Lecture 5:Formation of NOx in SI Engines

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NO Formation in SI Engines

For computation of rate of formation of NO using Eq. 2.11 data are required on;

(i)	Thermodynamic state of the combustion gases
(ii)	Equilibrium concentration of O. OH, O_2, N, N_2 and NO in the burned gases.

Thermodynamic Combustion Models

Temperature of the burned gases and subsequently the equilibrium composition for a given engine and air-fuel ratio may be computed using a thermodynamic model from

(a)	measured cylinder pressure – crank angle history
(b)	Use of empirical burn rates, or
(c)	Use of fundamental combustion models that are based on flame propagation models or multi-dimensional combustion models.

Thermodynamic combustion models for SI engines are zero-dimensional and are only time dependent. Space coordinates of the combustion chamber are not taken into account. Two types of thermodynamic combustion models are used:

- One Zone Combustion Model: It is the simplest form of thermodynamic combustion models where the burned gas after combustion is assumed to mix instantaneously with gases burned earlier and the unburned gases so that all the cylinder gases at a given instant is uniform in composition and temperature. This model is too simplistic and unreal. It is unable to predict Excepting gross engine performance parameters such models are unable to predict engine performance and emissions with an acceptable degree of accuracy.

- Two Zone Combustion Models: Two zone models consist of an unburned mixture zone and a second zone consisting of the burned gases. The unburned and burned zones are separated by a thin reaction zone (flame front) of negligible thickness and hence the mass of charge in the flame front can be neglected.

    Two zone fully mixed model: This model assumes that the burned gases produced on combustion of the charge element during the given time period instaneously mixes with the burned gases produced earlier. Thus, all the burned gases at a given instant are uniform in temperature and composition. The unburned gases are in a separate zone and obviously at a different and much lower temperature. The pressure in the entire cylinder is however uniform.

    Two zone unmixed model: At the extreme is an *unmixed multi-zone model* where no mixing occurs between the burned gases produced by the mixture elements that burn at different instants in the cycle. The unmixed model predicts that a temperature gradient exists in the burned gases. The difference in temperatures of an early burnt element (near spark plug) with a late burn element at the far end of the combustion chamber of around 400 K have been experimentally measured supporting that the burned gases are not uniform in temperature and composition supporting the *unmixed combustion model*. Although, the actual situation in the combustion chamber may be somewhere between the *fully mixed* and *unmixed* models, but the unmixed model is more realistic.

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Using unmixed model and an empirical relation giving mass fraction burned as a function of crank angle, the computed engine cylinder pressure - crank angle (P-θ) history is shown on Fig. 2.5 .

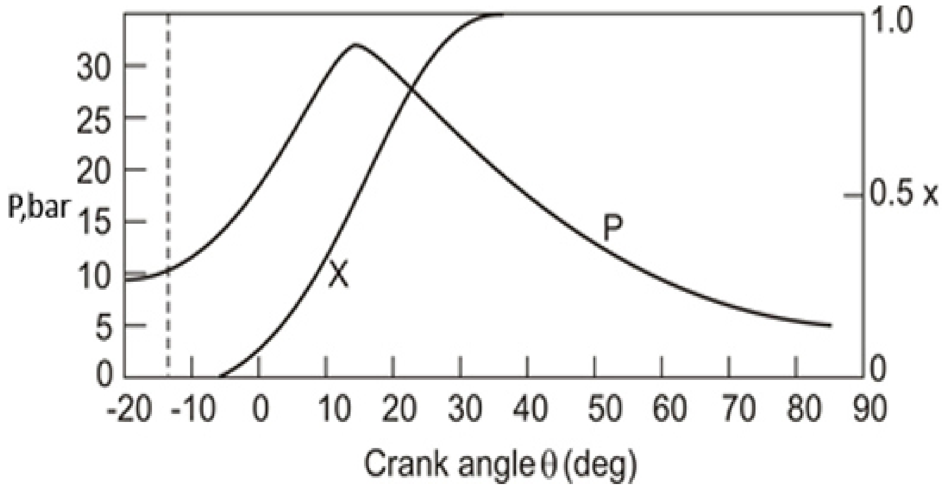

Figure 2.5	Computed cylinder pressure- crank angle (P-**θ**) history using unmixed combustion model and an empirical combustion rate function.

Fig 2.6 shows the variation in temperature with respect to crank angle for (i) the unburned mixture (T_u) (ii) the charge element that burned at the beginning of the combustion process (T_b at x =0) and (iii) the charge element that burned last at the end of combustion(T_b at x = 1.0). As seen the charge element close to the spark plug that burns in the beginning itself reaches a much higher temperature compared to the element that burns last. The difference in the calculated temperatures of two elements at a given crank angle is seen close to 400 K

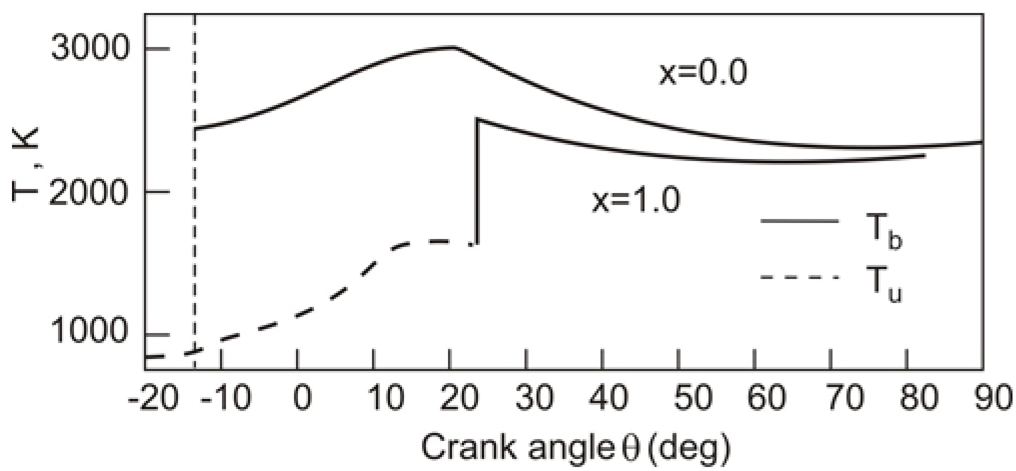

Figure.2.6	Unburned gas temperature ($\boldsymbol{T_u}$), burned gas temperature for the first burned element (T_b for $\boldsymbol{x}$=0) and the last burned element (T_b for $\boldsymbol{x}$ =1.0).

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NO concentrations were computed by numerically integrating the Eq. 2.11. NO concentration in the above two elements as a function of crank angle are shown in Fig 2.7. The equilibrium concentrations of NO for the two elements are also shown in this figure. In the early burned element as the peak temperature reaches significantly high values due to compression to peak cylinder pressure (the first burned element attains the highest temperature of all), the kinetically controlled NO reaches to near equilibrium levels. Later, as the temperature starts falling as a result of expansion, NO starts decomposing. The rate of decomposition is controlled by the backward reactions of NO kinetics (Reactions 2.1 to 2.3) until the NO chemistry freezes due to falling temperatures.

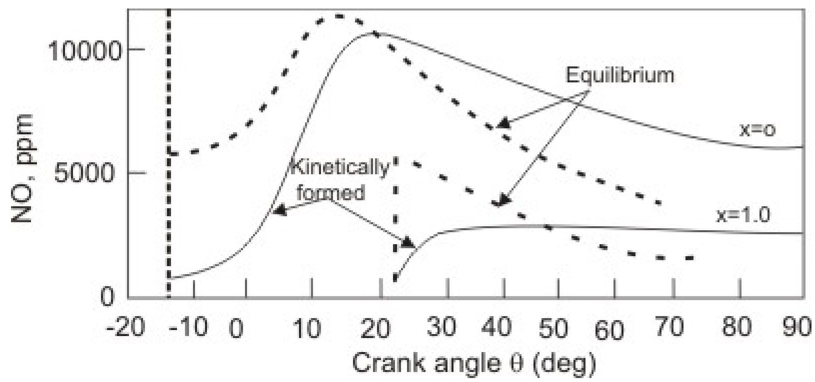

Figure 2.7	Kinetically formed NO in an early burned and a late burned charge element. Equilibrium NO concentration in each of these elements is also shown.

The net mass fraction of NO emissions in the exhaust is computed as the weighted average of the frozen mass NO fraction over all the burned gas elements.

$$\bar{x}_{NO} = \sum x_{NO} \cdot \Delta x$$

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Effect of Addition of Diluents on NO Formation

Burned residual gases left from the previous cycle act as charge diluents. A part of exhaust gas is also recirculated back to the engine for diluting the intake charge to reduce NO formation. This process is known as exhaust gas recirculation (EGR). Dilution by the burnt residual gases is also called as 'internal EGR'. The combustion temperatures decrease as a result of charge dilution and the lower combustion temperatures result in lower NO levels. The effect of different diluents on NO emissions is shown on Fig. 2.8(a) The equal volume of different diluents gives different NO reductions. CO_2 and H_2O being tri-atomic gases have higher specific heat and give larger NO reductions than the same volume of N_2, He or Ar. The NO emission data with different diluents correlates very well with heat capacity (mass flow rate of the dilutent x specific heat) irrespective of the chemical nature of the diluents as shown in Fig. 2.8(b) . It shows that the effect of charge dilution on NO is almost entirely due to the heat capacity of the diluting gases. The specific heat of the exhaust gas is higher than for air due to presence of substantial fractions of CO_2 and H_2O. Hence, EGR results in lower combustion temperatures compared to those from dilution by nitrogen alone or by leaning of mixture.

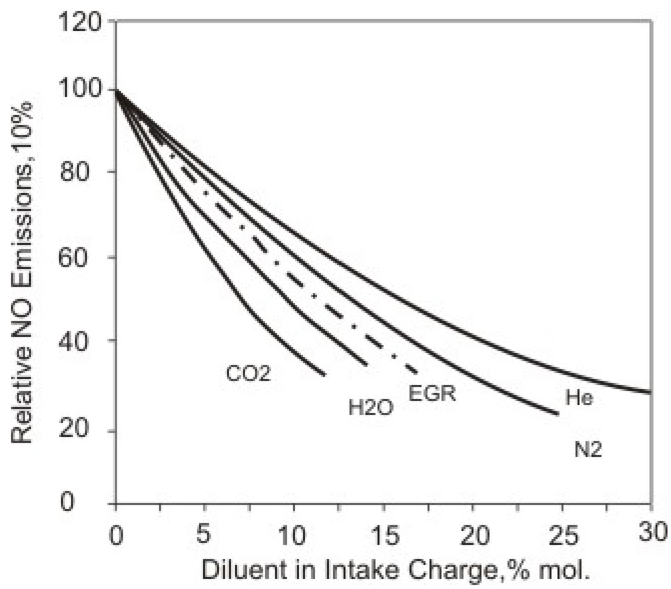

Figure 2.8(a)	Effect of content of various diluents in intake air on NO reduction in a SI engine

A negative effect of charge dilution is reduction in oxygen concentration in the charge and slowing down of flame propagation speed and the rate of combustion. It causes further reduction in the burned gas temperature and beyond a limit causes misfired combustion resulting in lower fuel efficiency and higher unburned hydrocarbon emissions

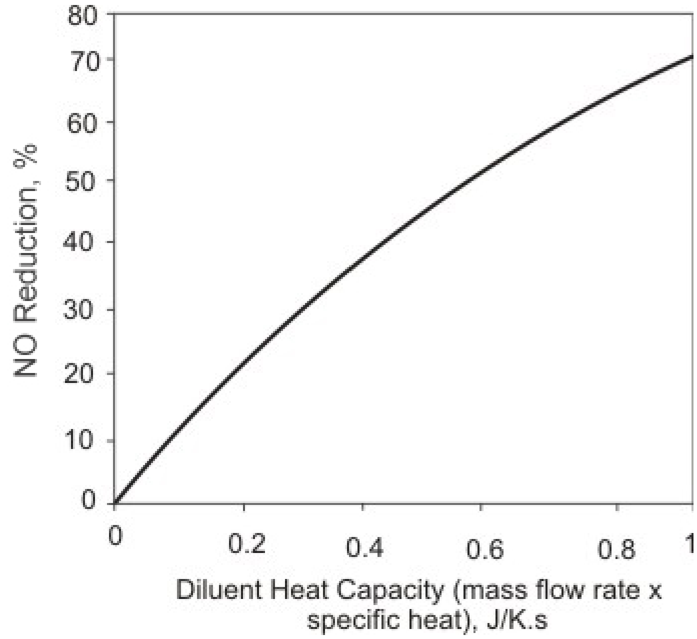

Figure 2.8(b)	NO reduction correlates well with diluent's heat capacity in a SI engine.

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