], and complex chemical kinetical model [29]. On the basis of the extended Zeldovich mechanism, other mechanisms were also proposed. Miller et al.[30] concluded that the extended Zeldovich mechanism failed to take into account the species of N_2O and related reactions in lean mixtures and high-pressure condition so that the combination of extended Zeldovich mechanism with N_2O mechanism was proposed and used.

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Those mechanisms come to the solutions of equilibrium concentrations of combustion species. For the 12 species scheme, the H, O, N, H_2, OH, CO, NO, O_2, H_2O, CO_2, N_2, and Ar are considered in the combustion products. Equilibrium Constant Method and the minimizing Gibbs energy method are two ways to determine the equilibrium concentrations of products in chemical reaction. The method of minimizing Gibbs energy is based on the theory that the reaction under constant pressure and temperature will occur spontaneously along the direction where the total Gibbs energy of mixture drops[13–15]. The total Gibbs energy of the mixture reaches its minimum when the chemical equilibrium is achieved. In this method, the Gibbs energy of each component in the mixture has to be known and the amounts of reactants need to be determined in advance. Normally, the fuel is taken as one mole and the amount of air is derived by the fuel-air equivalence ratio. Then, the concentrations of products at equilibrium can be determined when the target function reaches its optimal value. Equilibrium Constant Method determines the concentrations of products by constructing the required independent equations[16–21]. In that case, the atomic conversation theory and product dissociation reactions are involved. In the dissociation reactions, the generated species is the mixture of reactants and products. When it reaches the equilibrium, the reaction rate of reactions is equal to the reaction rate of products, from which the equilibrium constant is derived. For the solution convenience, the sum of products is assumed to be one mole. Researchers have found that this set of nonlinear equations can be simplified into a 4×4 nonlinear system to improve calculation speed and reduce the complexity [20].

Two types of the methods result in the solution of nonlinear equations. Newton-Rapson iteration method is the most known and widely used method for the solution of nonlinear equations. It uses the linear equation obtained by the Taylor expansion of the original nonlinear equation to gradually approach the exact solution. It is commonly seen in solving various engineering problems in various fields[31–34] as well as the equilibrium computation of combustion products in internal combustion engine[21,35,36]. Mehrnoosh D. et al. [21] investigated the performance and emission of a four-stroke SI engine fueled by gasoline and CNG (Compressed Natural Gas). The set of equations about the emission was solved by the Newton-Raphson iteration method. Adnan R. et al. [35] modeled the combustion process based on Equilibrium Constant Method on MATLAB and calculated 18 combustion products with Newton-Raphson method. Perini F. et al. [36] presented a rich emission model where the nitric oxide was predicted based on Equilibrium Constant Method and Newton-Raphson was used for solving an 11 equilibria acts nonlinear system.

In practice, however, engineers and researchers found that unmodified Newton-Raphson iteration method did not perform well in the solution of multivariable nonlinear equations such as the equations formed from the chemical equilibrium of combustion products in IC engines. In that case, the initial value plays an important role in the convergence, otherwise, a local minimum may be obtained. In order to overcome those problems, Reynolds W. C., the pioneer of the chemical equilibrium calculation, carefully designed a valid method, named STANJAN, using the element potential[14]. In STANJAN, the element potentials and phase moles are unknown variables. It minimizes the well designed dual problem in element potentials space with fixed total moles by the steepest descent roughly and uses the Newton-Raphson iteration to get convergence when it closes to the minimum. Then, it maximizes this minimum by adjusting the value of total moles using the steepest ascent method and uses the Newton-Raphson iteration to adjust the element potentials and value of total moles so that it get convergence. The matrix conditioning is used to prevent the matrix from singular or nearly singular. The initial value and the set of base species are obtained from the initializer via the simplex method and pseudo-Gibbs energy. STANJAN is a widely used method for chemical equilibrium analysis and had been used in CHEMKIN and as a solver for Chemical calculation provided by the Colorado State University. The Gibbs function continuation (GFC) method is another different method for chemical equilibrium calculation, which was proposed by Pope S.B. [15]. In GFC, $\tilde{\mathbf{g}}$ and λ are taken as the variables changing with a pseudo time s instead of λ and $\mathbf{N}_m$ in STANJAN. When the pseudo-time changes from 0 to 1, the pseudo-Gibbs function changes from an initial value to the true Gibbs function and the constrained potential $\bar{\lambda}(s)$ turns to the constrained potential satisfied the nonlinear equations[15,37,38]. There are also some other improvements for equilibrium solution. Scoggins J. B. et al. [39] used Gibbs function continuation method to calculate the linearly constrained multiphase chemical equilibrium compositions. Néron A. et al. [40] developed a general thermodynamic method to real industrial problems under energy constraint and kinetic constraint. Both Rossi C. C. R. S. et al. [41] and Belov G. et al. [42] used linear programming to calculate the chemical equilibrium. Aithal S M [43] modified the Newton-Raphson iteration method by adding a relaxation factor to prevent the step size from being too large. Rakopoulos C. D. et al. [20] suggested that the initial value for iteration could be obtained according to the assumption of complete combustion since the equilibrium concentrations are close to the value calculated from the perfect combustion, which is easy to be calculated and had been demonstrated to be effective.

The optimization problems in artificial intelligence have greatly promoted the development of optimization. A large number of optimization algorithms, such as the particle swarm optimization (PSO) [44–46], genetic algorithm (GA)[47,48], ant colony optimization (ACO), ANN based optimization algorithms[49–52], trust region method[53–56], and interior point method, have been proposed and used to solve the nonlinear equations. Therefore, the Trust-region dogleg, PSO, and GA are also added to this paper for investigation besides Newton-Raphson and STANJAN. The basic NO formation against time in terms of extended Zeldovich is introduced in Section 1. In order to solve the equation, twelve equilibrium species are considered. In addition, the commonly used Gibbs energy minimization method and Equilibrium Constant Method are presented in Section 2. The equilibrium constant for each decomposition reaction is also provided. The investigated optimization algorithms are described in Section 3 but other methods are omitted. The performances for all the methods are analyzed in Section 4. After that, the sensitivities of combustion products to temperature, pressure, and equivalence ratio are analyzed using the well performed Trust-region dogleg method. Finally, NO prediction of a four-stroke diesel engine is presented.

2. Nitric oxide model

Generally, the NO in diesel emission products is original from the reaction of atmospheric nitrogen and oxygen in high-temperature conditions. According to the well-known extended Zeldovich mechanism, the NO formation is based on the following equations.

$$\mathrm{O} + \mathrm{N_2} \underset{k_{r1}}{\overset{k_{f1}}{\rightleftharpoons}} \mathrm{NO} + \mathrm{N} \tag{1}$$

$$\mathrm{N} + \mathrm{O_2} \underset{k_{r1}}{\overset{k_{f1}}{\rightleftharpoons}} \mathrm{NO} + \mathrm{O} \tag{2}$$

$$\mathrm{N} + \mathrm{OH} \underset{k_{r3}}{\overset{k_{f3}}{\rightleftharpoons}} \mathrm{NO} + \mathrm{H} \tag{3}$$

As the N atom varies slowly, the change of N atom is viewed as zero. Then, according to the law of mass action, the change of NO concentration is finally derived as[57].

$$\frac{d[NO]}{dt} = \frac{2R_1(1-\beta^2)}{1 + \beta R_1/(R_2 + R_3)} \tag{4}$$

where [] denotes the concentrations of corresponding species in moles per cubic centimeter, R_1, R_2 and R_3 are the equilibrium reaction rates corresponding to equations(1)–(3). And the β in equation (4) is the