Contemporary Engineering Sciences, Vol. 7, 2014, no. 1, 19 - 37
HIKARI Ltd, www.m-hikari.com
http://dx.doi.org/10.12988/ces.2014.3951

A Quasi-dimensional Three-zone Combustion Model of the Diesel Engine to Calculate Performances and Emission Using the Diesel-Ethanol Dual Fuel

Paramust Juntarakod

Department of Mechanical and Aerospace Engineering
King Mongkut's University of Technology North Bangkok
1518 Pracharat 1 Road, Wongsawang, Bangsue, Bangkok 10800, Thailand
paramust_kmitnb@hotmail.com

Thanakom Soontornchainacksaeng

Energy Management Systems and Monitoring & Verification Control,
Research & Development Center Science and Technology Research Institute
Department of Mechanical and Aerospace Engineering
King Mongkut's University of Technology North Bangkok
1518 Pracharat 1 Road, Wongsawang, Bangsue, Bangkok 10800, Thailand
tss@kmutnb.ac.th

Abstract

In the present study, develop the multi zone thermodynamic model for the simulation of a small diesel engine operating on the mixture of diesel and ethanol and comparing results with an experiment. This paper discussed analytically and provides data of nitrogen oxide and performance parameters such as power, speci-

fic fuel consumption and thermal efficiency, indicated mean effective pressure. For this purpose, quasi-dimensional phenomenological three zone combustion process (unburned, adiabatic core region and boundary layer gas) has been modeled based on equilibrium constants method with MATLAB program to calculate the mole fractions of 11 combustion products when the new equilibrium constants function developed by Gill which are lowly-highly temperature dependent. To compute diesel engine cycles, zero-dimensional compression and expansion model have given by Ferguson and developed with new assumptions. These results involve various combination sequence effects of compression ratio (23-25), equivalence ratio (0.8-0.9), burn duration angle (60-70 CA) and engine speed (1000-1500 rpm) which volume fraction of fuel compositions (10-30% ethanol) (Diesel-Ethanol blend).
The results of the study as the power was calculated by this method are the error range within around 5% or 0.5 kW from the maximum experiment results. The specific fuel consumption was less than 5% or 15-20 g (Fuel)/kW-hr from experiment results. The resulted show that nitrogen oxide has changed very little, corresponding results of various sequence effects. The performance parameters were changed with varying engine computing conditions. Maximum performance parameters be raised by increases the engine speed and equivalence ratio, its can increase the thermal efficiency are approximately value 15-20%.

Keywords: Newton-Raphson iteration; Nitrogen Oxide; Engine Performances; Three zone Combustion modeling; Burned; Unburned Adiabatic core region Boundary layer gas

1 Introduction

Three zone thermodynamic model by numerical method which employed three zones for the combustion process: (1) unburned, (2) adiabatic core region, and (3) boundary-layer gas of a internal combustion engine has been studied and since published automotive engineering work by Caton [1], Sahin [2] and Kodavasal [3] with validated experiment. They documented which have demonstrated the use of novel combustion techniques the new methodology as two zone combustion to achieve low nitric oxide emissions with concurrent high thermal efficiencies. It has attracted great attention due to its superior potential applications, resulting in a reduction in the time scales and costs of the design process experiment or commercial program. For examples in this methodology of two zone thermodynamic model by numerical method and compare with experiments.
Hanson et al. [4] provided results from a heavy-duty, direct-injection compression-ignition engine using gasoline with various injection strategies. Their work centered on 1300 rpm operation at two different loads: IMEP of 11.5 and 6.5 bar. Using 41% and 30% EGR, for the high and moderate loads, respectively, they reported low emissions with about 50% net indicated thermal efficiency.

Kokjohn et al. [5] applied the work of Hanson et al. [4], but using both a dual-fueled diesel engine and pre-mixed charge compression ignition concept to comparing, resulted in a net indicated thermal efficiency of 50%. In document, he used in-cylinder blends of gasoline and diesel to extend the range of operation of the diesel engine type combustion. They were able to better match the desired ignition and combustion properties to specific (but changing) fuel blends. They demonstrated successful operation for several operating conditions. One such case was a 1300 rpm, 11 bar $imep_{net}$ condition, that resulted in negligible emissions and a 50% net indicated thermal efficiency. This was achieved using an overall lean mixture (u = 0.77), a high level of EGR (45.5%) and an inlet pressure of 200 kPa. Combustion was stable and repeatable.

Wilhelmsson et al. [6] presented work that was based on the diesel engine with supercharging using the mixture of natural gas and n-heptane. Although they stated that natural gas appeared to be an ill-suited fuel for pure diesel engine operation, they were able to adopt an operating strategy to minimize emissions while attaining a relatively high efficiency. They reported net indicated thermal efficiencies of 45% and 50% for two cases.

In recent paper, the study of two zone thermodynamic model by numerical method of a diesel engine has more focused on equilibrium constants functions were developed by Gill [7] which are lowly-highly temperature dependent, because of a new time specific energy polynomial temperature-pressure function than the old time function of JANAF [8] and CHEMKIN [9] for solving nonlinear equations. In this study, the derivations of governing equations for the reaction combustion equations were performed by assuming 11 combustion products. A system of 11 nonlinear equations appears in the derivation of the reaction combustion equations and it can be solved using Newton–Raphson methods prior to its implementation into MATLAB program [10]. The first example of the new method was presented by Paramust [11]. Since then, other three zone thermodynamic model by numerical method have been reported Buttsworth [12], Ramachandran [13], Adnan [14] and Mohammad [15] but with equilibrium constants functions specific energy polynomial temperature function from JANAF as different form this in this methodology.

Now a day, some methods have been proposed for three zone thermodynamic model of the combustion systems such as, for examples, a combustion chamber of gasoline engine combustor of gas turbine and premixed combustion flame and alternative fuel combustion. When the parameters of the combustion equation are uncertain or unknown, adaptive equilibrium constants can be solved using numerical techniques as following Ramachandran [13], Adnan [14] and Mohammad [15].

The thermodynamic model which employed three zones for the combustion process at this present is a three-zone thermodynamic [1 and 2] and developments have included the effect of compression ratio (r), equivalence ratio (ϕ),burn duration angle (ϕ_b), pressure intake ratio (P_{in}/P_0), engine speed (rpm) and volume fraction of two fuels (V_p/V_s). The design that provides the most effective operation is not yet known, but these types of features are clearly important. The most important assumptions were that,

1) The working medium was considered a mixture of 11 species.
2) All 11 species were considered as ideal gas of combustion products.
3) The mixture fuels are limited to $C_{\alpha}H_{\beta}O_{\gamma}N_{\delta}$ species.

The study described in this paper provides the emission that is nitric oxide and performance parameters of a small diesel engine such as power, specific fuel consumption, furthermore also be considered, thermal efficiency and indicated mean effective pressure operating on diesel and ethanol. Results were compared with an experiment Tanakom [16] and [17].

2 Modeling and Analysis

2.1 A Three-zone, Zero-dimensional model

The following is the derivative version of the equations modified based on Kreiger [18] which using for determination of three-zone of unburned, burned (adiabatic core region) and boundary-layer gas to analyze the rate of temperature, pressure and mass transfer based on equally pressure of a diesel engine. Consider the schematic of an engine cylinder while combustion products are occurring in combustion stroke as in Fig. 1.

Assumptions: Pressure (P) in the burned and unburned zones is equal, $\dot{P}_u = \dot{P}_b$

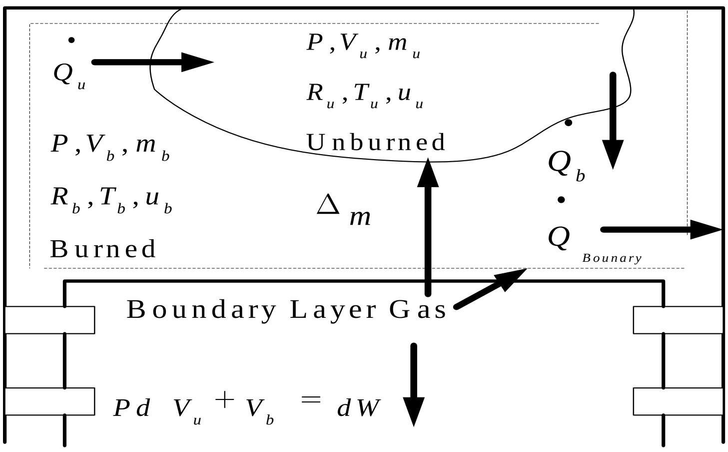

Figure 1 : Burned, unburned and boundary-layer gas based on constant pressure

The method is assumed that the fuel-air is supplied from a perfect system (port injection of fuel or induction) and mixed completely. No chemical reactions take place in the unburned zone (zone is said to be frozen)

$$\frac{\partial x_u}{\partial T} = \frac{\partial x_u}{\partial P} = 0, \frac{\partial M_u}{\partial T} = \frac{\partial R_u}{\partial T} = \frac{\partial M_u}{\partial P} = \frac{\partial R_u}{\partial P} = \frac{\partial u_u}{\partial P} = 0$$

The total cylinder volume and mass is taken up by the burned and unburned volumes and masses only, Determining is defined from Amagat's law [20]. $V = V_b + V_u, m = m_b + m_u$. It can write $m_{u1} - \Delta m = m_{u2}, m_{b1} - \Delta m = m_{b2}$. This leads to $\dot{m}_u = \dot{m}_b$.

2.2 The thermodynamic model

The mathematical engine model was applicable in detail mass and energy balance for four stroke diesel engine and is based on three zone thermodynamic analysis of the ideal fuel-air cycle. The method is assumed that the fuel-air is supplied from a perfect system and mixed completely. Mass balance, the equation of state for an ideal gas is,

$$PV = mRT \tag{1}$$

The rate of change of mass within any open system is the net flux of mass across the system boundaries. Hence for a control volume enclosing the air-fuel mixture, we have,

$$\dot{m} = \sum_i \dot{m}_i \tag{2}$$

From the first law of thermodynamics,

$$\dot{E} = \dot{Q} - \dot{W} + \sum_i \dot{m}_i \ H_i \tag{3}$$

Taking the derivative of Eq. 2 and 3 as the function of the crank angle θ yields as,

$$\frac{dm}{d\theta} = \sum_i \frac{dm_i}{d\theta} \tag{4}$$

$$\frac{d(mu)}{d\theta} = \frac{dQ}{d\theta} - \frac{dW}{d\theta} + \sum_i \frac{dm_i}{d\theta} \ h_i \tag{5}$$

2.3 Thermodynamic properties

The specific heat change as the function of the crank angle in eq. (2) and eq. (5), those indicate the enthalpy change with respect to temperature and pressure, which was obtained from curve fitted polynomial equation. Table 1 shows the thermodynamics properties expressed as a function of crank angle, pressure and temperature. Where, Lewis [20] has represented the thermodynamic properties of fuels and air Ferguson [21] and Heywood [22] proposed the thermodynamic properties of air and combustion products by the form of coefficient $a_1, a_2, a_3 ... a_5$.

3 Methodologies for Analysis

3.1 The Mathematical model of a cylinder engine

In the combustion stroke, we consider the temperature in the term of burned mixture (T_b) and unburned (T_u) as separate open systems. Recalling eq.(5) and combining all the derivatives of thermodynamic properties will enable the pressure and temperature to be expressed as a function of crank angle, pressure, unburned gas temperature and burned gas temperature.

Table 1. The thermodynamic properties.

Air and Combustion products	**Fuels**
$\frac{c_P}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$	$\frac{c_P}{R} = a_0 + b_0 T + c_0 T^2$
$\frac{h}{RT} = a_1 \ln T + \frac{a_2}{2} T + \frac{a_3}{3} T^2 + \frac{a_4}{4} T^3 + \frac{a_5}{5} T^4 + \frac{a_6}{T}$	$\frac{h}{RT} = a_0 + \frac{b_0}{2} T + \frac{c_0}{3} T^2 + \frac{d_0}{T}$
$\frac{s^0}{R} = a_1 \ln T + a_1 T + \frac{a_3}{3} T^2 + \frac{a_4}{4} T^3 + \frac{a_5}{4} T^4 + a_7$	$\frac{s^0}{R} = a_0 \ln T + b_0 T + \frac{c_0}{2} T^2 + e_0$
Internal energy, Volume, Entropy, Enthalpy	
$\frac{du}{d\theta} = \left(c_P - \frac{Pv}{T} \frac{\partial \ln v}{\partial \ln T} \right) \frac{dT}{d\theta} - \left(v \left(\frac{\partial \ln v}{\partial \ln T} + \frac{\partial \ln v}{\partial \ln P} \right) \right) \frac{dP}{d\theta}, \left(\frac{\partial h}{\partial T} \right)_P = C_P$	
$\frac{dv}{d\theta} = \frac{v}{T} \frac{\partial \ln v}{\partial \ln T} \frac{dT}{d\theta} - \frac{v}{P} \frac{\partial \ln v}{\partial \ln P} \frac{dP}{d\theta}, \frac{ds}{d\theta} = \left(\frac{C_P}{T} \right) \frac{dT}{d\theta} - \frac{v}{T} \frac{\partial \ln v}{\partial \ln T} \frac{dP}{d\theta}$	

$$\frac{dP}{d\theta}, \frac{dT_b}{d\theta}, \frac{dT_u}{d\theta}, \frac{dW}{d\theta} = f_1(L, P, T_b, T_u) \tag{6}$$

Modified algorithm from Ferguson [21] as following the arbitrary heat release conditions and solving the above equations with appropriate input data enable determination of the indicated work, enthalpy and heat loss throughout the system. Those can be expressed as a function of pressure and temperature.

$$\frac{dP}{d\theta} = \frac{A + B + C}{D + E} \tag{7}$$

$$\frac{dT_b}{d\theta} = \frac{-h \left(\frac{\pi b^2}{2} + \frac{4V}{b} \right) x^{1/2} \ T_b - T_W}{\mathrm{v} m \mathrm{c}_{\mathrm{Pb}} x} + \frac{v_b}{\mathrm{c}_{\mathrm{Pb}}} \left(\frac{\partial \ln v_b}{\partial \ln T_b} \right) \left(\frac{dP}{d\theta} \right) + \frac{h_u - h_b}{x \mathrm{c}_{\mathrm{Pb}}} \left[\frac{dx}{d\theta} - \ x - x^2 \ \frac{C}{\mathrm{v}} \right] \tag{8}$$

$$\frac{dT_u}{d\theta}=\frac{-h\left(\frac{\pi b^2}{2}+\frac{4V}{b}\right)1-x^{1/2}\quad T_u-T_W}{\mathrm{v}mc_{\mathrm{Pb}}\ 1-x}+\frac{v_u}{c_{\mathrm{Pu}}}\left(\frac{\partial\ln v_u}{\partial\ln T_u}\right)\left(\frac{dP}{d\theta}\right)\tag{9}$$

From the derivatives of eq. (7–9) let us defined the constant term with respect to the combination of the thermodynamic properties equations are,

$$A=\frac{1}{m}\left(\frac{dV}{d\theta}+\frac{VC}{\mathrm{v}}\right)\tag{10}$$

$$B=h\frac{\left(\frac{dV}{d\theta}+\frac{VC}{\mathrm{v}}\right)}{\mathrm{v}m}\left[\begin{array}{l}\frac{v_b}{c_{\mathrm{Pb}}}\frac{\partial\ln v_b}{\partial\ln T_b}x^{1/2}\frac{T_b-T_u}{T_b}+\\ \frac{v_u}{c_{\mathrm{Pu}}}\frac{\partial\ln v_u}{\partial\ln T_u}\ 1-x^{1/2}\ \frac{T_b-T_u}{T_b}\end{array}\right]\tag{11}$$

$$C=-\ v_b-v_u\ \frac{dx}{d\theta}-v_b\frac{\partial\ln v_b}{\partial\ln T_b}\frac{h_u-h_b}{c_{\mathrm{Pb}}T_b}\left[\frac{dx}{d\theta}-\frac{(x-x^2)C}{\mathrm{v}}\right]\tag{12}$$

$$D=x\left[\frac{v_b^2}{c_{\mathrm{Pb}}T_b}\left(\frac{\partial\ln v_b}{\partial\ln T_b}\right)^2+\frac{v_b}{P}\frac{\partial\ln v_b}{\partial\ln P}\right]\tag{13}$$

$$E=\ 1-x\ \left[\frac{v_u^2}{c_{\mathrm{Pu}}T_u}\left(\frac{\partial\ln v_u}{\partial\ln T_u}\right)^2+\frac{v_u}{P}\frac{\partial\ln v_u}{\partial\ln P}\right]\tag{14}$$

3.2 Chemical equilibrium with the fuel mixture

The basis of the equilibrium combustion products with fuel mixture model $C_\alpha H_\beta O_\gamma N_\delta$ is a solution to the atom balance equations from the chemical reaction equation of fuel and air forming and the subscript 1 and 2 represent the one of the Diesel and Ethanol respectively as shown in Table 2.

Table 2. The diesel and ethanol mixture fuel [20, 21]

Name	Structure	Atom	Fuel-Air Ratio (Stoich)
Diesel	$C_{14.4}H_{24.9}$	α_1=14.4,β_1=24.9	14.3
Ethanol	C_2H_6O	α_2=2,β_2=6,$\gamma_2=1$	8.94

This mixture equation is given in Eq.15 for the condition of equivalence ratio ϕ, where ν_1 through ν_{11} are mole fractions of the product species, ε is the molar fuel-air ratio required to react with one mole of air. This process based on the work of modified [21, 22] as given below,

$$\begin{array}{lcl} \varepsilon\phi(1-\chi_1)C_{\alpha1}H_{\beta1}O_{\gamma1}N_{\delta1} & & \nu_1CO_2+\nu_2H_2O+\nu_3N_2 \\ +\varepsilon\phi(\chi_1)\ \chi_2C_{\alpha2}H_{\beta2}O_{\gamma2}N_{\delta2} & \rightarrow & +\nu_4O_2+\nu_5CO+\nu_6H_2 \\ +0.21O_2 & & +\nu_7H+\nu_8O \\ +0.79N_2 & & +\nu_9OH\nu_{10}NO+v_{11}N \end{array} \tag{15}$$

Where, x_1 is the molar ratio of multi-fuel having the condition, $0 < x_1 < 1$. x_2 are the fuel in the second and third which having the condition, $x_1 + x_2 = 1$. There is the conservation of 4 atoms, C,H,O and N from mixture equation, so atom balancing can be written,

$$\text{C} \quad \varepsilon\phi(1-\chi_1)\alpha1+\varepsilon\phi\chi_1\chi_2\alpha2=(y_1+y_5)N \tag{16}$$

$$\text{H} \quad \varepsilon\phi(1-\chi_1)\beta1+\varepsilon\phi\chi_1\chi_2\beta2=(2y_2+2y_6+y_7+y_9)N \tag{17}$$

$$\text{O} \quad \varepsilon\phi(1-\chi_1)\gamma1+\varepsilon\phi\chi_1\chi_2\gamma2+0.42=(2y_1+y_2+2y_4+y_5 +y_8+y_9+y_{10})N \tag{18}$$

$$\text{N} \quad \varepsilon\phi(1-\chi_1)\delta1+\varepsilon\phi\chi_1\chi_2\delta2+1.58=(2y_3+y_{10}+y_{11})N \tag{19}$$

Where, N is the total number of moles and y is the mole fraction. Thus, the total number of mole fraction must be equal to one and this gives,

$$\sum_{i=1}^{11} y_i - 1 = 0 \tag{20}$$

The expression for atom balance of each equation can be eliminated by dividing (eq. 17-19) by eq. 16. The equation can be written as next equation.

$$2y_2+2y_6+y_7+y_9-\left[d_1(y_1+y_5)\right]=0 \tag{21}$$

$$2y_1+y_2+2y_4+y_5+y_8+y_9+y_{10}-\left[d_2(y_1-y_5)\right]=0 \tag{22}$$

$$2y_2+y_{10}+y_{11}-\left[d_3(y_1+y_5)\right]=0 \tag{23}$$

where

$$d_1=\frac{(1-\chi_1)\beta1+\chi_1\chi_2\beta2}{(1-\chi_1)\alpha1+\chi_1\chi_2\alpha2},\ d_2=\frac{(1-\chi_1)\gamma1+\chi_1\chi_2\gamma2+\dfrac{0.42}{\varepsilon\phi}}{(1-\chi_1)\alpha1+\chi_1\chi_2\alpha2},\ d_3=\frac{(1-\chi_1)\delta1+\chi_1\chi_2\delta2+\dfrac{1.58}{\varepsilon\phi}}{(1-\chi_1)\alpha1+\chi_1\chi_2\alpha2}$$

Eq. (20-23) have 11 unknowns ($y_1, y_2, y_3 .... y_{11}$), therefore in order to solve for these 11 unknowns other 7 more equations are needed which may be derived from the consideration of equilibrium among products. The equilibrium constant can be related to the partial pressure of the reactants and products. And the partial pressure of a component is defined relative to the total pressure and the mole faction, thus the equilibrium constant can be rewritten as Table 3.

The equilibrium constant in Table 3, K_1 through K_7 are curve fitted form Gill [7] and their expressions are of the from,

$$K_P = \exp\left(\Delta a_1 \left(\ln T - 1 \right) + \frac{\Delta a_2 T}{2} + \frac{\Delta a_3 T^2}{6} + \frac{\Delta a_4 T^3}{12} + \frac{\Delta a_5 T^4}{20} - \frac{\Delta a_6}{T} + \Delta a_7 \right) \tag{24}$$

Through algebraic manipulations, the ten equations can be reduced into four equations with four unknowns. The equations are nonlinear and solved by using the Newton-Raphson method [10]. Each of these may be expanded in Taylor's series $f_j(y_3, y_4, y_5, y_6) = 0$, where $j = 1,2,3,4$ (neglecting the second order and higher order) as,

$$f_j + \frac{\partial f_j}{\partial y_3}\Delta y_3 + \frac{\partial f_j}{\partial y_4}\Delta y_4 + \frac{\partial f_j}{\partial y_5}\Delta y_5 + \frac{\partial f_j}{\partial y_6}\Delta y_6 = 0 \tag{25}$$

Table 3. Dissociation of mole fraction of Equilibrium Constant Method (ECM).

$$\begin{aligned}
K_1 &= \frac{P_{CO}\sqrt{P_{O2}}}{P_{CO2}} = \frac{y_5 y_4^{1/2} P^{1/2}}{y_1} \rightarrow y_1 = c_1 y_5 y_4^{1/2}, \text{ where } c_1 = \frac{P^{1/2}}{K_1} \\
K_2 &= \frac{P_{H2O}}{P_{H2}\sqrt{P_{O2}}} = \frac{y_2}{y_4^{1/2} y_6 P^{1/2}} \rightarrow y_2 = c_2 y_4^{1/2} y_6, \text{ where } c_2 = K_2 P^{1/2} \\
K_3 &= \frac{P_{OH}}{\sqrt{P_{H2}}\sqrt{P_{O2}}} = \frac{y_9}{y_4^{1/2} y_6^{1/2}} \rightarrow y_9 = c_3 y_4^{1/2} y_6^{1/2}, \text{ where } c_3 = K_3 \\
K_4 &= \frac{P_H}{\sqrt{P_{H2}}} = \frac{y_7 P^{1/2}}{y_6^{1/2}} \rightarrow y_7 = c_4 y_6^{1/2}, \text{ where } c_4 = \frac{K_4}{P^{1/2}} \\
K_5 &= \frac{P_O}{\sqrt{P_{O2}}} = \frac{y_8 P^{1/2}}{y_4^{1/2}} \rightarrow y_8 = c_5 y_4^{1/2}, \text{ where } c_5 = \frac{K_5}{P^{1/2}} \\
K_6 &= \frac{P_N}{\sqrt{P_{N2}}} = \frac{y_{11} P^{1/2}}{y_3^{1/2}} \rightarrow y_{11} = c_6 y_3^{1/2}, \text{ where } c_6 = \frac{K_6}{P^{1/2}} \\
K_7 &= \frac{P_{NO}}{\sqrt{P_{O2}}\sqrt{P_{N2}}} = \frac{y_{10}}{y_4^{1/2} y_3^{1/2}} \rightarrow y_{10} = c_7 y_4^{1/2} y_3^{1/2}, \text{ where } c_7 = K_7
\end{aligned}$$

Functions f_j are evaluated from the solution of interested functions (eq.20-23) the independent set of derivatives is obtained by solution of matrix equation that results from differentiating with respect to mole faction. The above can be arranged as set of linear equations in the matrix form,

$$\left[\frac{\partial f_i}{\partial y_i} \right] [\Delta y] - [-f] = 0 \tag{26}$$

This set of linear equations can then be solved for y_3, y_4, y_5, y_6 and iterative procedures undertaken until the corrections are less than a specified tolerance (δ).

For convenience, defining following partial derivatives and defining the constant values for a simple studied and the Jacobian of solution are given as Table 4.
Eq.26 may be solved using by Gauss elimination. The second approximation is then $\{y\}_{k+1} = \{y\}_k + \{\delta\}_k \quad y = 3,4,5,6$. The process of forming the Jacobian, solving Eq.24 and calculating new values for $\{y\}$ is repeated until a stop criterion is met, results in the molar concentrations of the 11 product species[11].

3.3 Heat release and Calculation of ignition delay

The rate of heat release from the cylinder walls has been calculated using temperature condition T_θ of each crank angle for unburned, adiabatic core region and boundary-layer gas is,

$$\frac{dQ_i}{d\theta} = hA_\theta (T_\theta - T_W) \tag{27}$$

In cylinder derivative volume at each crank angle position is calculated as,

$$\frac{dV}{d\theta} = \frac{V_0(r-1)}{2}\left[\sin\theta + \frac{\varepsilon}{2}\sin 2\theta\left(1-\varepsilon^2\sin^2\theta\right)^{-1/2}\right] \tag{28}$$

The rate of heat release has been estimated from Wiebe's heat release model [21] shown as,

$$\frac{dQ_c}{d\theta} = a(m+1)\left(\frac{Q_{av}}{\Delta\theta_c}\right)^m \left(\frac{\theta-\theta_i}{\Delta\theta_c}\right)^m \exp\left[-a\left(\frac{\theta-\theta_i}{\Delta\theta_c}\right)^{m+1}\right] \tag{29}$$

3.4 Nitric Oxide Computations

The nitric oxide in exhaust gas is well accepted for calculating from the extended Zeldovich Mechanism [20, 21]. The oxidizing of nitrogen be on the chain mechanism, basic reactions are,

$$\mathrm{O+N_2} \Leftrightarrow \mathrm{NO+N} \tag{30}$$

$$\mathrm{N+O_2} \Leftrightarrow \mathrm{NO+O} \tag{31}$$

$$\mathrm{N+OH} \Leftrightarrow \mathrm{NO+H} \tag{32}$$

These equations can be derived for the change in nitric oxide concentration or can be written in derivation term of time. And the nitrogen atoms are assumed to be in steady state (*i.e.*, the net change of the nitrogen atoms is much smaller than its concentration). The other species, such as N_2, O_2, OH, H and O are assumed to be equal to their equilibrium values. For these conditions, the following formation rate for nitric oxide may be derived (eq. 30-32):

$$\frac{d[NO]}{dt} = \frac{2R_1[1-\beta^2]}{(1-BK)} \tag{33}$$

Where the terms are:

$$R_1 = k_1^+[O]_e[N_2]_e = k_1^-[NO]_e[N]_e \tag{34}$$

$$R_2 = k_2^+[N]_e[O_2]_e = k_2^-[NO]_e[O]_e \tag{35}$$

$$R_3 = k_3^+[N]_e[OH]_e = k_3^-[NO]_e[H]_e \tag{36}$$

$$\beta = \frac{[NO]_a}{[NO]_e}, \quad K = \frac{R_1}{R_2 + R_3}$$

$[NO]_a$ is the actual nitric oxide concentration and $[NO]_e$ is the equilibrium concentration for species.

3.5 Engine Performances

A study of gases as models of internal combustion engines is useful for qualitatively illustrating some of the important parameters influencing combustor performances, that is, the work output w_{CV} from fuel-air cycle. In theoretical of control volume, the combustor performances can be calculated by meaning of the indicated values which the following definitions are done by the gas. That is thermal efficiency, specific fuel consumption and the indicated mean effective pressure.

Thermal Efficiency (%, neglected combustion loss)

$$\eta = w_{CV}[1+\phi F_s(1-f)]/\phi F_s a_0(1-f) \quad 37)$$

Specific fuel consumption

$$SEC = m_f / w_{CV} \tag{38}$$

The indicated mean effective pressure (bar)

$$IMEP = w_{CV}[1+\phi F_s(1-f)]/V \tag{39}$$

Where, the stoichiometric fuel-air ratio by mass is F_s, residual fraction is f, available energy of fuel is a_c (LHV), and V is the constant volume of a cylinder.

Table 4. Constant values and the jacobians of solution.

$D_{ij} = \frac{\partial y_i}{\partial y_i} \frac{i = 1,2,7,8,9,10,11}{j = 3,4,5,6}$
$D_{14} = \frac{\partial y_1}{\partial y_4} = \frac{1}{2}\frac{c_1 y_5}{y_4^{1/2}}$ $D_{24} = \frac{\partial y_2}{\partial y_4} = \frac{1}{2}\frac{c_2 y_6}{y_4^{1/2}}$, $D_{84} = \frac{\partial y_8}{\partial y_4} = \frac{1}{2}\frac{c_5}{y_4^{1/2}}$, $D_{94} = \frac{\partial y_9}{\partial y_4} = \frac{1}{2}\frac{c_3 y_6^{1/2}}{y_4^{1/2}}$
$D_{15} = \frac{\partial y_1}{\partial y_5} = c_1 y_4^{1/2}$ $D_{26} = \frac{\partial y_2}{\partial y_6} = c_2 y_4^{1/2}$, $D_{76} = \frac{\partial y_7}{\partial y_6} = \frac{1}{2}\frac{c_4}{y_6^{1/2}}$, $D_{96} = \frac{\partial y_9}{\partial y_6} = \frac{1}{2}\frac{c_3 y_4^{1/2}}{y_6^{1/2}}$
$D_{103} = \frac{\partial y_{10}}{\partial y_3} = \frac{1}{2}\frac{c_7 y_4^{1/2}}{y_3^{1/2}}$ $D_{104} = \frac{\partial y_{10}}{\partial y_4} = \frac{1}{2}\frac{c_7 y_3^{1/2}}{y_4^{1/2}}$, $D_{113} = \frac{\partial y_{11}}{\partial y_3} = \frac{1}{2}\frac{c_6}{y_3^{1/2}}$

4 Engine and operating conditions

The main engine specifications for numerical simulation are summarized in Table 5. The engine selected for this study is a small diesel single cylinder, cooling system by radiation method, rated output 6.5 kW at 2400 rpm and configuration with a bore and stroke of 90 and 94 mm, respectively. For the Wiebe combustion parameters, the following values were used as recommended by Heywood [21], m

= 2.0 and a = 5.0 which a moderate load and moderate speed operating condition was examined. Table 6 lists examples of the values of other parameters (and ‘‘how obtained’’) which were needed in this work. Table 7 lists some of the parameters for case 1. The engine was assumed that the fuel-air is supplied from a perfect system (by port injection of fuel or induction) and mixed completely.

Table 5 : The engine specifications for calculation.

Item	Value
Number of cylinders	1
Bore, Stroke, Stroke/2(rod Length)	0.090, 0.094,0.15
RPM	1000
Equivalence ratio	0.8
Compression ratio	23
Burn duration angle	60-70

Table 6 : Common engine and fuel input parameters.

Item	Value used	How obtained
Fuel LHV (MJ/kg)	45.73	Diesel [20,21]
Fuel LHV (MJ/kg)	29.71	Ethanol [20,21]

Table7 : Descriptions of case : 1st, Fuel are D100, D90E10 and D70E30

Case 1st	Descriptions
1. (Base)	Table 5
2.(r)	r=25, ϕ=0.8, $\theta_b = 60$ and rpm=1000
3.(ϕ)	r=25, ϕ=0.9, $\theta_b = 60$ and rpm=1000
4.(ϕ_b)	r=25, ϕ=0.9, $\theta_b = 70$ and rpm=1000
5.(P_{in}/P_0)	r=25, ϕ=0.9, $\theta_b = 70$ and rpm=1000
6. (rpm)	r=25, ϕ=0.9, $\theta_b = 70$ and rpm=1500

5. Methodology and Discussion

5.1 Methodology

The main idea of this study is to complete a systematic assessment of the various features that the resulted are in low nitric oxide and high performance parameters [1]. By considering each feature in a step-by-step fashion, the impact of each feature can be quantified that.

The order that the features were added was arbitrary. For the five features considered, equivalence ratio, burn duration angle and engine speed, 19 different arrangement are possible for one output which this study used the mixture percentage of diesel and ethanol fuels such as D100 (Diesel 100%) D90E10 (Diesel 90%, Ethanol 10%) and D70E30 (Diesel 70%, Ethanol 30%) in computed, so the total 57 different arrangement are possible for one output of three mixed diesel fuel. Table 8 is a description of the case: 1st sequence.

The following results are based on a set of assumptions and approximations which did not consider a few engine characteristics. For example, combustion stability, cycle-to-cycle variations, or other combustion issues are not included. In addition, knock or other abnormal combustion phenomena are not considered [1].

Some items are not known. For example, the burn duration angle (θ_b) will be a function of a port direct-injection of fuel, air pressure induced and open-close inlet valves and exhaust valves. For this work, a simple schedule was assumed the 60 CA. The burn duration angle was assumed equal to the greater of 60 CA or the burn duration angle plus 10 CA for special cases. The sensitivity of this assumption is examined below.

5.2 Discussion

The study discussed in this paper provides nitric oxide and performance parameters of a small diesel engine such as power, specific fuel consumption, furthermore also be considered, thermal efficiency and indicated mean effective pressure operating on diesel and ethanol. By considering each feature in a step-by-step fashion, the impact of each feature will be quantified of the fourth of different sequences of the five features considered as in Table 8.

The resulting will be reported, and the reasons for the high performance will be determined that. The fourth section describes the thermodynamic model results as,

1) Comparison of the thermodynamic model results with the experimental results.
2) Thermal efficiencies and indicated mean effective pressures.
3) Powers and specific energy consumption.
4) The thermodynamic model results of nitric oxide.

Table8 The examples of different sequences, fuel are D100, D90E10 and D70E30

No	1st	2nd	3th	4th
1.	Base (Table 7)	Base (Table 7)	Base (Table 7)	Base (Table 7)
2.	r=25	rpm=1500	$\theta_b = 70$	$\phi = 0.9$
3.	$\phi = 0.9$	r=25	rpm=1500	$\theta_b = 70$
4.	$\theta_b = 70$	$\phi = 0.9$	r=25	rpm=1500
5.	rpm=1500	$\theta_b = 70$	$\phi = 0.9$	r=25
Output	Nitric oxide (NO_x) P (kW), SFC (g/kW), Thef (%), IMEP (kPa)			

6 Results

6.1 Comparison of thermodynamic model results and experimental results

In order to compare a realistic case, Table 5 the engine specification was used for the thermodynamic model calculation. This engine was applicable in diesel fuel (Table 6). The thermodynamic model (Power_Model and SEC_Model) was run at equivalence ratio of 0.8, compression ratio of 23 while using different engine speed varied from 1000, 1500, 2000 and 2500 rpm respectively. These values are compared with some actual test data (Power_Test and SEC_Test) [16]. According to fig. 2, it can be seen that the relative power and SEC results change of engine speed increases, which can be seen from the curves are almost the same of the actual test (Consistent with actual test data from specification engine).

The results of the study as the power was calculated by the methods differ by around 5% or 0.5 kW from the maximum experiment results. The specific fuel consumption was less than 3% or 20 g(Fuel)/kW-hr from experiment results. The results show that the thermodynamic model is consistent with the real test of both models in each engine speed. So, the thermodynamic model can be applied to predict the primary engine for use with other conditions, as shown in the following 6.2 to 6.4.

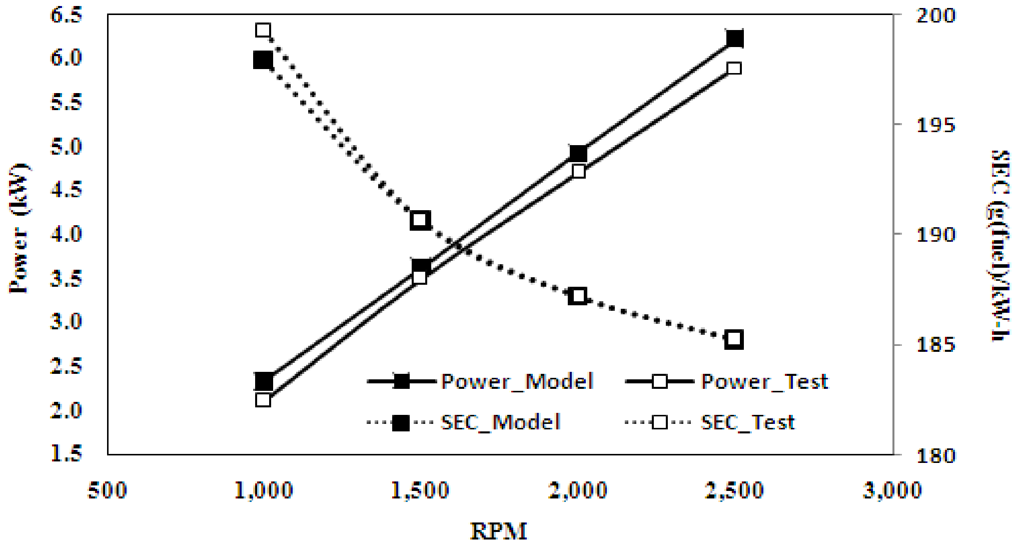

Figure 2 : Comparison the power and SEC model with the experimental results[16]

6.2 Thermal efficiencies and Indicated mean effective pressures

Fig. 3 shows, thermal efficiencies and indicated mean effective pressures for this operating condition for each case as described in Table 7 and Table 8.

The greatest thermal efficiency increases were achieved for the increase of burn duration angel and engine speed and the decrease of equivalence ratio. But, the increase of compression ratio affects resulted in a slight increase. In the case of mixed fuel, the result is higher thermal efficiencies, greater than 10% every time there is a change for the sequence. The maximum is 70% of thermal efficiency for D70E30 (Diesel 70%, Ethanol 30%). And case 3th, the trend of resulted curve raises thermal efficiency more than other case. Reasons for the increased oxygen content in ethanol. Result in a more complete combustion thus increasing the amount of ethanol that result in greater efficiency.

The greatest indicated mean effective pressures increases were achieved for the increase of all case and sequences, but similar value of fuels. The maximum is 1800 kPa (18 bars) of indicated mean effective pressures. The condition of resulted burn duration angel was the greater slope of the graph than other types.

6.3 Powers and Specific energy consumptions

Fig. 4 shows, powers and specific energy consumption for this operating condition for each case as described in Table 7 and Table 8. The greatest thermal efficiency increases were achieved for the increase of engine speed (rpm) and the decrease of burn duration angel. But, the increase of compression ratio and equivalence ratio affect resulted in a slight increase. Diesel fuel (D100) has a higher power than others (D90E10 and D70E30). Power than any other fuel is about 0.25 kW. The condition of round per minute (rpm) reported the greater slope of the graph than other types. The maximum power is 3.6 kW of (D100) and equal of cases. And case 2^{nd}, the trend of resulted curve raises power more than other cases.

The greatest specific energy consumption was achieved for the increase of equivalence ratio and equivalence ratio affect resulted in a slight increase. . Diesel and ethanol blend (D70E30) has higher specific energy consumption than others and diesel (D100) is the minimum value. . The maximum was 245 g/kW-hr of diesel and ethanol blend (D70E30) in case 4th for increased equivalence ratio 0.8 to 0.9. Specific energy consumption, the difference is less than 10 g/kW-hr.

6.4 The thermodynamic model results of nitric oxide

The variations of computed NO_X emissions and four different cases with five difference sequences are shown in Fig. 5. It shows that NO_X emission with changed diesel and ethanol blend, NO_X emission increases were achieved for the increase of engine speed and compression, but, the decrease of equivalence ratio and burn duration angle. The maximum is 330 ppm on case 2^{nd} on increase the sequence of engine speed and compression ratio.

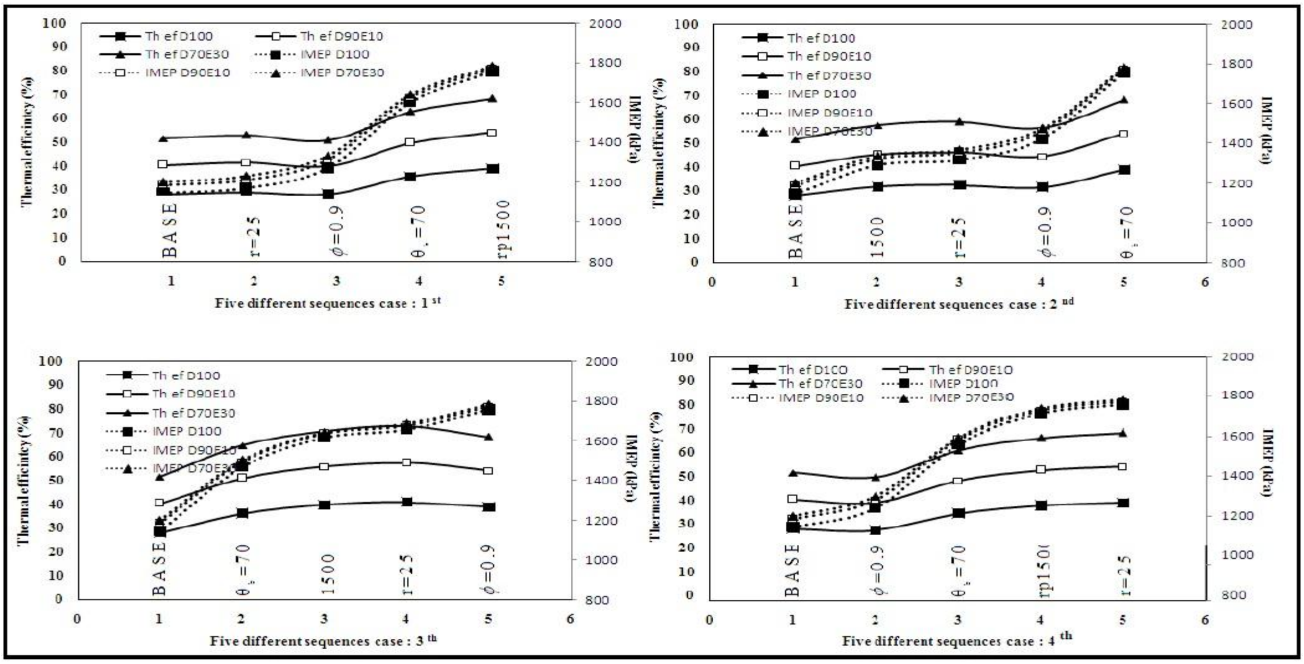

Figure 3: Thermal efficiencies and Indicated mean effective pressures

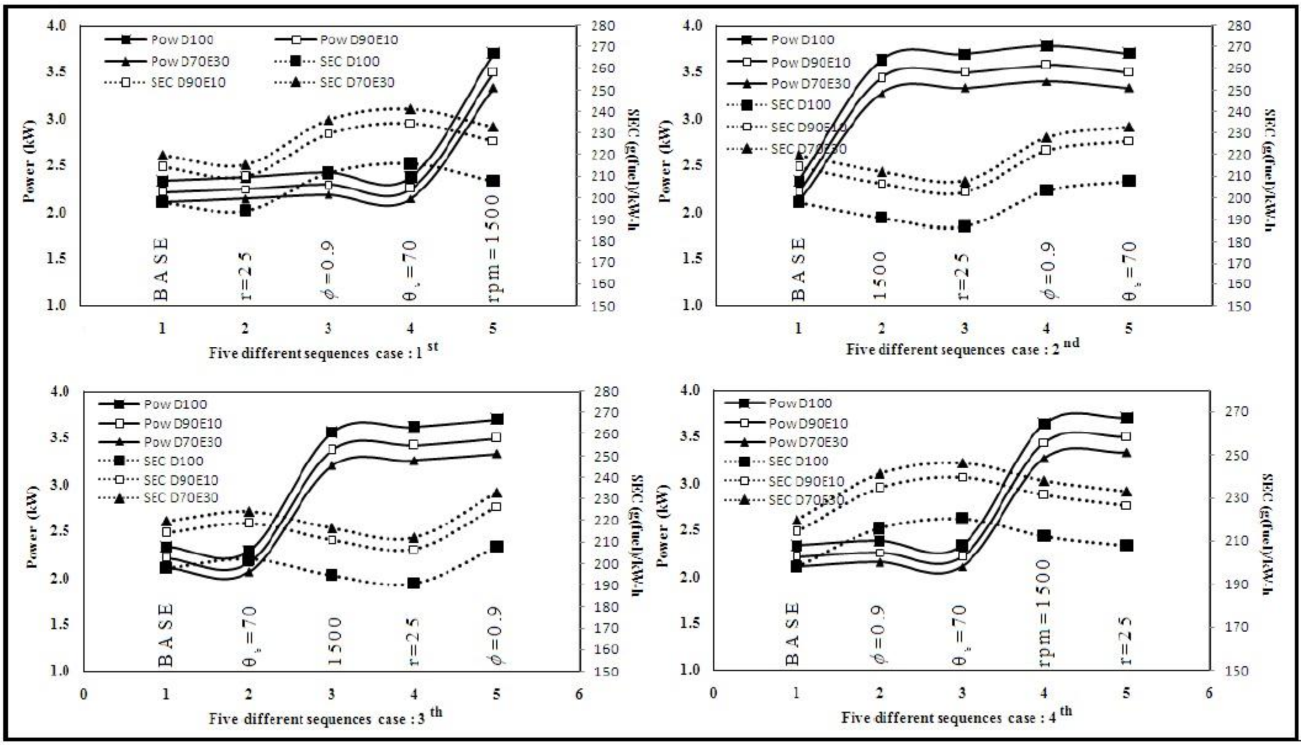

Figure 4 : Powers and Specific energy consumption for five different sequences

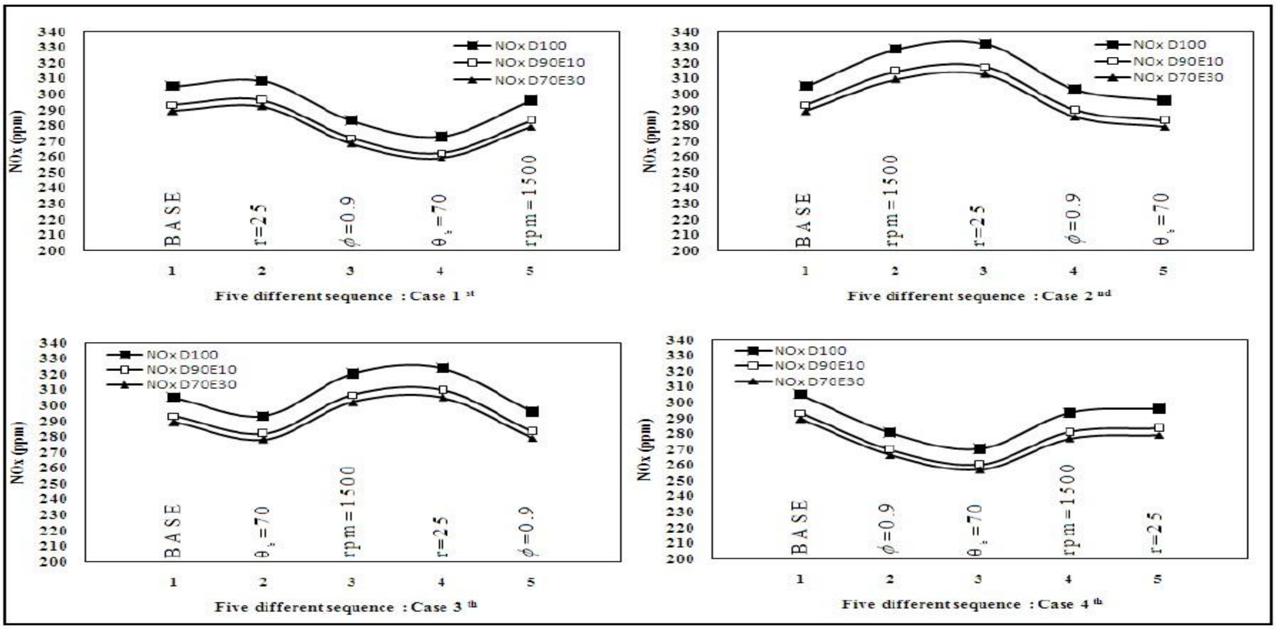

Figure 5 : **Nitrogen oxides emission for five different sequences**

7 Conclusions

The results of the study as the power was calculated by the methods differ by around 5% or 0.5 kW from the maximum experiment results. The specific fuel consumption was less than 3% or 20 g (Fuel)/kW-hr from experiment results. The resulted show that nitrogen oxide has changed very little, corresponding results of various sequence effects. The performance parameters were changed with varying engine computing conditions. Maximum performance parameters were raised by increases the engine speed and equivalence ratio, its can increase the thermal efficiency are approximately value 18-20%.

Acknowledgements

This research was supported by Energy Management Systems and Monitoring & Verification Control, Research & Development Center [ES-MVC]. Science and Technology Research Institute (STRI). King Mongkut's University of Technology North Bangkok,Thailand.

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Received: September 11, 2013