Integrated modeling of nitrogen oxides formation in diesel engines*

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Abstract To account for the effects of both chemistry and flow turbulence, the present study proposes an integrated NO sub-model that combines the extended Zel'dovich mechanism and engine CFD computations to simulate the NO histories in a diesel engine. NO_x sub-model parameters and pollutant formation mechanisms can be more easily investigated by solving the NO_x sub-model. The new NO formation model incorporating the effects of both chemical kinetics and turbulent mixing was applied to simulate a diesel engine with a quiescent combustion chamber, and one with a re-entrant combustion chamber; the premise of the model being the reaction rate is mainly determined by a kinetic timescale and a turbulent timescale. The results indicate that the predicted NO formulation from the new model agrees well with the measured data. As the utilization of fossil fuels continues to increase, the control of NO_x emissions is a worldwide concern; and it is imperative to understand fully the NO_x reaction processes in combustion systems. This technology has the potential to enhance the application of various combustion techniques used to reduce NO_x emissions from practical combustion systems.

Keywords: nitrogen oxides (NO_x), combustion, turbulence, diesel.

Nitrogen oxides consist of nitric oxide (NO), nitrogen dioxide (NO_2), and nitrous oxide (N_2O). NO and NO_2 are collectively referred to as NO_x. N_2O survives only in the hotter, fuel-rich, flame regions and is destroyed downstream[1]. It has been reported[2] that the mole ratio of NO_2 to NO_x is about 0.1—0.3 in diesel engines. According to Reitz[3], the engine NO_x data is consistent with the EPA, and the NO_x mass is multiplied by the ratio of NO_2 to NO molecular masses (1.533). NO is the predominate oxide of nitrogen produced in diesel engines.

Nitrogen oxides are a significant threat to the environment, and the control of NO_x emissions is a world-wide concern as the utilization of fossil fuels continues to increase. Advances in the science of NO_x reactions, mathematical modeling, and increased performance of computer systems have made comprehensive modeling of NO_x formation and destruction a valuable tool to provide insights and understanding of the NO_x reaction processes in combustion systems. This technology has the potential to enhance the application of various combustion techniques used to reduce NO_x emissions from practical combustion systems.

Computer modeling of the NO_x formation and destruction process in combustion systems has involved many approaches. The most common approach couples a simplified description of the NO_x reaction process with a detailed, "comprehensive" description of the combustion and flow processes. This approach for modeling the NO_x reaction processes requires a joint solution of detailed CFD equations for turbulent flow, combined with reduced chemical reaction mechanisms, and is referred to as "comprehensive modeling", and it is emphasized here.

Comprehensive modeling of NO_x reaction processes in combustion systems requires simulation of both the turbulent fluid dynamics and the chemical kinetics in the system being modeled. Hundreds of elementary reactions are required to provide a detailed description of the NO_x reaction process in laminar combustion systems. However, it is not currently feasible to use such generalized reaction mechanisms to model this process in a turbulent, reacting system in which large reaction kinetics schemes are coupled with the turbulent fluid dynamics. Consequently, global reactions or reduced mechanisms, which are called NO_x submodels, are typically used in comprehensive combustion codes to describe the NO_x reaction processes.

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In engines, the combustion occurs at high pressure and the cylinder pressure rises during most of the combustion, so burned gases produced early in the combustion process are compressed to a higher temperature than will be reached immediately after combustion. NO formation in the post-flame gases almost always dominates any flame-front-produced NO. It is appropriate to assume that the formation of trace pollutant species does not affect the flame structure, which is governed by fast fuel-oxidizer reactions. Therefore, NO sub-models are commonly de-coupled from the generalized combustion model and executed after the flame structure has been predicted. Another advantage of this approach is computational efficiency. Further, solving the pollutant model equations jointly with the combustion model equations is far more complex. As a consequence, NO_x sub-model parameters and pollutant formation mechanisms can be more easily investigated by solving the NO_x sub-model using restart files for a pre-calculated flame structure.

NO_x or NO can be formed or destroyed by at least four separate reaction processes in the gas phase. These are classified as: thermal NO, prompt NO, fuel NO, and NO reburning. Most of the NO_x produced in engines was found to be thermal NO, and the extended Zel'dovich mechanism is widely used for NO_x submodel in engines[3, 4]. According to the extended Zel'dovich mechanism, the resulting NO formation rate expression in ($gmol/cm^3$) is[5]

$$\left.\frac{d[NO]}{dt}\right|_{Zeldovich} = 2k[O][N_2] \quad (1)$$

There is a significant difference between the NO data predicted from the extended Zel'dovich mechanism and those obtained from experiments. In some previous implementations, Reitz[3] has introduced a calibration factor, β, adjusted to allow NO_x predicted from the extended Zel'dovich mechanism to match engine NO_x data, i.e.

$$\frac{d[NO]}{dt} = \beta \left.\frac{d[NO]}{dt}\right|_{Zeldovich} = 2\beta k[O][N_2] \quad (2)$$

A value of β was assumed to be 0.78 for the cases investigated by Reitz. This indicated that the predicted data by the extended Zel'dovich mechanism is over estimated by about 30%, i.e. Zel'dovich mechanism results in very fast formation rates for engine NO emission. It is very possible that the effects of turbulence on the NO reaction rates must be considered.

Similar to the Eddies Dissipation Concept, a NO submodel was proposed as follows[6]:

$$\frac{d[NO]}{dt} = \min\left\{\left.\frac{d[NO]}{dt}\right|_{Zeldovich}, \left.\frac{d[NO]}{dt}\right|_{EDC}\right\} \quad (3)$$

where $\left.\frac{d[NO]}{dt}\right|_{EDC} = \frac{C_{NO}\rho m_{NO}\varepsilon}{k}$.

Some researchers[5, 9] integrated the effect of turbulent pulsation on the temperature or concentration in the gas phase into the reaction rates. These models are complicated and some closure methods must be developed for each unclosed fluctuation term.

The thermal NO reactions take place in a few tens of microseconds, and are highly dependent on temperature, residence time, and atomic oxygen concentration[5]. In the diesel combustion chamber, the temperature and O concentration are non-uniform. Non-uniform burned gas temperature and composition result from the non-uniform fuel distribution during combustion. Reactions of NO depend on temperature and atomic oxygen concentration, with the reaction rate of NO determined by the mixing of high temperature eddies (containing less O and more N) and low temperature eddies (containing more O). If the chemistry solutions were solely used, the species conversion rates would be regarded as kinetics-controlled and this will result in very fast combustion rates.

The NO reactions have a typical time-scale on the order of 1 ms in the combustion zone[4, 5]. It is of the same order as the integral time-scale of turbulence in the vicinity of TDC of compression stroke[7]. Since these time-scales are nearly the same order of magnitude, the NO reactions could be partly controlled by the breakup of turbulent eddies which could result in a slower reaction rate. To account for the effects of both chemistry and flow turbulence, the present study proposes an integrated NO submodel that combines the extended Zel'dovich mechanism and engine CFD computations to simulate the NO histories in a diesel engine.

1 Model formulation

In this study, a NO sub-model was formulated to incorporate the effects of both chemical kinetics and turbulent mixing. The premise of the model is that the reaction rate is mainly determined by a kinetic timescale and a turbulent timescale. The kinetic timescale is the time needed for a species to reach its

equilibrium state under perfectly homogeneous conditions. The turbulent timescale is the time of eddy breakup in order to mix O contained in low temperature eddies and N contained in hot reaction products, supposing that inhomogeneities exist in the mixture. The model is expressed as

$$\frac{d[NO]}{dt} = \frac{[NO]_e - [NO]}{\tau_{kin} + C_{NO}\tau_{turb}} \quad (4)$$

where $[NO]$ is the current concentration, $[NO]_e$ is the equilibrium concentration which is expressed as $[NO]_{eq} = (k_{NO}[N_2][O_2])^{1/2}$ [4], and τ_{kin} is the kinetic timescale and is expressed as[4]

$$\tau_{kin} = ([NO]_e - [NO]) \Big/ \left.\frac{d[NO]}{dt}\right|_{Zeldovich}$$

The turbulent timescale τ_{turb} is the eddy turnover time and is equal to $\alpha k/\varepsilon$ [3] with α the model constant, k and ε the turbulent kinetic energy and its dissipation rate, respectively.

The sub-model expressed by equation (4) has the same formalization with the characteristic-time model for turbulent combustion, and then it is called the characteristic-time model for NO formation.

At mean temperatures above 1600—1800 K, thermal NO formation by the Zel'dovich mechanism is significantly increased[5]. NO formation occurs at the molecular scale as a result of collisions between reacting molecules. Subsequently, when the temperature increases, NO formation is strongly influenced by turbulence since the turbulence has significant effects on the transport properties and on the preparation of the reactants. In other words, the NO formation relies on laminar chemistry at the lower temperature (< 1800 K), and then becomes influenced by turbulence when the temperature is increased. The model is so formulated that the turbulence starts to have effect at temperatures above 1800 K by the use of the progress variable C_{NO}. The variable C_{NO} is a function of the temperature of each computational cell and is expressed as[8]

$$C_{NO} = 3.23\exp(10.5(T - 1800)/T)$$

If turbulent effects on the reaction rate are excluded, Eq. (4) can be simplified to a kinetics-controlled reaction rate as

$$\frac{d[NO]}{dt} = \frac{[NO]_e - [NO]}{\tau_{kin} + C_{NO}\tau_{turb}} = \frac{[NO]_e - [NO]}{\tau_{kin}} = \left.\frac{d[NO]}{dt}\right|_{Zeldovich} \quad (5)$$

A relation between the kinetic timescale and the equilibrium concentration of NO is obtained by rewriting the kinetics-controlled reaction rate (5)

$$[NO]_e - [NO] = \tau_{kin}\left.\frac{d[NO]}{dt}\right|_{Zeldovich} \quad (6)$$

By combining Eqs. (4) and (6), a new formula to compute the NO reaction rate can be obtained as

$$\frac{d[NO]}{dt} = \frac{\tau_{kin}}{\tau_{kin} + C_{NO}\tau_{turb}}\left.\frac{d[NO]}{dt}\right|_{Zeldovich} \quad (7)$$

The formula includes the effects of both chemical kinetics and flow turbulence on the reaction rate, and the turbulence that affects the NO formation rate by property transport, heat flux, and mixture preparation during the combustion process.

In the present study, the NO sub-model was implemented into STAR-CD3.22. The STAR-CD3.22 provides the NO sub-model with the species, thermodynamic, and turbulent information of each computational cell. The effects of both chemical kinetics and turbulent mixing are incorporated for solving the NO sub-model. The NO sub-model utilities return the new species information. Other numerical models for diesel engine combustion computations in STAR-CD3.22 include a RNG k-ε turbulence model modified for the variable-density engine flow[10], a wave breakup model of Reitz[11] adopted to model the spray dynamics, an ignition model based on the multi-step Shell ignition model[3], a wall heat transfer model with modified temperature wall function to account for the density variation in the boundary layer[12], and a combustion model extending the laminar-and-turbulent characteristic-time model of Abraham et al.[13].

2 Experiments and results

The present model was applied to simulate a Tacom diesel engine[14] with the specification and operating conditions shown in Table 1. This engine has a shallower bowl (i.e. quiescent chamber) and fuel spray is confined inside the combustion chamber without strong wall impingement. The cylinder mass-averaged nitric oxide histories were produced by the dumping technique (total cylinder sampling). The concept of the total cylinder sampling is to rapidly quench the NO reactions in the engine cylinder at a given crank angle by causing the cylinder contents to rapidly flow from the cylinder into a large evacuated receiving tank. Analysis of the receiving tank con-

tents gives an approximation of the mass averaged concentration of NO in the cylinder at the given crank angle. Repetition of the experiment at different crank angles then gives a history of cylinder average NO for a given operating condition.

The computations used tetradcane ($C_{14}H_{30}$) as the fuel due to the similar C/H ratio. The computational grid together with the droplets distribution in the combustion chamber is shown in Fig. 1, where injection started at −9 deg. ATDC.

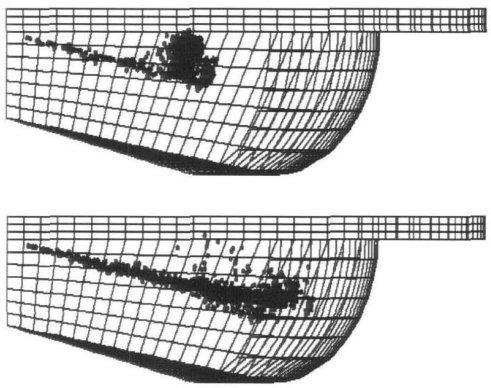

Fig. 1. Perspective view of computational grid and fuel droplet distribution for the Tacom engine. (a) At TDC; (b) 5 deg. ATDC.

The computed and measured cylinder pressures for cases 1 and 2 are shown in Fig. 2 and the agreements are very good. However, comparison of cylinder pressure alone is not enough to verify numerical models and temperature histories since the overall process also involves the fuel energy release rate and heat loss. The computed heat release rate data are also compared with those obtained by applying a zero-dimensional model to the measured pressure data as seen in Fig. 3. It can be seen that overall the predicted results agree well with the experimental data.

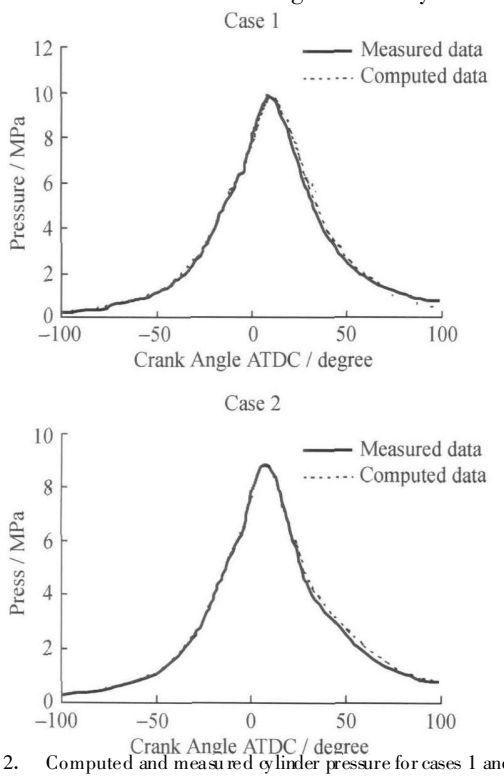

Fig. 2. Computed and measured cylinder pressure for cases 1 and 2.

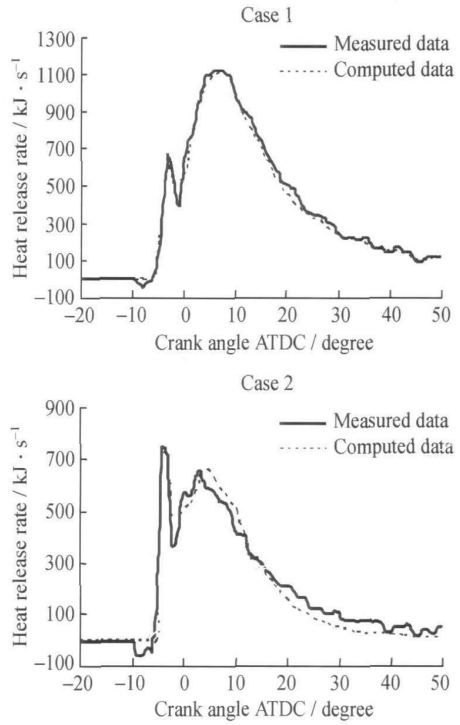

Fig. 3. Computed and measured heat release rate for cases 1 and 2.

Table 1. Tacom engine conditions

Engine type	4-Stroke; DI
Cylinder bore × stroke (mm)	114.3× 114.3
Connecting rod length (mm)	228.6
Displacement volume (L)	1.173
Combustion chamber	Quiescent
Piston crown	Mexican hat
Bowl diameter (mm)	88.9
Maximum depth (mm)	12.7
Compression ratio	16.0
Number of nozzle orifice× diameter (mm)	8× 0.18
Spray angle (from cylinder head)	7.5 degree
Inlet air pressure (kPa)	179
Inlet air temperature (K)	333
Swirl ratio (normal)	1.0
Engine speed (rpm)	1500
Fuel	Amoco Premier #2
Peak injection pressure (MPa)	65 for case 1 and 55 for case 2
Start of injection (CA deg. ATDC)	−9
Injection duration (CA degree)	16 for case 1 and 11 for case 2
Fuel injected (g/cycle)	0.067 for case 1 and 0.039 for case 2

NO formation in the combustion chamber was very sensitive to the gas temperature. The investigation above shows that the present STAR-CD3.22 can capture the gas temperature histories in the combustion chamber.

The computed NO formation histories of cases 1 and 2 are shown in Fig. 4 and are compared with the total cylinder content dumping experiment data. It can be seen that the present NO sub-model (i.e. Eq. (7)) predicts NO formation histories very well.

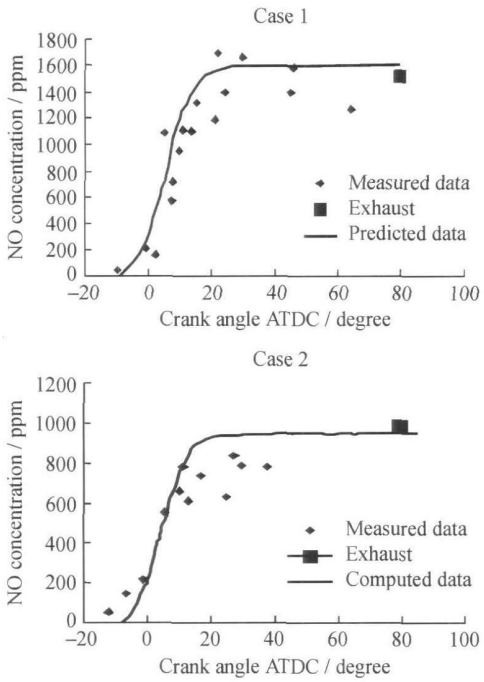

Fig. 4. The computed and measured NO histories for cases 1 and 2.

Engine emission experiments[15], where injection timing and loads were varied, were performed. The test engine is 485QDI Engine, which has a re-entrant combustion chamber and a smaller displacement volume than the previous engine discussed above. The specifications and operating conditions are shown in Tables 2, 3, and 4.

Table 2. 485QDI engine specifications

Engine type	4-Stroke; DI
Cylinder bore× stroke (mm)	85× 95
Connecting rod length (mm)	190
Displacement volume (L)	0.5388
Combustion chamber	Re-entrant
Piston crown	ω
Bowl diameter (mm)	45
Maximum depth (mm)	20
Compression ratio	18.0
Number of nozzle orifice× diameter (mm)	4× 0.28
Spray angle (from cylinder head)	20 degree
Inlet air pressure (kPa)	185
Inlet air temperature (K)	400
Swirl ratio (normal)	2.0
Engine speed	2000 rpm
Fuel	Diesel #0
Peak injection pressure	65 MPa

Table 3. Test conditions with varying loads

Load (%)/Torque (Nm)		50/55	58.7/65	68/75	80/85	86.5/95
Fuel injected (g/cycle)	8Degree BTDC	0.0122	0.0140	0.0157	0.0173	0.0192
	6Degree BTDC	0.0131	0.0148	0.0164	0.0182	0.0199

Table 4. Test conditions with varying fuel injection timing (load 68%)

Injection timing (BTDC)	2	4	6	8	10	12
Fuel injected (g/cycle)	0.0171	0.0167	0.0163	0.0158	0.0155	0.0152

The test engine was operated on a test bench instrumented for typical dynamometer experiments. A multipurpose control system was used for measuring and controlling torque, speed, inlet air temperature, exhaust temperature, etc; a Yike Fuel Consumption Meter (FCM-05) was used for measuring fuel consumption; a Bosch Smoke Analyzer (FQD-102A) was used for measuring the smoke density; a HORIBA Gas Analyzer (MEXA-7100) was used for measuring NO, HC, CO. In all tests the engine was allowed to warm up for 15 min to reach equilibrium. This is determined by monitoring the exhaust and coolant temperatures. More details about this engine and measurements are available from Yao[15].

The present model was also applied to model the engine-out NO. All model constants were kept the same. The effect of the loads and fuel injection timing on NO formation was investigated, and the computed and measured engine-out NO data are shown in Fig. 5 for comparison. As shown in Fig. 5, a good level of agreement was obtained and the general trends of reduced NO with fuel injection timing retard and increased NO with increasing loads are well captured by the present NO sub-model.

The measured engine-out NO data in the test was NO_x mass, i.e. the Summation of NO and N_2O mass, and the predicted NO data was only NO mass.

A calibration factor according to EPA was used to adjust NO data predicted from NO model to match engine NO data.

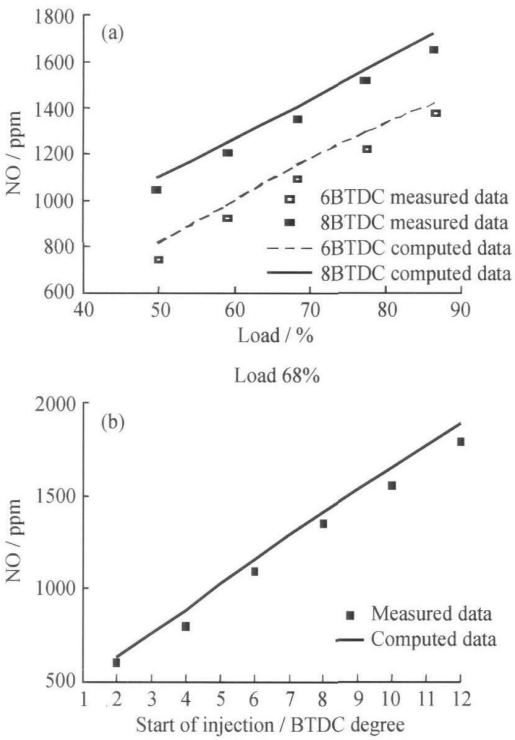

Fig. 5. Comparison between computed NO data and measured engine-out data[15] with varying loads (a) and varying fuel injection timing (b).

3 Summary and conclusion

A new NO sub-model was presented and implemented into the STAR-CD3.22 to simulate diesel engines NO formation. Exhaust NO was well predicted for a wide range of diesel engine operating conditions without any adjustment to kinetic constants.

The results show that the NO formation in the actual engine was controlled by the breakup of turbulent eddies and by chemical kinetics simultaneously. The sole use of the extended Zel'dovich mechanism will result in a significant difference between the NO data predicted and measured. It is necessary to incorporate the effects of flow turbulence into the extended Zel'dovich mechanism to simulate the NO formation correctly.

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