(Extended Abstract for SOMCE '95)

APPLICATION OF ASPEN PLUS IN COMBUSTION MODELING

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INTRODUCTION

Modern process simulators are useful tools to imitate chemical reactions, analyse product streams and change reactor parameters without using expensive equipments, laboratory materials and precise measuring instruments. In this work ASPEN PLUS Release 9.1-3 (1994) was employed to simulate the combustion reactions of premixed gaseous flames. This simulator incorporates up to date databank for pure component properties as well as combustion databank based on JANAF Tables [1]. By using the minimization of total Gibbs free energy method adiabatic flame temperature for several stoichiometric fuel/air mixtures were calculated. Analysis of combustion products with concentrations as low as 1 PPB was carried out for over twenty species and compared with previous works.

PROCEDURE

The flow diagram of the combustion process of premixed flames includes separate streams of fuel and air at 300K and 1 atm. flowing into a mixer which provides perfect mixing. Mixture stream then enters the reactor and after an equilibrium reaction leaves as combustion products. ASPENPLUS enables selection of several types of reactors for different application. i.g: Stoichiometric. Equilibrium, Yield, Plug Flow, Batch and Gibbs reactors. In the case of a multireaction system such as combustion of a hydrocarbon fuel involving numerous dissociating, recombination and elementary reactions Gibbs reactor is preferred because reactants with initial amounts and conditions and only the product components are required to be specified. Details of the reactions involved, stoichiometry, and equilibrium constants are not necessary for calculation of products concentration.

Methane, Ethane, Propane, LPG (60% n - C_4H_{10} and 40% C_3H_8) and Hydrogen are popular fuels and studied here. Among the long list of possible species present in the product stream, twenty three components, detected in most hydrocarbon combustion processes were included in this model. These species in respective order are: N_2, H_2O, CO_2, CO, O_2, H_2, OH, NO, H, O, HO_2, NO_2, N_2O, HNO, N, NH, CHO, HCN, CH_2O, CN, CH, C_2H_4, and C_3H_6. Reactor pressure was taken constant I atm., but reactor temperature was specified with a tolerance of IK in each run. Choosing the reactor temperature above or below the adiabatic flame temperature results in positive or negative reactor heating duties respectively. So an adiabatic reactor with heating duty of zero represents a self sustained reaction at the flame temperature of the fuel/air mixtule.

RESULTS AND DISCUSSION

By sensitivity analysis the reactor temperature was varied for each fuel and adiabatic performance of the reactor was indicated precisely. Fig. (1) shows the summary of results for calculation of flame temperatures. Table (1) shows the analysis of combustion products for different fuels at soichiometric concentrations reacting to equilibrium at the appropriate flame temperatures. These results are in agreement with reported measured or calculated recognized works, some of which are summarized in Table (2) [2,3 and 4]. The effect of changing reaction temperature on the concentration of product species was studied and the results for stoichiometric methane/air mixture are shown in Fig. (2) and (3). Another sensitivity analysis carried out was to study the effect or varying fuel/air ratio (O, equivalence ratio) at the specified flame temperature. The results for methane are shown in Fig. (4) and (5). It should be mentioned that the accuracy of species concentrations as well as calculated flame temperatures strongly depend on the number of products species chosen and included in the simulation model. Precision of thermochemical data and different solution techniques are also responsible.

REFERENCES

1. JANAF, Thermochemical Tables. Dow Chemical Company, Michigan, 1979.
2. Hamidi, A.A. and Farshchi, F. Proc, 1st. Int. Non Renewable Energy Sources Congress. Iran Univ. of Tehcnology 1993, 667-679.
3. Gaydon, A.G. and Wolfhard, H.G. Flames, Their Structure, Radiation and Temperature. 4th ed. Chapman and Hall, London 1979.
4. Barnard, J.A. and Bradley, J.N. Flame And Combustion 2nd ed. Chapman And Hall, London 1985, 13.

Fig.(1) Adiabatic Flame Temperature for Stoichiometric Mixtures

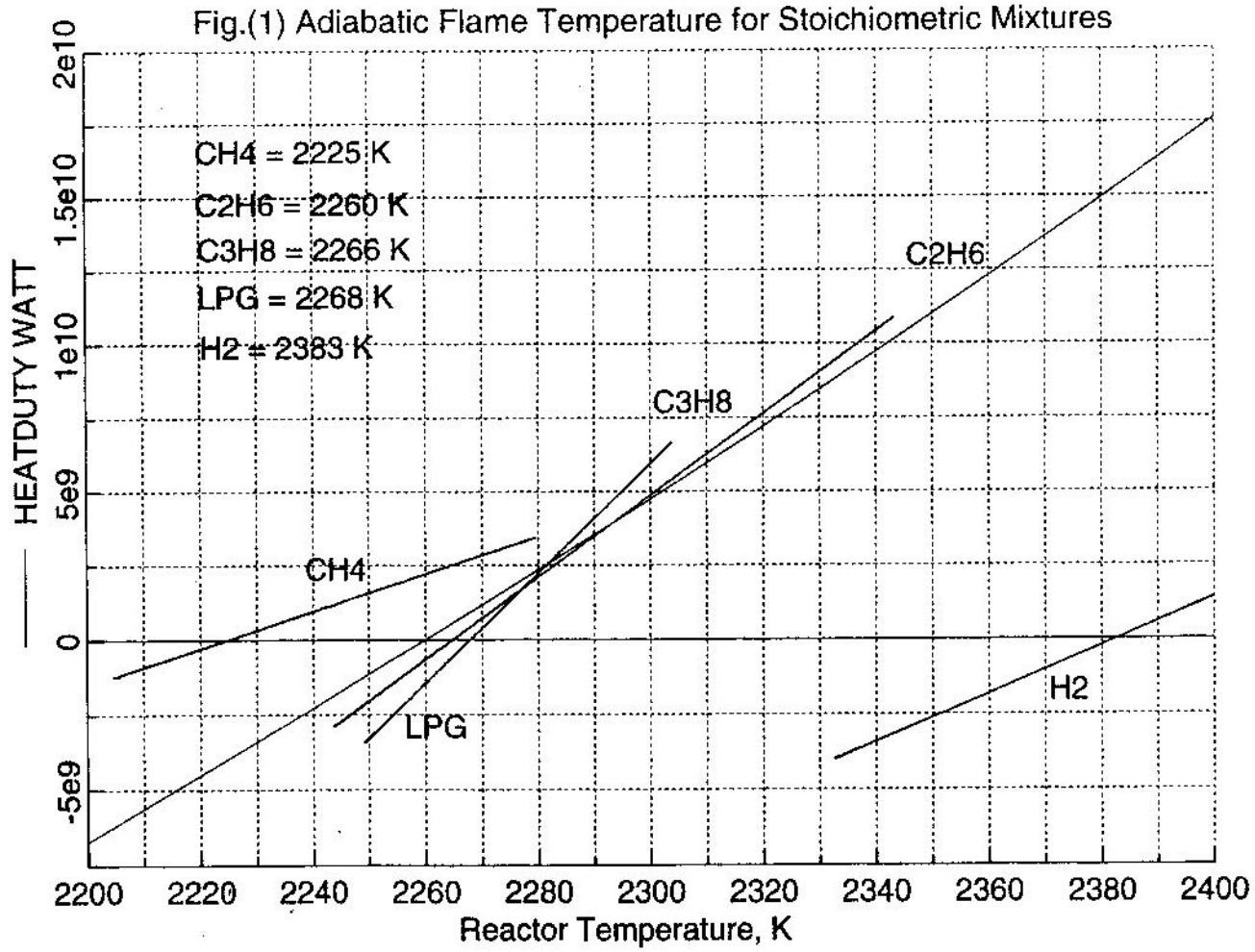

Table (1) Analysis of Combustion Products

Product Species	CH_4 2225 K	C_2H_6 2260 K	C_3H_8 2266 K	LPG 2268 K	H_2 2383 K
N_2	0.70864	0.71715	0.72082	0.72214	0.64434
H_2O	0.18336	0.15831	0.14836	0.14479	0.32351
CO_2	0.08536	0.09745	0.10266	0.10453	-
CO	0.00896	0.01166	0.0125	0.01279	-
O2	4553 PPM	5541 PPM	5511 PPM	5909 PPM	4754 PPM
H_2	3615"	3488"	3313"	3248"	15330"
OH	2924"	3266"	3277"	3278"	7009"
NO	1980"	2372"	2468"	2503"	2678"
H	393"	466"	470"	471"	1827"
O	215"	293"	312"	319"	548"
HO_2	880 PPB	1050 PPB	1073 PPB	1080 PPB	1882 PPB
NO2	330"	415"	438"	446"	370"
N_2O	94"	113"	117"	119"	120"
HNO	51 "	60 "	60 "	61 "	143 "
N	14 "	21 "	23 "	23 "	75 "
HN	<1"	1"	1"	1"	6"
CHO	<1 "	1 "	1 "	1 "	-

Tables (2) Analysis of Combustion Products From Other Sources

Product Species	CH_4		C_2H_6	C_3H_8	
	2207 K [2]	2222 K[3]	2240 K [2]	2247 K [2]	2219 K [4]
N_2	0.7087	0.709	0.7178	0.7210	0.7341
H_2O	0.1834	0.18	0.1585	0.1484	0.1423
CO_2	0.0854	0.085	0.0976	0.1028	0.1004
CO	0.0089	0.009	0.0115	0.0124	0.0099
O_2	0.0045	0.004	0.0055	0.0058	0.0048
H_2	0.0036	0.004	0.0035	0.0033	0.0032
OH	0.0028	0.003	0.0032	0.0032	0.0027
NO	0.0020	0.002	0.0024	0.0025	0.0020
H	0.0004	0.0004	0.0005	0.0005	0.0035
O	0.0002	0.0002	0.0003	0.0003	0.0020

Fig.(2) Concentration Variations with Temperature in CH4 Flame

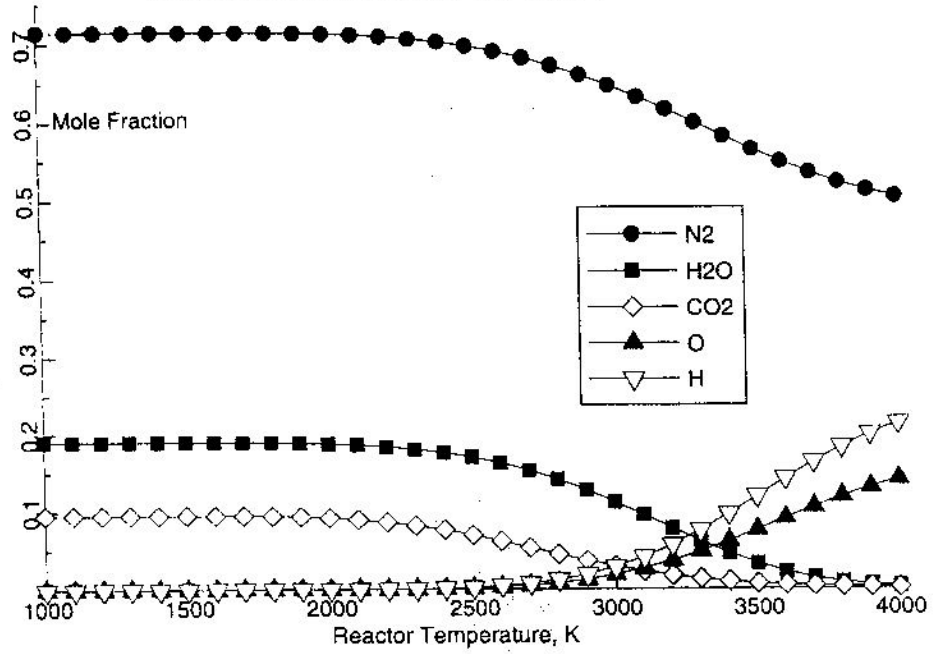

Fig.(3) Concentration Variations with Temperature in CH4 Flame

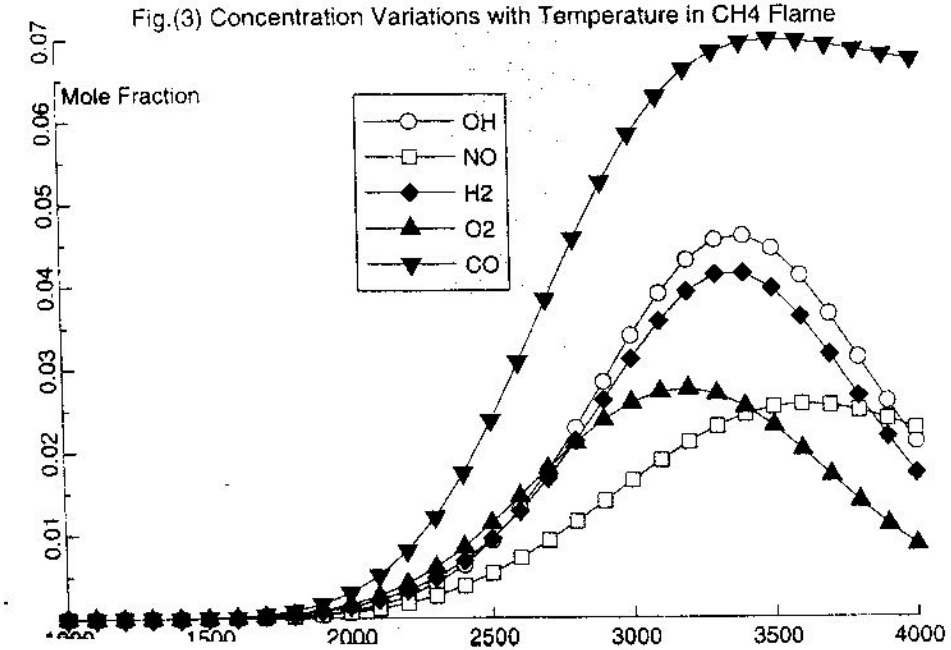

Fig.(4) Concentration Variations with Fuel Ratio in CH4 Flame

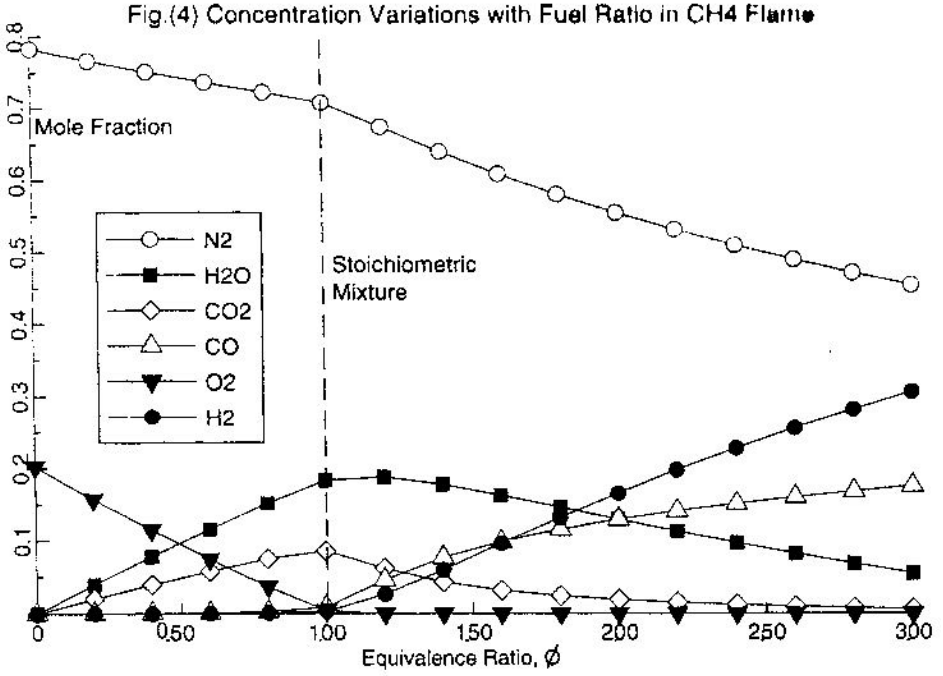

Fig.(5) Concentration Variations with Fuel Ratio in CH4 Flame