



Figure 5.1: Thermal NO production Rate Sensitivity with Temperature

The rate of NO formation governed by equation 5.5 is a function of T , global species O_2 and N_2 concentration and concentration of O atoms and OH radicals. The global species concentration is known from the combustion simulation using simplified reaction mechanism, however O and OH radical concentrations are not known a priori and have to be determined. It is known that the kinetics of thermal NO formation is much slower than the main hydrocarbon oxidation rate, and most of the thermal NO is formed after completion of combustion. Therefore, the thermal NO formation process can often be decoupled from the main combustion reaction mechanism and the NO formation rate can be calculated by assuming equilibrium concentrations of O atoms and OH radical as illustrated by ANSYS Fluent user guide [13].

Determining O radical concentration

- Equilibrium Chemistry Approach

$$[O] = 3.97 * 10^5 T^{-1/2} e^{-31090/T} [O_2]^{1/2} \text{mol/m}^3 \quad (5.6)$$

- Partial Equilibrium Approach

The O atoms concentration has been observed to be more abundant than their equilibrium levels. The level of thermal NO can be under predicted by as much as 28% when considering Equilibrium Approach [13]. The more accurate partial equilibrium approach accounts for third-body reactions in the O_2 dissociation recombination process and generally leads to a higher partial O atoms concentration.

$$[O] = 36.64 T^{1/2} e^{-27123/T} [O_2]^{1/2} \text{mol/m}^3 \quad (5.7)$$

Determining OH radical concentration

- Exclusion of OH Approach

The third body reaction in the extended Zeldovich mechanism contributes to the formation of NO at near-stoichiometric conditions or in fuel-rich mixtures and is negligible for fuel lean conditions which leads to the following assumption $k_{f2} [O_2] \gg k_{f3} [OH]$.

- Partial Equilibrium Approach

$$[OH] = 2.129 * 10^2 T^{-0.57} e^{-4595/T} [O]^{1/2} [H_2O]^{1/2} \text{mol/m}^3 \quad (5.8)$$

5.3 Calculating NO Mass Fraction

The NO species transport equation needs to be solved for obtaining the NO mass fraction (Y_{NO}) distribution due to convection, diffusion and volume sources. The governing convection diffusion equation for NO transport is given by,

$$\underbrace{\frac{\partial \rho Y_{NO}}{\partial t}}_{\text{Transient term}} + \underbrace{\nabla \cdot (\rho \vec{u} Y_{NO})}_{\text{Convection term}} = \underbrace{\nabla \cdot (\rho D_{eff} \nabla Y_{NO})}_{\text{Diffusion term}} + \underbrace{S_{Y_{NO}}}_{\text{Source term}}$$

where $S_{Y_{NO}}$ is the source term accounting for production of NO calculated from the rate of change of concentration of NO in equation eq. (5.5).

$$S_{Y_{NO}} = M_{NO} \frac{d[NO]}{dt} \text{Kg/m}^3 - s \quad (5.9)$$

The NO concentration can be obtained from the NO mass fraction using the relation

$$[NO] = \frac{p Y_{NO}}{RT}$$

Since the thermal NO production is very sensitive to temperature distribution as illustrated earlier, an accurate temperature distribution is a prerequisite for reasonable NO prediction.

Calculation of S_ϕ , ρ and ρD_{eff} for NO transport

The implementation details of the passive scalar transport equation for NO mass fraction was presented above. However, it requires the calculation of the source term S_ϕ , density ρ and mass diffusivity D_{eff} . The source term for NO transport given by eq. (5.5) is re-stated here as follows

$$S_{Y_{NO}} = M_{NO} \quad 2 k_{f1} [O] [N_2] \quad \frac{\left(1 - \frac{k_{b1} k_{b2} [NO]^2}{k_{f1} k_{f2} [N_2] [O_2]}\right)}{\left(1 + \frac{k_{b1} [NO]}{k_{f2} [O_2] + k_{f3} [OH]}\right)} \quad (mol/m^3 - s)$$

The following quantities are known from the main combustion calculations

- Temperature(T) distribution.
- The velocity field (\vec{u}).
- The mass fraction Y_s of the participating chemical species and pressure(p) distribution.
- Turbulent viscosity μ_t .

From the molecular weights and the available mass fractions of the stable species the weighted density is computed as follows $\rho = M_{avg} \frac{P}{RT}$, $M_{avg} = \sum_s f_s M_s$ where M_s is the molar mass of specie s. The effective molecular diffusivity is given by

$$\rho D_{eff} = \frac{\mu_o}{Sc} + \frac{\mu_t}{Sc_t}$$

where Sc and Sc_t are the Schmidt number and turbulent Schmidt number respectively and μ_o is the laminar viscosity computed using Sutherland law for Transport

$$\mu_o = A_s \frac{T^{3/2}}{T + T_s}$$

where $A_s = 1.67212 \times 10^{-6}$, $T_s = 170.672$. The average Schmidt number for NO in air of 0.85 is used for calculations. The turbulent Schmidt number of 0.7 is used for comparison with ANSYS Fluent.