Exhaust Emissions

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BASED UPON S.C. SORENSEN
CHAPTER 6 PART 1

Common Exhaust Pollutants

- Unburned Hydrocarbons, CHx, HC's, partially oxidized hydrocarbons, etc.
- Oxides of Nitrogen, NO, NO2, N2O2, etc.
- Carbon Monoxide
- Particulate Matter (soot), soluble, insoluble
- Sulfur and Sulfur Oxides
- Carbon Dioxide

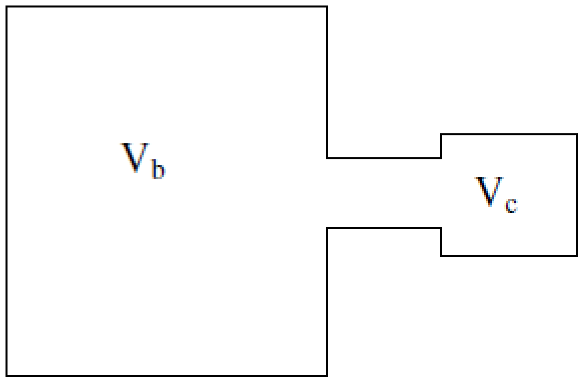
Noxious Gas Production During Combustion

- SI Engines
  - NOx
  - CHx, HC's
  - CO
- CI Engines
  - NOx
  - CHx, HC's
  - CO
  - particulate (soot)
- Stationary Combustion
  - NOx
  - CHx, HC's
  - CO
  - particulate (soot)
  - sulfur compounds

Hydrocarbon Formation

- Flame Quenching
- Crevices
- Absorption by the oil film
- Bulk quenching
- high at excess fuel conditions

‘Noxious’ because of the contribution to photochemical smog



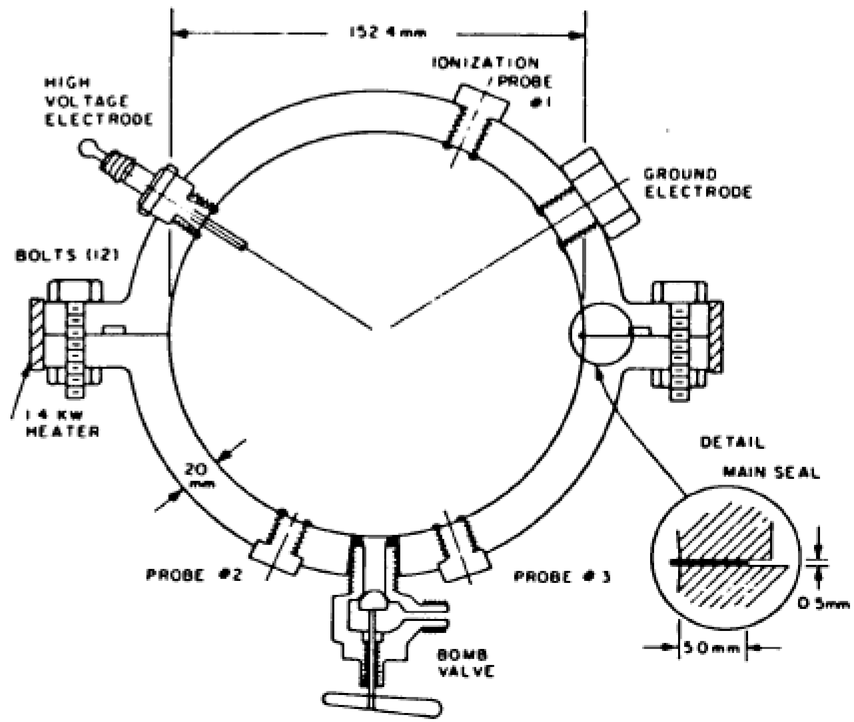


Figure 6.2: Combustion bomb used for HC emissions research

Oxides of Nitrogen

- high temperatures
- frozen equilibrium
- dissociation with time
- peak at stoichiometry

'Noxious' because of the contribution to photochemical smog

NOx Kinetics

Table 6.1: Equilibrium constant for Reaction 6.6, and equilibrium concentration of NO for an initial gas composition of 98% N_2 and 2 % O_2.

Temperature - K	K_p	x_{NO}
1500	$1.07 \cdot 10^{-5}$	$9.06 \cdot 10^{-4}$
2000	$4.00 \cdot 10^{-4}$	$5.24 \cdot 10^{-3}$
2500	$3.52 \cdot 10^{-3}$	$1.35 \cdot 10^{-2}$
3000	0.0149	$2.25 \cdot 10^{-2}$
3500	0.0416	

$$N_2 + O_2 \rightleftharpoons 2NO$$

$$K_p = \frac{p_{NO}^2}{p_{N_2} \cdot p_{O_2}} = \frac{x_{NO}^2}{x_{N_2} \cdot x_{O_2}}$$

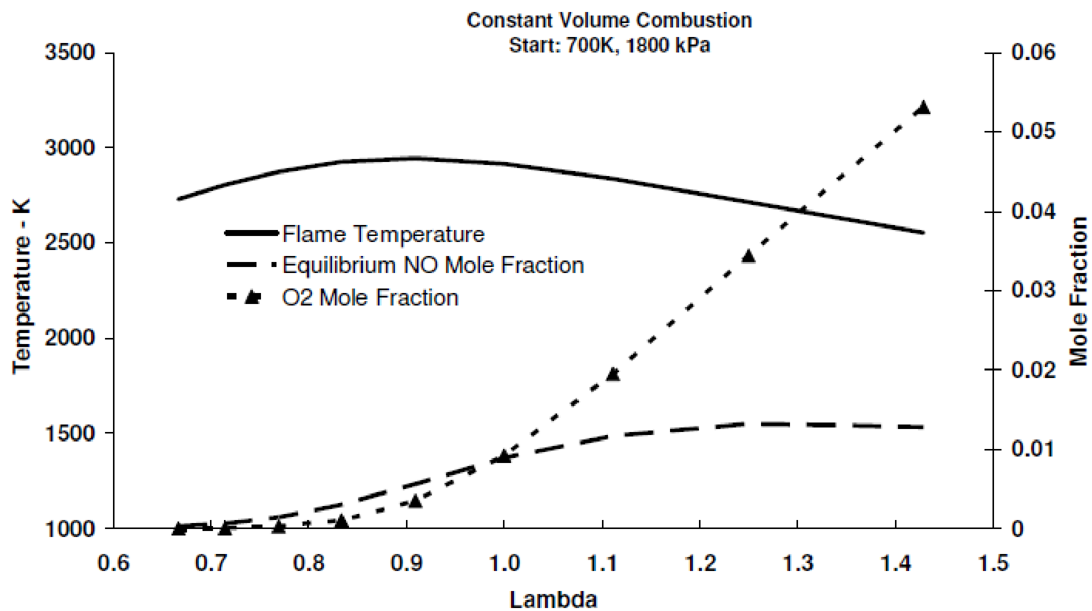


Figure 6.3: Equilibrium flame temperature, and equilibrium concentrations of NO and O_2 for constant volume combustion of iso-octane and air as a function of excess air ratio.

NOx: Equilibrium and Actual

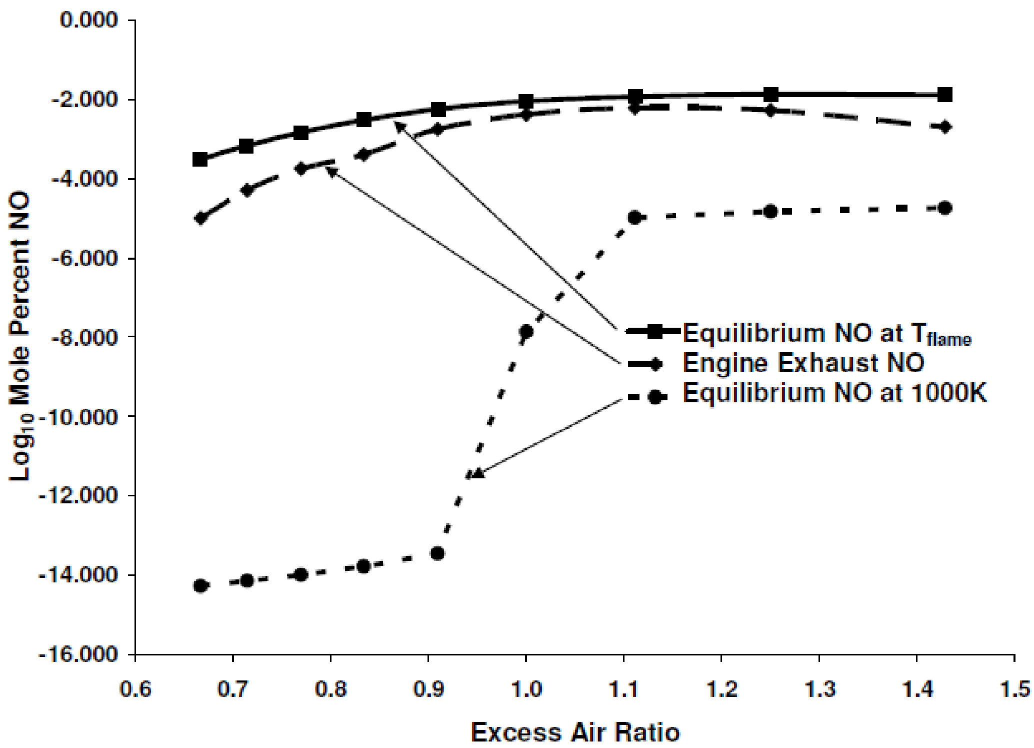


Figure 6.4: Equilibrium of concentrations NO at peak temperature and pressure, at exhaust conditions (1000K, 1 atm) compared to typical NO_x emissions from a spark ignition engine operating at full load.

NOx: Temporal Development

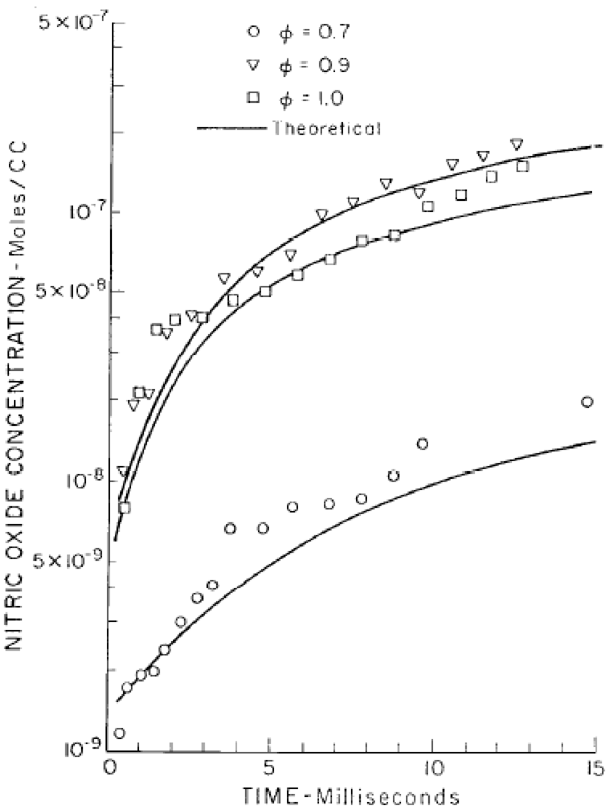


Figure 6.5: The temporal development of the NO concentration in the period after the flame in a constant volume bomb.

NOx: Equilibrium and Reaction Kinetics

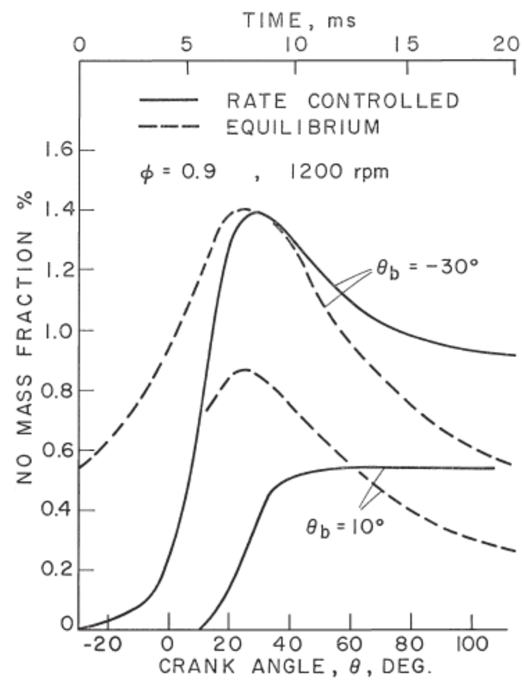


Figure 6.6: A comparison of the NO concentrations from equilibrium conditions and from reaction kinetics controlled conditions for two locations in the combustion chamber of a spark ignition engine.

Zeldovich Mechanism

$$N_2 + O \rightarrow N + NO \quad [2f]$$
$$N + NO \rightarrow N_2 + O \quad [2b]$$
$$O_2 + N \rightarrow O + NO \quad [3f]$$
$$O + NO \rightarrow O_2 + N \quad [3b]$$

$$N + OH \rightarrow NO + H \quad [4f]$$
$$H + NO \rightarrow OH + N \quad [4b]$$

$$k_{2f} = 7 \cdot 10^{13} \exp(-37800/T) \tag{6.8}$$

$$k_{2b} = 1.55 \cdot 10^{13} \tag{6.9}$$

$$k_{3f} = 1.33 \cdot 10^{10} \cdot T \cdot \exp(-3600/T) \tag{6.10}$$

$$k_{3b} = 3.2 \cdot 10^{9} \cdot T \cdot \exp(-19700/T) \tag{6.11}$$

$$k_{4f} = 7.1 \cdot 10^{13} \exp -450/T) \tag{6.12}$$

$$k_{4b} = 1.7 \cdot 10^{14} \cdot \exp(-24560/T) \tag{6.13}$$

Calculated Composition

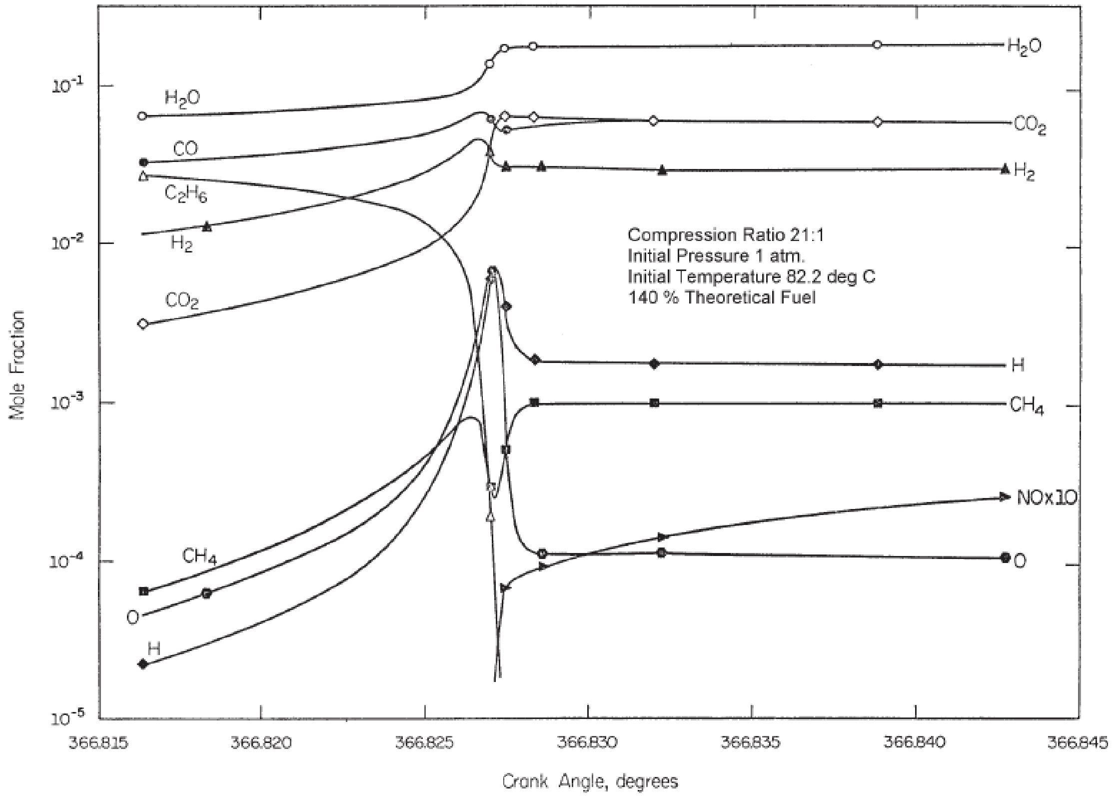


Figure 6.7: Calculated composition of the combustion gasses immediately before and after homogeneous charge compression ignition at high pressure and temperature. The pressure and temperature after the combustion are 190 atm and 3000 K. An elapsed time of $2.5 \cdot 10^{-6}$ s. corresponds to 0.03 crank angle degrees.

NOx: the Time Constant

$$\tau = \frac{R_o T}{p} \frac{1}{k_{2b} x_{N,e} + k_{3b} x_{O,e} + k_{4b} x_{H,e}}$$

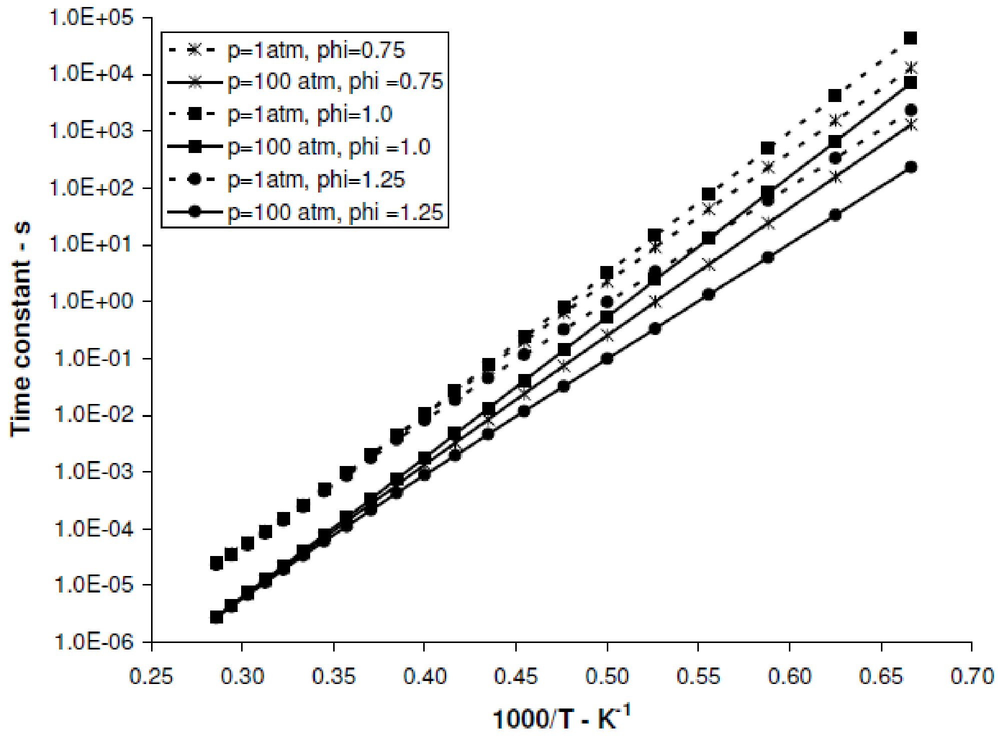


Figure 6.8: Calculated values of the time constant for the NO reactions as a function of temperature, pressure and equivalence, iso-octane was the fuel used to form the combustion products.