

ABSTRACT

A complete FORTRAN computer program is presented which can be used to compute the equilibrium composition of 19 species and all the relevant information regarding the final state of the products after either constant pressure or constant volume combustion in any hydrocarbon - air system. The data required by the program are: fuel formula ($C_nH_mO_l$), fuel specific heat constants, reactant pressure, reactant air temperature, fuel temperature and finally if the combustion takes place at constant pressure or constant volume. The output data are: the equilibrium composition of the products, the enthalpy or internal energy of the products, the specific heat of the products and finally the adiabatic flame temperature of the products.

The second part of the thesis presents an approximate formula by means of which the adiabatic flame temperature of fuel - air systems can be calculated as functions of reactant pressure, reactant temperature, equivalence ratio, carbon number of the fuel and the type of combustion (constant volume or constant pressure). The formula has been developed by fitting of the data from the output of the chemical equilibrium program to a functional expression. This formula provides a very fast and easy means of predicting flame temperatures compared to equilibrium calculations. It is applicable to any fuel within the paraffin, naphthene, olefine, aromatic and alcohol families for a wide range of reactant conditions.