

NO<sub>x</sub> and CO Production in Pulsed Jet Combustion:  
Thermochemical Analysis

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A thermochemical model of Pulsed Jet Combustion (PJC) is proposed and used for the parametric study of the effect of various governing parameters on the level of NO<sub>x</sub> and CO production during burning of methane - air mixtures.

The PJC system under study consists of the main chamber of volume  $V_0$  and the prechamber of volume  $V_p$ . Prior to ignition, the former is filled with a homogeneous fuel-air mixture with the equivalence ratio  $\phi_p > 1$ , while the latter is filled with the fuel-lean mixture with  $\phi_0 < 1$ . Initial temperature and pressure in the PJC system are  $T_0$  and  $P_0$ . The diameter of the orifice between the prechamber and the main chamber is  $D_0$ . Ignition source is located in the prechamber.

After ignition, a turbulent plume is generated in the main chamber by the jet of combustion products escaping from the prechamber. The plume is composed of multiple vortices of various size. Combustion of fuel-lean mixture in the main chamber is resumed in the vortices due to mixing with the high-temperature combustion products. The vortices grow in size by engulfing new portions of fresh mixture and the mixture from other vortices and due to thermal expansion caused by chemical reaction. The combustion process terminates when the entire mixture has burned out.

The final composition of the combustion products includes H<sub>2</sub>, H<sub>2</sub>O, CO, CO<sub>2</sub>, and NO. The maximum rate of pressure rise, the maximum pressure, and the final level of CO and NO are dependent of  $T_0$ ,  $P_0$ ,  $V_0$ ,  $\phi_0$ ,  $\phi_p$ ,  $V_p$ , initial distribution of vortices size (fractions of  $D_0$ ), and heat loss to chamber wall.

The mathematical model of the PJC system is based on the mass, volume, and energy balance equations for vortices and the whole system, coupled with the equation of state and with the balance equations for chemical species.

Initially, the mixture in prechamber was assumed to burn under constant volume conditions and expand isentropically into the main chamber. The vortices thus formed in the main chamber have been grouped according to their size in  $n$  groups. The size distribution was assumed to have a Gaussian shape with the mathematical

expectation  $D_0$ . The distribution curve was approximated by piece-step function with certain characteristic sizes of vortices.

Mass transfer between the vortices of various groups have been modelled by the following equation:

$$\frac{dm_i}{dt} = uS_i \cdot \sum_{j=0}^n \left[ \left( \frac{V_j}{V_0} \right) \rho_j - \left( \frac{V_i}{V_0} \right) \rho_{iu} \right] \cdot \sum_{j=1}^n S_j$$

where  $m_i$ ,  $\rho_i$ ,  $S_i$ ,  $V_i$  are the mass, mixture density, surface area, and volume of vortices of group  $i$ , respectively,  $t$  is time,  $i=0$  corresponds to unburned mixture ( $S_0 = 0$ ),  $u$  is the average rate of mass transfer. In summation  $i$  is not equal to  $j$ . As the estimate for the average rate of mass transfer,  $u$ , the value of characteristic velocity fluctuation in the expanding jet has been used.

The kinetic scheme for methane oxidation and NO formation was as follows:



Reaction (4) was used for modeling prompt NO formation. The use of  $\text{CH}_4$  in the both parts of reaction equation ensured prompt NO production only in the reaction zone where  $\text{CH}_4$  was available. In detailed reaction mechanisms prompt NO is produced due to reactions with the radicals like  $\text{CH}$  and  $\text{CH}_3$ . Reaction (5) was used for modeling thermal NO formation (Zel'dovich NO). The corresponding reaction constants for reactions (1) to (5) have been chosen by fitting the predicted and measured laminar flame velocities and NO levels in laminar flame structure at different initial values of fuel - air ratio, pressure and temperature. For reaction (5), the rate constant incorporates the equilibrium constant of  $\text{O}_2$  dissociation.

Variation of various species mass in vortices of group  $i$  was modelled by equations like.

$$dm_{ki} = dm_{ki}^r + x_k dm_i$$

where the first term describes the variation the  $k$ -th specie mass due to chemical reaction, while the second term is due to engulfing mixture from the ambient space. Thus, the mixing and reaction processes were assumed to proceed simultaneously

The heat loss to chamber wall has been modelled with due regard for radiation heat flux as well as the convective heat transfer between the unburned and the wall.

The governing equations were solved by the Runge-Kutta method for different initial mixture composition, and different values of  $u$ ,  $D_0$ ,  $T_0$ , and  $P_0$ . For realistic estimates of  $u$ , some gasdynamic calculations of 2-D cylindrical jets were performed by using an available computer code.

The results of calculations have allowed to optimise the set of governing parameters for obtaining the highest rate of pressure rise at a reasonably low level of NO and CO content in combustion products.

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