

Real time model for oxides of nitrogen emissions from a slow speed marine diesel

Dr L Goldsworthy

*Faculty of Maritime Transport and Engineering
Australian Maritime College*

A thermodynamic model is presented for predicting oxides of nitrogen (NO_x) emissions from slow speed marine diesel engines. The model is zero-dimensional, uses chemical kinetics for NO_x formation in multiple burnt gas zones, and runs in real time on a standard PC. The mean fuel/air mixture strength at which NO_x forms and the rate of dilution of the burnt gas by unburnt air, are adjustable. Two MAN B&W IMO NO_x-compliant slow speed diesels are modelled. Effects such as variations in fuel spray interaction with load are accounted for in the calibration of the model. The effect of dilution rate and equivalence ratio on NO_x formation is studied. It is shown that, under certain conditions, there is a critical burnt gas dilution rate which maximises NO_x. The model responds adequately to changes in engine load and to NO_x control measures such as water injection, injection timing retard, exhaust gas recirculation and humidification.

INTRODUCTION

Worldwide, ship oxides of nitrogen (NO_x) emissions have been estimated at about 10 million tonnes per annum, equivalent to about 50% of the land based NO_x emissions from the USA or 14% of total NO_x emissions from fossil fuels.¹ NO_x emissions participate in photochemical smog, acid rain and eutrophication. Marine sourced emissions can have significant impact on air quality on land, especially near busy coastal waterways.

The Air Pollution Annex to Marpol (Annex VI) aims to limit NO_x emissions to 17g/kWh for slow speed marine diesels under a test cycle.² It is likely that further restrictions will occur.

Marpol Annex VI prescribes four load points at which NO_x is to be measured, with the overall NO_x output found by weighting the varying load measurements. Measurements for test cycle E3 (propeller law) are used in the present study.

The NO_x model is developed for use in a machinery space simulator for training marine engineers³ and in a predictive emissions monitoring system. Inclusion of an intelligent NO_x model in the simulator mathematical model allows engineers to develop an awareness of the ways in which engine operating conditions and NO_x control measures affect NO_x output and fuel

consumption. The model could potentially be used onboard to predict actual emissions of a ship equipped with NO_x certified engines, as part of an environmental performance monitoring system under ISO 14000.

NO_x MODELLING

Models for prediction of NO_x emissions from diesel engines essentially consist of models for predicting gas temperature, pressure and composition, combined with models for predicting NO_x using this computed combustion history. The NO_x formation chemistry is generally decoupled from the combustion chemistry. The complexity of combustion models ranges from zero-dimensional, fully mixed (single zone) models using semi-empirical equations for calculating burning rate, to the modern three-dimensional CFD models. Basic models have a role for applications where rapid execution is required. The insights into the combustion process gleaned from CFD modelling and modern measurement techniques, for mapping in-cylinder combustion and NO formation, can be used to refine real time models.

Dec and Cnaan⁴ used planar laser induced fluorescence (PLIF) on a quiescent DI diesel engine of 140mm bore, at 1200 rev/min. They demonstrated that nitric oxide (NO) forms mainly in a thin layer on the fuel-lean side of the diffusion flame, around the periphery of the jet. NO is the primary constituent of NO_x. It is uncertain how these studies relate to slow speed marine propulsion engines. Zabetta and Kilpinen⁵ postulate that in low speed engines, any mixing will tend to be on the fuel-lean side of the jet. The fuel spray penetrates the relatively quiescent mass of

AUTHOR'S BIOGRAPHY

Laurie Goldsworthy has been a lecturer in thermodynamics and computer aided design at the Australian Maritime College (AMC) since 1985. His area of research interest is marine diesel engine combustion and emissions. Laurie is currently expanding AMC's involvement in marine engine research.

air, and a layer forms on the periphery of the spray where the mixture strength grades from rich to lean. There will be a relatively long time available for the NO-rich gases around the periphery of the fuel spray to mix with colder surrounding unburnt gases. In high speed engines, the high air motion may result in significant air penetration into fuel-rich zones. Thus, NO formation mechanisms which are favoured for fuel-rich conditions may be more relevant in high speed engines. Also, in low speed engines, there may be enough time and enough heating of very fuel-lean areas ahead of the flame, for NO formation mechanisms which are favoured for lower temperatures and leaner mixtures, to produce significant NO.

Paro⁶ describes the use of metal surfaces in proximity to the burning fuel spray to cool the burnt gases and reduce NOx.

Thus, essential features of NO formation in low speed engines probably involve NO formation on the lean side of the flame and mixing of NO-rich regions with unburnt gases. Cooling of the NO-rich regions by metal surfaces may be a significant factor. Incorporation of these features into a real-time model in a meaningful way is a major aim of the present study

A number of basic models which are potentially simple enough to operate in real time have been developed. These models are all zero-dimensional, in that they do not attempt to resolve the in-cylinder processes spatially.

Tree and Cooley⁷ describe recent work where the inverse of a single time-weighted adiabatic flame temperature was correlated with the log of fuel specific NOx. They assumed NOx was formed in a thin layer on the lean side of the turbulent diffusion flame. The time-weighted adiabatic flame temperature was calculated using a simple chemical kinetic model with temporally resolved temperatures. This required the calculation of adiabatic flame temperature at a number of stages throughout the cycle. The resulting correlation was good, demonstrating the value of calculating adiabatic flame temperature throughout the NO formation period. Previous correlations have found a linear relationship between the logarithm of fuel-specific NOx against the inverse of a single adiabatic flame temperature calculated at top dead centre or peak pressure.⁸

Dodge et al⁹ and Goldsworthy¹⁰ calculated adiabatic flame temperature at a number of stages throughout the burn duration, as an input to a semi-empirical correlation for NOx against flame temperature. NOx models which use correlations with adiabatic flame temperature, rather than following the evolution of NOx using chemical kinetics, are unlikely to predict the impact of variations in duration of NOx formation.

Easley et al¹¹ described ongoing development of a characteristic time model for NO formation and decomposition in high speed direct injection diesel engines. They assumed two zones surrounding the burning spray, one for NO formation and one for NO decomposition. Adiabatic flame temperature calculated at start of combustion was used to characterise the NO formation process. NO formation and decomposition rates were based on the extended Zeldovich mechanism¹² with two nitrous oxide reactions added.

Heider et al¹³ described a two-zone model for NO emissions from diesel engines. A fully mixed combustion model provided the mean temperature and heat release history, primarily using measured pressure history. A burned zone and an unburned zone were used in the NO predictions. The two zones were allowed to mix. The rate of mixing between the two zones was the primary

parameter which was used to calibrate the model for a given engine. Turbulent mixing was considered to be more important than flame radiation or convective heat transfer, in determining the temperature of the burnt gas zone. The mixing process was characterised by the temperature difference between the two zones, which started at its maximum value at the beginning of combustion and finished at zero at the end of expansion. The extended Zeldovich mechanism for NO was integrated over the temperature history of the burnt gas zone, assuming stoichiometric air/fuel ratio throughout.

Models which represent NO formation in a single zone are unlikely to represent the range of temperature and composition histories during which NO forms. In reality, NO will begin to form in different regions at different times throughout the burn history

Weisser¹⁴ developed a zero-dimensional model for a medium speed diesel engine which allowed for the formation of NOx in multiple burnt gas zones. The zones were formed sequentially during combustion, and allowed to mix with unburnt air at a rate dependent on the turbulence levels. It was assumed that the combustion process occurred at stoichiometric mixture strength and produced burnt gas at the adiabatic flame temperature and at chemical equilibrium. The individual zones were defined by the period during which they were formed, rather than by their spatial distribution. Mixing between the burnt gas zones was not allowed.

Similarly, the present study employs multiple burnt gas zones, adiabatic flame temperature, chemical kinetics, NO formation on the lean side of the flame, mixing of the burnt gas with unburnt air and extra cooling by metal surfaces. Unlike Weisser's¹⁴ model, detailed spray and turbulence calculations are not performed, as the model has to run in real time on a standard PC. Turbulent mixing rates are derived empirically from the burn rate, which is inferred from measured peak cylinder pressure and engine power at a number of representative engine-operating conditions.

THE COMBUSTION MODEL

AMC's marine diesel simulator mathematical model predicts power output, cylinder pressure, heat release rate, exhaust temperature and thermal efficiency using a simple combustion model.¹⁰ The model employs a modified Whitehouse Way method for calculation of burning rate. The whole combustion space is considered as a single zone for the combustion model, which calculates a single, varying-bulk gas temperature throughout the cycle. The multi-zone model for NOx emissions has been superimposed onto this simple combustion model.

NOx MODEL

Representative NO zones

To create a realistic temperature history for the NO formation regions, a number of zones are created as combustion proceeds. The zones attempt to represent the gas mixture where NO forms, starting from a given time in the combustion process. A typical NO zone corresponds to a single step in the combustion calculations. The initial mass of an NO zone is the mass of the fuel/air mixture consumed during the corresponding step in the combustion calculations. Thus, a number of zones of known mass are created and the evolution of NO in each of those zones is followed kinetically. The first zone represents the earliest NO formation. The last zone represents the NO formation which begins at the

end of combustion. The number of zones is much less than the total number of calculation steps for the combustion period. At the end of combustion, the total NO is found by averaging the NO from subsequent zones and summing the average values, weighted according to the mass of fuel burnt between the starting angles of the subsequent zones. This approach essentially follows the kinetic evolution of NO in representative parcels of burnt gas.

The temperature history of each NO zone is followed by a simplified energy analysis which accounts for compression/expansion, heat transfer and mixing of the gas with unburnt air. The starting temperature for each NO zone is the constant pressure adiabatic flame temperature at that time. The constant pressure adiabatic flame temperature is known to be representative of diffusion flame temperatures.¹⁵ The fuel/air equivalence ratio for the flame temperature calculations is set at a single value less than one (fuel-lean) for all zones, and this value is an input to the model.

In a slow speed engine, the turbulence levels during combustion will be determined by the rate of injection/combustion as well as the swirl velocity.¹⁶ The major part of the combustion process will be mixing rate controlled. Thus, the burn rate is controlled by the turbulence levels, which control the mixing of fuel and air as well as the mixing of the burnt gas with unburnt charge. In the present model, the rate of mixing is controlled by the burn rate. The burn rate is determined by setting the combustion model parameters to give the required cylinder pressure development. The rate of mixing of unburnt charge with an NO zone is defined as the fractional zone mass change per second. For example, a dilution rate of $25s^{-1}$ signifies a change of mass of 2.5% of the original zone mass, per millisecond.

The chosen equivalence ratio determines the NO zone temperature and composition. This allows for the formation of NO in fuel-lean areas ahead of the flame and in diluted post-combustion gases. Even if the combustion occurs near to stoichiometric conditions, the gases well ahead of the flame will be subject to lower temperatures than the stoichiometric flame temperature. Combustion will occur, and NO will form, over a range of temperatures and compositions. Combustion products will diffuse into the unburnt gas ahead of the flame, and oxygen will

diffuse from the unburnt air to the flame. The present model attempts to simulate these complex processes with NO zones which follow broadly representative temperature and composition histories.

The heat transfer rate is taken as a proportion of the total cylinder heat transfer rate, weighted by the mass of the NO zone. Local cooling of burnt gas zones by metal surfaces may be an important NOx control measure. This is modelled by allowing the heat transfer rates from the NO zones to be greater than the overall heat transfer rate, by applying a single multiplying factor to the heat transfer rates from the NO zones, up to 20deg after top dead centre (TDC). The extra cooling due to the proximity of the metal surfaces would be most important around TDC where the clearance space is small. Setting this extra cooling to zero at 20deg after TDC increases NOx by only about 1.5% compared with allowing it to act throughout the burn.

To reduce computation time the number of zones is set at 10.

As the unburnt air mixes with the burnt gas, the equivalent fuel/air mixture strength is calculated. This is then used in the calculation of equilibrium composition which is, in turn, used in the NO kinetics calculations. The temperature of the air mixing into the NO zones is found by assuming adiabatic compression/expansion from the cylinder conditions just prior to ignition. This same temperature is used as the reactants temperature for the initial flame temperature calculations. The kinetics model could be improved by using a two zone model instead of a fully mixed model for the combustion process, to give more accurate representation of the state of the unburnt gas.

The zones are distributed through time by setting one zone at the start of combustion, one at maximum cylinder pressure and two zones in between. A further six zones are distributed between maximum pressure and end of burn. The earliest zones produce the maximum NO, so more zones are allowed where NO production is greatest.

NO kinetics

A number of reduced kinetics schemes were evaluated.¹⁷ The scheme developed by Zabetta and Kilpinen^{5,18} was chosen be-

Table 1: Reference engine operating conditions - Indicative data supplied by MAN B&W for a 7L70MC mk6 IMO NOx-compliant engine with VIT

load	100%	75%	50%	25%
speed (rev/min)	108	98.1	85.7	68.0
scavenge pressure (MPa absolute)	0.360	0.280	0.200	0.138
exhaust pressure (MPa absolute)	0.327	0.253	0.181	0.125
fuel/cylinder/s (kg/s)	0.13678	0.10088	0.06839	0.0360
air/cylinder/s (kg/s)	7.3095	5.885	4.190	2.164
scavenge temperature (°C)	41	34	29	34
power (MW)	19.810	14.858	9.905	4.953
compression pressure (MPa abs)	13.1	10.1	7.5	5.1
maximum pressure (MPa abs)	14.1	12.6	9.9	7.0
cylinder cooling load (kW)	3000	2400	1890	1335
injection angle (degrees after BDC)	179.0	178.5	179.5	179.5
measured NOx (g/kWh)	13.6	17.6	19.1	16.5

cause it was derived in the context of large marine propulsion diesels, and a relatively-simple solution technique was available. It involves the extended Zeldovich mechanism, a two-step 'N₂O Intermediate' path and five additional reactions, called the 'N₂O Extension' path, which involves oxidation of N₂O to NO via NH and HNO intermediates. This scheme is likely to give significant NO production in fuel lean areas. Nitrous oxide reactions are important in this context.^{19,20} The nitrous oxide pathway also assumes more importance with water injection or exhaust gas recirculation.²⁰

Mostly NO is formed initially. This is partially oxidised to NO₂ in the exhaust. Final NO_x output in g/kWh is calculated by assuming that all NO produced becomes NO₂.²

A small proportion of engine NO_x is derived from fuel-bound nitrogen (up to 10% for engines operating on residual fuel oil²¹). Precise modelling of this source of NO requires a degree of detail in modelling of the combustion chemistry, which is prohibitive given the small contribution to NO_x.¹⁴ Bazari²² assumed that all fuel-bound nitrogen is converted to NO. This simplified approach would give some measure of the impact of changes in fuel nitrogen on NO_x, if the nitrogen content of the fuel was known. The data used in the present study are for an engine operating on test bed gas oil, hence NO_x from fuel-bound nitrogen will be negligible.

REFERENCE CONDITIONS

The primary engine simulated is a MAN B&W 7L70MC mk6, direct injection, turbocharged, aftercooled, uniflow scavenged, slow speed marine diesel, with the following specifications:

- Number of cylinders = seven
- Bore = 0.70m
- Stroke = 2.268m
- Effective compression ratio = 12.60
- Ratio of connecting rod length to stroke = 1.2037
- Fuel calorific value = 42700kJ/kg
- Fuel carbon to hydrogen ratio (mass) = 7
- Specific humidity of charge air = 0.01071kg/kg dry air (ISO reference humidity)

Measured Data

Indicative data were supplied by MAN B&W for the modelled engine, and inferred from design data and shop trial data, as detailed in Table 1. The engine has variable injection timing (VIT). The load/speed relationship is the propeller law.

FITTING THE MODEL TO THE SUPPLIED DATA

Setting the combustion model

A fixed delay time between start of injection and start of combustion was set for all load points. This was set at the time for a 1.5deg delay at 100% load. This represents a delay time of 2.3ms. Indicative delay data from MAN B&W for an L42MC test engine for a number of fuels of varying CCAI showed a delay time of 1.4ms to 1.9ms at 100% load and similar or lower delay times at 25% load. The delay time would change with operating conditions but definitive data were not available.

The combustion model allows matching to measured data by adjusting burn rate, injection timing and heat transfer rate. Relative injection timings over the load range were inferred from available data. Initially, the 75% load point was matched for peak pressure and power, using an injection timing of 178.5deg after bottom dead centre (BDC). This gave a good match to a typical pressure vs crank angle plot for a real engine. Measured pressure traces for a K98MC with VIT were used as a guide for this initial setting. In a real engine with VIT, timing is advanced as speed increases then retarded at high loads to reduce maximum pressure. Shop trial data over the load range for a 7L70MC with VIT were plotted and used to set the timings relative to the 75% load point. A MAN B&W service letter on VIT²³ and design data were used to relate VIT control pressure to injection timing.

Mechanical efficiency was obtained from shop trial data for a 7L70MC. The nominal fuel injection rate was set at $5.4 \times 10^{-6} \text{m}^3/\text{deg}$ on the basis of shop trial data and design data for a 7L70MC.

The model burn settings were chosen to give close match of power and peak pressure. The predicted performance data are presented in Table 2. The predicted pressures for the four reference load conditions are plotted in Fig 1. To apply the model at any load, the values of burn parameters at the four load points are interpolated using the load index.

Within a reasonable range of injection timing, predicted NO_x depends primarily on the value of maximum pressure predicted. Thus, different combinations of the burn rate constants will yield similar predicted NO_x if the peak pressure is correctly predicted. At 75% load, for variations in injection timing of 0.5deg either side of the reference value of 178.5deg after BDC, the range of variation of predicted NO_x is only 3% if the burn constants are adjusted to give the same maximum pressure and power.

The scavenging efficiency will be lower at low loads, where the

Table 2: Engine combustion model outputs at the reference conditions, 7L70MC

load	100%	75%	50%	25%
maximum pressure (MPa)	14.1	12.6	9.9	7.0
power output (MW)	19.81	14.86	9.91	4.95
compression pressure (MPa)	13.1	10.3	7.4	5.1
air temperature at injection (°C)	559	544	535	545
maximum pressure rise rate (MPa/deg)	0.31	0.49	0.52	0.38
exhaust temperature before turbine (°C)	333	284	257	259
cylinder cooling load (kW)	3006	2391	1869	1325
crank angle at peak pressure (deg after BDC)	188.8	189.9	190.9	189.9

mass flow rate of air through the engine is much lower. A lower scavenging efficiency will result in lower charge purity and thus reduced NO_x. This is similar to the effect of exhaust gas recirculation. To simulate the effect of scavenging efficiency, a linear increase in the residuals ratio (ratio of residuals mass to charge mass) over the load range is imposed. Thus, charge purity is varied from 100% at full load to 97.5% at 25% load.

PREDICTION OF NO_x VARIATION WITH LOAD

The trend for NO_x to increase as load decreases is dominant. This is explained as follows:

- The air temperatures at the start of combustion are determined by the scavenging temperature and the speed of compression.
- Subsequent air temperatures are determined more by the ratio of maximum cylinder pressure to compression pressure. This ratio increases as load decreases, from 1.08 at 100% load to 1.37 at 25% load.
- Higher air temperature leads to higher flame temperature, so this increasing pressure ratio produces higher flame temperature.
- The amount of NO produced depends on the temperature during formation and the duration of high temperature.
- The burnt gas from combustion before maximum pressure produces most of the NO. This gas is subject to further compression during NO formation, increasing the duration and level of high temperature.
- The degree of compression of the burnt gas increases as load decreases because the ratio of maximum cylinder pressure to compression pressure increases.
- The duration increases as load decreases, because engine speed decreases. In addition, the mass of fuel burnt before maximum pressure increases as load decreases, from about 20% at full load to 52% at 50% load, then decreasing slightly to 44% at 25% load.

Thus, the dominant trend is for NO_x to increase as load decreases. Other factors such as interaction between fuel jets and changing scavenging efficiency can disrupt this trend.

Setting of kinetics model parameters

The present model is a highly simplified representation of the governing processes. This simplified approach is required to allow the model to operate in real time on a standard PC. Thus, it is necessary to adjust parameters to give the required outputs. The available parameters for adjustment are flame temperature, dilution rate, and initial equivalence ratio of the NO zones. It is assumed that, by adjusting the model parameters to match the four measured load points, the model will respond adequately at any load to normal variations in operating conditions as well as NO_x control measures, because it is based on real physical processes.

Flame temperature

The adiabatic flame temperature is an upper estimate of the combustion temperature. Factors such as flame radiation and non-equilibrium chemistry may result in a lower actual temperature than the adiabatic flame temperature. Current CFD models tend to underpredict combustion temperature and thus NO_x, especially for slow speed engines, where the grid size is a limita-

tion. NO_x may be underpredicted by a factor of 2 to 5.^{16,24} In the present study, predicted NO_x is in the range of measured NO_x when using adiabatic flame temperature as the starting temperature for the NO zones.

Effect of initial equivalence ratio

The effect of initial equivalence ratio for the NO zones at 75% load, for a range of dilution rate factors, is shown in Fig 2. Maximum NO_x is predicted at initial equivalence ratio of 0.95 to 0.97, depending on dilution rate. Similar results were found at all loads. This effect is a result of the interplay between decreasing temperature and increasing oxygen content and is well known in premixed spark ignition engines, where maximum NO_x occurs for equivalence ratio just fuel-lean of stoichiometric.²⁵

A common approach in engine combustion models is to assume that combustion occurs, and burnt gas is formed, at stoichiometric mixture strength. In reality, combustion will occur over a range of mixture strengths. In addition, the gases well ahead of the flame will be subject to heating by the flame. Thus, the most representative initial fuel/air mixture strength for the burnt gases in the present context may be less than stoichiometric.

Maximum dilution rate

For an upper estimate of the rate of mixing, the mass of the NO zones at end of combustion was compared with the total cylinder mass. The maximum amount of mixing is allowed when the mass of the NO zones equals the total cylinder mass at the end of combustion. NO formation and decomposition is virtually complete by the end of the combustion process.

At an initial equivalence ratio of 0.96, the estimated maximum allowable dilution rate over the load range is about three times the burn rate at all loads, where dilution rate and burn rate have the units s⁻¹. At 100% load, this represents a dilution rate of 5.4s⁻¹ at the maximum burn rate of 1.8kg/s. The rate of change of mass of an NO zone, due to dilution by unburnt charge, is found by multiplying the initial zone mass by the dilution rate.

Effect of dilution

The effect of dilution rate factor is shown in Fig 3. The dilution process provides oxygen while reducing temperature. At a critical dilution rate, the increased oxygen increases NO formation rate and the decreasing temperature reduces NO decomposition. A maximum NO_x value occurs for intermediate dilution rates, at a dilution rate factor of 0.2 to 0.3, depending on initial equivalence ratio. Thus, it is possible to simulate a measured NO_x level using two different values of dilution rate. Similar results were found at all loads.

Weisser¹⁴, using a zero-dimensional model of medium speed diesels, showed this effect of maximum NO_x for intermediate dilution rates. By modelling the turbulence levels in the combustion chamber, Weisser demonstrated that the higher dilution rate is the correct choice. This approach has been adopted in the present work. Weisser also demonstrated that the turbulent time scale which determines combustion rate will be similar to that which determines the rate of mixing of unburnt air with burnt gas. In the present study, a dilution rate factor of 1 represents the situation where unburnt air mixes into the burnt gas zones at the same rate as that at which unburnt air is consumed by combustion.

Matching the measured values

A single value of initial equivalence ratio combined with a single value of dilution rate factor over the load range did not give the required dependence of NO_x on load. For all such combinations, the NO_x output tended to increase as load decreased. This is the measured trend except at 25% load, where measured NO_x falls to a value between the full load value and the 75% load value. Thus, the 25% load point was a dominating factor in searching for the right combination of settings. The 25% load point is not critical as far as complying with IMO Annex VI is concerned, as it only has a 15% weighting. However, it is of considerable interest from a modelling point of view and for engine operation in areas of more severe NO_x restriction than the current IMO levels. The auxiliary blower will be operating at 25% load and this will influence the mass flow rate into the engine.

Whether the NO_x value at 25% load is higher or lower than at higher loads, depends very much on the particular fuel nozzle configuration.²⁶ The interaction between the sprays from individual holes in the nozzle has considerable effect on NO_x.²⁷ The main factor seems to be the availability of oxygen to the high temperature burnt gases. The interaction between the sprays will change with load. Two approaches are available in the present model to account for changes in oxygen availability. One is to vary the initial equivalence ratio, the other is to change the dilution factor.

Given that the common approach in engine modelling is to assume a constant initial equivalence ratio for combustion, and that the modelling of dilution rates in the present model is a gross simplification of the turbulent processes in the engine, dilution factor was chosen as the parameter to be adjusted with load.

It is observed that, for stoichiometric initial equivalence ratio, the NO_x values measured at intermediate loads are under-predicted for any value of dilution factor. A constant initial equivalence ratio of 0.96 is chosen. It is the equivalence ratio for maximum NO_x at intermediate dilution factor. Any value of initial equivalence ratio between 0.92 and 0.98 would suffice.

Dilution factor is adjusted to match predicted and measured NO_x. The required values of dilution factor against engine load are plotted in Fig 4.

This is the chosen reference configuration for the kinetics model for the 7L70MC. To apply the model at any load, the values of dilution factor at the four load points can be interpolated using load index.

Predicted NO_x history

The zonewise NO history for 75% load is shown in Fig 5. A definite peak in the NO concentration occurs for the early burned gases, but is not apparent for the late burned gases. Calculations for the early burned gas show that at the crank angle corresponding to the maximum value of NO concentration, NO is still being produced by the kinetics mechanism, but the rate of decrease of NO concentration due to dilution begins to outstrip the rate of production. Decomposition of NO by the kinetics mechanism begins at a later crank angle, but never reaches a significant value compared with the early formation rates, because the falling temperature effectively freezes the kinetic mechanism. Similarly, NO decomposition is not significant in the later burned gases. The NO peak is absent for the later burned gases, because dilution is not as significant due to the lower combustion rate.

Thus, final NO concentration is generally formation-rate

limited in the present context. This is apparent for all load points.

Extra cooling for NO_x control

The effect of the extra cooling of the NO zones by metal surfaces is investigated. At the 75% load point, increasing the cooling rate factor from two to four gives 3% less NO_x. Reducing the cooling rate factor to zero gives 3% more NO_x. The factor is useful for illustrating the potential for NO_x control by increasing local cooling during NO_x formation. In real engines this is achieved by design of the spray pattern and by reducing piston temperature.

Application to other engines

For comparison purposes, published NO_x data²⁸ for an IMO-compliant MAN B&W 12K98MC slow speed engine are modelled. Measured NO_x is 12.5, 15.0, 15.3 and 15.4g/kWh at 100%, 75%, 50% and 25% load respectively.

The combustion model settings are partly derived from 12K98MC shop trial data and partly from the 7L70MC data supplied by MAN B&W. It is assumed that the combustion parameters for an IMO NO_x-compliant K98MC would be similar to those for an IMO NO_x-compliant L70MC. For the four ISO load points, predicted power output and maximum cylinder pressure are matched to the data by adjustment of the burn constants.

It is observed that, with initial equivalence ratio of 0.96 for the NO zones, and dilution rate factor decreasing linearly with load from 1.1 at 100% load to 0.54 at 25% load, NO_x simulated by the kinetic model can be matched with the measured values at the four ISO load points.

Work is underway to automate the procedure of matching the combustion model and the NO_x model to any given engine data set. Also, the performance of the model for engines driving a controllable pitch propeller will be assessed, as data become available. It is feasible that the model could be fitted to the parent-engine test data which would be given in the technical file of any engine certified in accordance with the NO_x Technical Code.² The model could then be used to predict the deviation, from the certified values, of the emissions of an in-service engine, under the influence of varying operating conditions.

NO_x CONTROL MEASURES

The model accounts for the impact of various NO_x control measures, primarily through changes in the stoichiometry of the combustion process. These affect the adiabatic flame temperature and the gas composition.

Water injection, fuel/water emulsion

Introduction of water into the combustion chamber reduces combustion temperature due to the absorption of energy for evaporation, increased specific heat capacity and reduced oxygen concentration. Water can be introduced in the charge air (humidification), through direct injection into the cylinder or through water/fuel emulsion. Water/fuel emulsions and, to a lesser extent, direct injection of water, place the water more directly in the combustion region, where it has maximum effect on NO_x production.

All the injected water does not reside in the combustion zone. This is accounted for by applying a water diffusion factor^{9,10}, which represents the proportion of the injected water present in

the reactants and products in the calculation of flame temperature. This factor is set to 0.8 to give sufficient prediction of the impact of water injection on NO_x. Tanner et al²⁴ have demonstrated the importance of the way in which the water is injected on the degree of NO_x control.

It is assumed that the water has evaporated before taking part in the combustion. The energy of evaporation is taken from the bulk gas.

Humidification

The water content of the charge air can be increased by injection of water into the inlet air, or by the method of Munters Euroform²⁹ whereby the charge air cooler is replaced by a humidifier which increases the air humidity to about 95%.

Wärtsilä is developing a combustion air humidification system⁶ in which a nozzle is used to inject water after the turbo-charger. It is claimed that there is about a 70% NO_x reduction from a medium speed engine for saturated air at about 70°C, without significant fuel consumption increase.

A disadvantage of humidification or injection of the water into the inlet air is that only a small proportion of the injected water will be present in the combustion region. In the present model, water added to the inlet air is assumed to take no energy from the charge air and is accounted for by adding to the initial charge air humidity.

Humidification for NO_x control is mainly being developed for medium speed engines. However, it is important that the model responds adequately to changes in inlet air humidity.

Exhaust gas recirculation (EGR)

EGR lowers the combustion temperature, thus lowering NO_x. EGR reduces combustion temperature by increasing the specific heat capacity of the cylinder gases and by reducing the overall oxygen concentration. Recent work by Wärtsilä NSD⁶ proposes the use of 'cooled rest gas', ie internal EGR with the retained gases cooled by water injection during compression.

The present approach simply allows for the presence of exhaust gas in the cylinder at start of compression, at the charge air temperature. The extent of EGR is defined as the ratio by mass of residuals to charge air (residuals ratio). The composition of the residuals is taken to be the same as the composition of the exhaust gases from the previous cycle.

Model prediction of parametric effects

Real data on NO_x control measures have been drawn from a number of sources for a range of engine types.^{21,30-33} While there is no guarantee that those data will be directly applicable to the particular engine being modelled, there appears to be similarity in the measured trends across the published data.

The predicted effect on NO_x emissions of water injection, injection retard, humidity of the inlet air, EGR and some combinations of these measures, are presented in Table 3. The results are compared with published data. Within the variability of the published data, the model sufficiently predicts the effects on NO_x and BSFC of direct water injection, injection timing retard, EGR and humidification.

Table 3: Predicted parametric effects on NO_x at full load, 7L70MC
(% change from reference condition in brackets)

Test Condition	NO _x /kWh	BSFC g/kWh	published data for comparison
Reference conditions	13.6	174.0	
Fuel/water emulsion or direct injection 50% water*	7.9 (-42%)	174.7 (+0.4%)	up to 50% NO _x reduction, 0% to 5% increase in fuel consumption ^{21,30,31}
Injection timing retard by 2 deg	11.9 (-13%)	177.3 (+1.9%)	10% NO _x reduction, 2% increase in fuel consumption ^{21,32}
70% water injection +2 deg retarded injection	5.2 (-61%)	178.2 (+2.4%)	60% reduction 3 to 4% fuel consumption rise ³³
humidification of scavenge air to 95% at 70(°C) 0.057kg/(kg air) at 0.36MPa)	6.8 (-69%)	182.8 (+5.1%)	70% reduction in NO _x , no rise in fuel consumption ^{6,29}
EGR† 6%	9.6 (-29%)	174.3 (+0.2%)	25% reduction in NO _x ^{21,33}

$$*\text{Water \%} = \frac{\text{mass of water}}{\text{mass of fuel}}$$

$$†\text{EGR \%} = \frac{\text{mass of residuals}}{\text{total cylinder mass}}$$

In contrast to published data, the combustion model predicts a significant increase in fuel consumption due to humidification at higher scavenge temperature. This is due to the increased scavenge air temperature. For the same humidity, but at normal scavenge temperature, the combustion model predicts negligible change in BSFC.

The model appears to slightly overpredict the reduction in NO_x due to EGR, but the available data are limited. In addition, the model assumes the recirculated gases are at the scavenge temperature. In a real engine they are likely to be at a higher temperature, which will lessen the NO_x reduction.

CONCLUSIONS

A thermodynamic model is presented for predicting NO_x emissions from slow speed marine diesel engines in real time, using chemical kinetics. Dilution of the burnt gas by unburnt air during NO formation is modelled.

For the MAN B&W 7L70MC slow speed engine which was modelled, the ratio of maximum pressure to compression pressure increases as load decreases. Thus, the degree of compression of the burnt gas increases as load decreases, resulting in higher temperature and longer duration of high temperature for NO formation. Additionally, more time is available for NO formation as speed decreases, and the mass of fuel burnt before maximum pressure increases as load decreases. These three factors result in the dominant trend of NO_x increasing as load decreases. The changing behaviour of interacting nozzle jets and scavenging efficiency can disrupt this trend.

Effects such as variations in fuel spray interaction with load are accounted for in the calibration of the kinetic model, by varying the dilution rate factor. A constant initial equivalence ratio for the NO_x values is set at a value less than 1. It is proposed that once the model is fitted to a sufficient number of measured load points, it will simulate NO_x adequately for a range of varying operating conditions, because it is based on real physical processes. More testing against real data is required to fully establish the capabilities of the model.

The model gives adequate prediction of the impact on NO_x and BSFC of the major primary NO_x control measures.

The model predicts that dilution of the burnt gas with unburnt air can increase or decrease NO_x, depending on conditions. Intermediate dilution rates give the highest NO_x. The model also predicts that NO production is generally formation rate limited.

REFERENCES

1. Corbett, JJ, and Fischbeck, P. *Emissions from Ships*. Science. Vol 298: pp 823-824 (1997).
2. IMO, *Protocol of 1997 to amend Marpol 73/78, Annex VI of Marpol 73/78 Regulations for the Prevention of Air Pollution from Ships and NO_x Technical Code*. (1998).
3. Goldsworthy, L, Jung Byung-Gun, Niekamp, P, and Earl, S. *Development of the Australian Maritime College PC Based Machinery Space Simulator*. MARTECH 2002 Conference Proceedings, Singapore (2002).
4. Dec, JE, and Canaan, RE. *PLIF Imaging of NO Formation in a DI Diesel Engine*. SAE 980147 (1998).
5. Zabetta, EC, and Kilpinen, P. *Improved NO_x Submodel for In-Cylinder CFD Simulation of Low- and Medium- Speed Compression Ignition Engines*. Energy and Fuels. Vol 15(6): pp 1425-1433 (2001).
6. Paro, D. *Development of the Sustainable Engine*. 23rd CIMAC Congress (2001).
7. Tree, DR, and Cooley, WB. *A Comparison and Model of NO_x Formation for Diesel Fuel and Diethyl Ether*. SAE 2001-01-0654 (2001).
8. Ahmad T, and Plee, L. *Application of Flame Temperature Correlations to Emissions from a Direct-Injection Diesel Engine*. SAE 831734 (1983).
9. Dodge, LG, Leone, DM, Naegeli, DW, Dickey, DW, and Swenson, KR. *A PC Based Model for Predicting NO_x Reductions in Diesel Engines*. SAE 962060 (1996).
10. Goldsworthy LC. *Simulating Primary Control Measures for Oxides of Nitrogen Emissions in a Slow Speed Marine Diesel Engine*. Sea Australia 2000 Conference Proceedings, Sydney (2000).
11. Easley, WE, Mellor, AM, and Plee, SL. *NO Formation and Decomposition Models for DI Diesel Engines*. SAE. Vol 582 (2001).
12. Lavoie, GA, Heywood, JB, and Keck, JC. *Experimental and Theoretical Study of Nitric Oxide Formation in Internal Combustion Engines*. Combustion Science and Technology. Vol 1: pp 313-326 (1970).
13. Heider, G, Woschni, G, and Zeilinger, K. *Two-Zone Calculation Model for the Prediction of NO Emissions from Diesel Engines*. MTZ. Vol 59(11): pp 770-775 (1998).
14. Weisser, G. *Modelling of Combustion and Nitric Oxide Formation for Medium-Speed DI Diesel Engines: A Comparison of Zero- and Three-Dimensional Approaches*, Swiss Federal Institute of Technology: Zurich (2001).
15. Strehlow, RA. *Combustion Fundamentals*. McGraw-Hill (1984).
16. Rodatz, P, Weisser, G, and Tanner, FX. *Assessment of CFD Methods for Large Diesel engines with a Common Rail Injection System*. SAE 2000-01-0948 (2000).
17. Goldsworthy, L. *Reduced Kinetics Schemes for Calculation of Oxides of Nitrogen Emissions from a Slow Speed Marine Diesel*. Energy and Fuels (American Chemical Society). submitted (2002).
18. Zabetta, EC, Kilpinen, P, Hupa, M, Stahl, K, Leppalahati, J, and Nieminen, J. *Kinetic Modelling Study on the Potential of Staged Combustion in Gas Turbines for the Reduction of Nitrogen Oxide Emissions from Biomass IGCC Plants*. Energy and Fuels. Vol 14: pp 751-761 (2000).
19. Miller, JA, and Bowman, CT. *Mechanism and Modelling of Nitrogen Chemistry in Combustion*. Prog. Energy Combust. Sci. Vol 15: pp 287-338 (1989).
20. Easley, WE, Mellor, AM, and Plee, SL. *NO Formation and Decomposition Models for DI Diesel Engines*. SAE 2000-01-0582 (2000).
21. Holtbecker, R, and Geist, M. *Emissions Technology, Sulzer RTA Series, Exhaust Emissions Reduction Technology for Sulzer Marine Diesel Engines*, Wartsila NSD (1998).
22. Bazari, Z. *A DI Diesel Combustion and Emission Predictive Capability for Use in Cycle Simulation*. SAE 920462 (1992).
23. MAN B&W, *Super-VIT Fuel Pumps: Adjustment and Maintenance*, (1987).
24. Tanner, FX, Brunner, M, and Weisser, G. *A Computational Investigation of Water Injection Strategies for Nitric Oxide reduction in Large-Bore DI Diesel Engines*. SAE 2001-01-1069 (2001).
25. Borman, GL, and Ragland, KW. *Combustion Engineering*. WCB/McGraw-Hill (1998).
26. Henningsen, S. *MAN B&W, Pers Comm*, MAN B&W (2002).

27. Weisser, G, Tanner, FX, Boulouchos, K, Kramer, J, and Holtbecker, R. *Integrating CRFD Simulations into the Development Process of Large Diesel Engine: A Status Report*. CIMAC 98 Paper No. 05.09 (1998).

28. Egeberg, C, and Ostergaard, A, *The MC Engine and its Future Development*. 23rd CIMAC Congress (2001).

29. Riom, E, Olsson, L, and Hagstrom, U. *NOx Emissions Reduction with the Humid Air Motor Concept*. 23rd CIMAC Congress (2001).

30. Lausch, W, and Fleischer, F. *NOx cut = fuel rise: incompatible*

opposites or not? MER (Marine Engineers Review), June 1996, p 23.

31. *The Green Diesel*, MER (Marine Engineers Review), May 1997, p14.

32. MAN B&W, *Emission Control Two-Stroke Low-Speed Engines*. MAN B&W(331-96.12) (1997).

33. Geist, MA, Holtbecker, R, and Chung, SY *Marine Diesel NOx Reduction Techniques - A New Sulzer Diesel Approach*. SAE 970321 (1997).

FIGURES

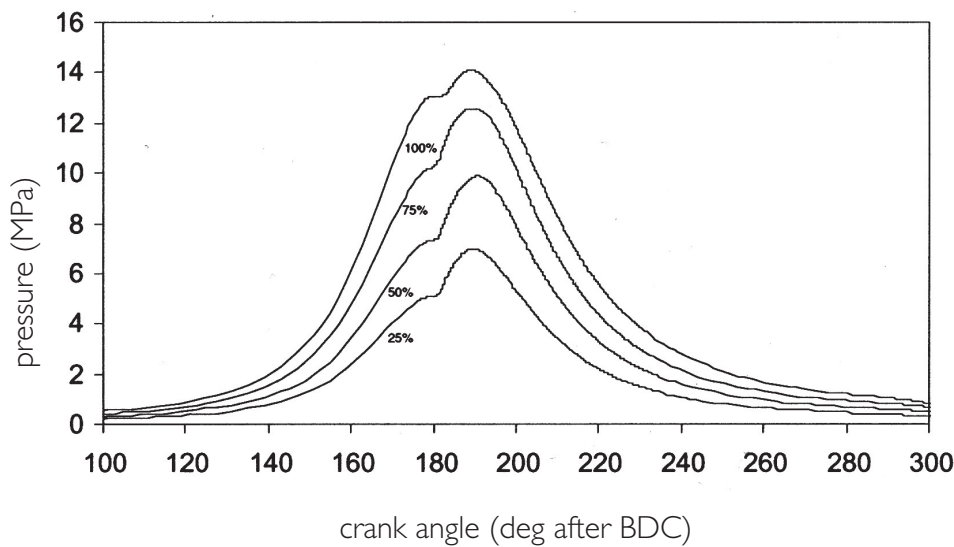


Fig 1: Simulated cylinder pressure v crank angle

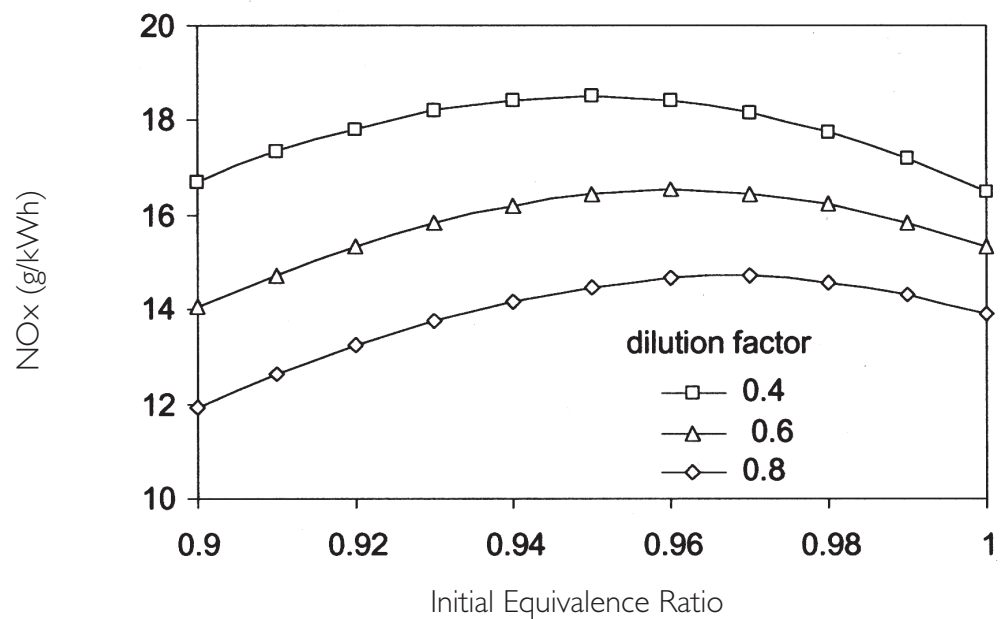


Fig 2: NOx v initial equivalence ratio, 75% load

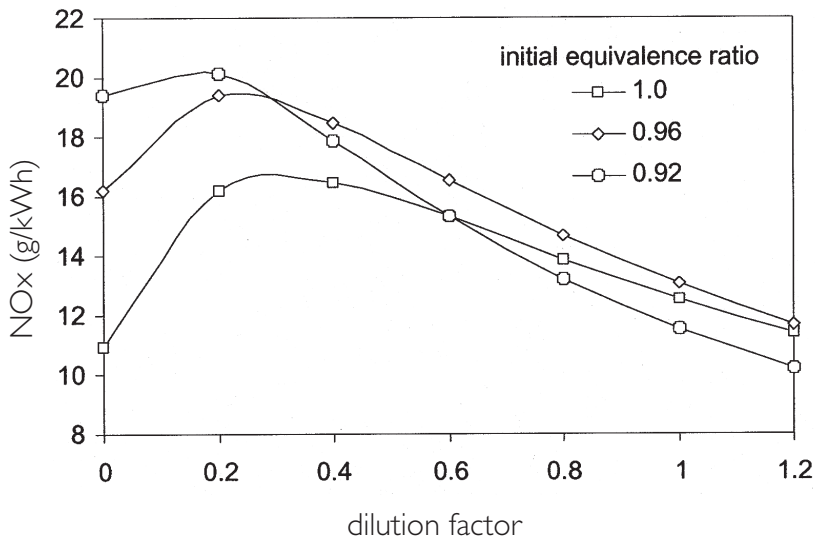


Fig 3: NOx v dilution rate factor, 75% load

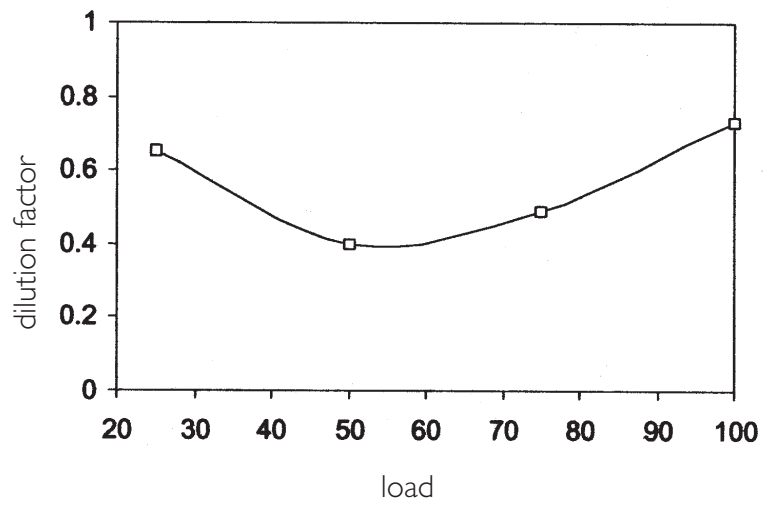


Fig 4: Dilution rate factor v load, initial equivalence ratio = 0.96

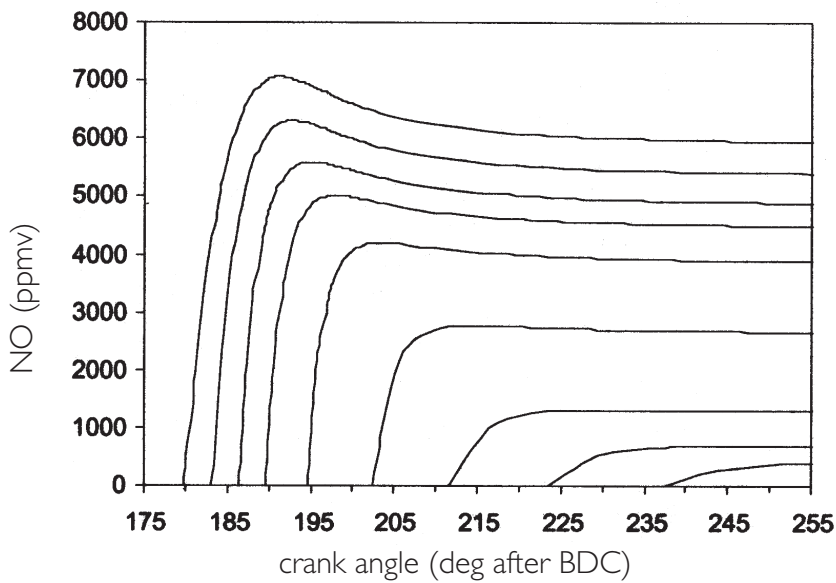


Fig 5: Zonewise NO at 75% load, reference settings, 7L70MC