UNIVERSITI PUTRA MALAYSIA

DEVELOPMENT OF COMPUTER PROGRAM TO ANALYSE COMBUSTION PRODUCTS RESULTING FROM INCINERATION OF SOLID FUELS

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This Work is Dedicated
To
My Parents and Sisters

Abstract of thesis presented to the Senate of Universiti Putra Malaysia in fulfilment of the requirements for the degree of Master of Science

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Numerous technologies have been developed to combust solid fuels and waste in a commercially useful manner. Impetus for technology development includes optimizing energy recovery, capitalizing upon economies of scale, maximizing the potential applications of solid fuels, and achieving compliance with present and expected environmental regulations. The goal of this research is to develop a computer program for analysing the chemical products from incineration of solid fuel. The objective is to compute the concentrations of 12 chemical products at a given temperature and excess air, with total flue gas pressure equals to 1 atm. Those concentrations can be used as thermodynamic indicators, for lowering the emissions by adequately organizing and conducting the combustion process. The computer program also takes into account the possibility of further extension.

The products of combustion concerned include; carbon dioxide CO_2, carbon monoxide CO, water vapor H_2O, hydrogen H_2, sulfur dioxide SO_2, sulfur trioxide SO_3, nitric oxide NO, nitrogen dioxide NO_2, hydrogen chloride HCl, chlorine Cl_2, oxygen O_2, and nitrogen N_2. Chemical combustion and equilibrium analysis form the

main part of this research. For the first analysis 6 equations are deduced from mole balance, and 6 other equations are deduced from the second analysis by using the chemical equilibrium constants. The 12 equations are non-linear, and therefore numerical method is used i.e. the Newton iteration method for its rapid convergence.

The output from this computer program are compared with the result of research carried out by the Institute of Nuclear Sciences (INS), which is based on the application of the developed model for computing the chemical thermodynamic equilibrium of a system formed by compounds and elements contained in the Kolubare [Yogoslavia] basin lignite. Combustion simulation was done for eight lignite compositions with temperatures from 800 to 1700 K, pressure 1 atm, and 25% excess air. The results obtained from the combustion of such a solid fuel show that there is no significant difference between the two sources [INS & Program] as proved by using statistical T-test whatever difference in the results that are noticed, vary from one compound to another. This is due to different models used in computing the chemical equilibrium constants and the number of products used. the results given by INS are related to more than 12 unknowns in comparison to the developed computer program.

It is recommended to add to the developed computer program the equation of energy, from which the adiabatic temperature can be computed. For the accuracy of the computer program, other compounds may be added such as H, OH, HO_2, N_2O, HNO_2, H_2O_2, SO, N, O, and CH_4. Beside this the humidity in the air should be taken into account. Additional subroutine may be inserted in the computer program, for computing some thermodynamic parameters and also amount of additional fuel in

case where the solid waste have unsufficient heating value. Options for designing furnace and the auxiliary equipments of an incinerator can also be included.

Abstrak tesis yang dikemukaken kepada Senat, Universiti Putra Malaysia sebagai memenuhi sebahagian keperluan untuk ijazah Master Sains

PEMBANGUNAN ATURCARA KOMPUTER BAGI MENGANALISIS PRODUK KIMIA YANG DIHASILKAN DARI PENUNUAN BAHAN API PEPEJAL

Oleh

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Pelbagai teknologi telah dibangunkan untuk membakar bahan api pepejal dan sisa dengan cara yang berguna dari segi komersial. Pemangkin bagi pembangunanan teknologi termasuk pengoptimuman pemulihan tenaga, pembiayaan skala ekonomi, memaksimumkan aplikasi berpotensi bagi bahan api pepejal, dan mencapai pematuhan peraturan-peraturan alam sekitar sekarang dan pada masa hadapan. Objektifnya ialah untuk mengira kepekatan bagi 12 produk kimia pada suhu dan udara lebih yang telah ditetapkan, dengan tekanan gas serombong menyeluruh bersamaan dengan 1 atmosfera. Kepekatan tersebut boleh digunakan sebagai penunjuk termodinamik, bagi mengurangkan keluaran dengan mengorganisasi dan menjalankan proses pembakaran secara sempurna. Aturcara komputer tersebut juga mengambil kira kemungkinan penambahan tugas penyelidikan.

Produk pembakaran termasuk karbon dioksida CO_2, karbon monoksida CO, wap air H_2O, hidrogen H_2, sulfur dioksida SO_2, sulfur trioksida SO_3, nitrik oksida NO, nitrogen dioksida NO_2, hidrogen klorida HCl, klorin Cl_2, oksigen O_2 dan nitrogen N_2. Pembakaran kimia dan analisis keseimbangan adalah kandungan utama

bagi penyelidikan ini. Bagi analisis pertama 6 persamaan telah dibuat kesimpulan dari persamaan mol dan 6 persamaan yang lain telah dibuat kesimpulan dari analisis yang kedua menggunakan permalar keseimbangan kimia. Kesemua 12 persamaan tersebut berbentuk tidak lelurus. Oleh yang demikian, kaedah berangka telah digunakan,

Keluaran (*output*) dari aturcara komputer ini dibandingkan dengan hasil penyelidikan yang dilaksanakan oleh Institute of Nuclear Science (INS), yang berasaskan penggunaan model yang telah dibangunkan bagi mengira keseimbangan termodinamik kimia bagi satu sistem yang dibentuk dari sebatian dan unsur terkandung dalam lignit lembangan Kolubare [Yugoslavia] dan pembakaran udara, kajian telah dibuat keatas lapan jenis lignit dalam keadaan pembakaran suhu 800 ke 1700 K, tekanan 1 atm, dan

dari pembakaran bahan api pepejal tersebut menunjukkan bahawa tidak ada perbezaan yang ketara dari kedua-dua sumber [INS dan aturcara], dan dibuktikan dengan mengguna kaedah statistik ujian-T. Mana-mana perbezaan keputusan yang ketara didapati berubah-ubah dari satu sebatian kepada yang lain. Ini disebabkan model-model yang berlainan yang digunakan dalam mengira keseimbangan kimia dan bilangan produk yang digunakan. Keputusan yang diberikan oleh INS adalah berhubung kait dengan lebih dari 12 anu jika dibandingkan dengan perisian komputer yang telah dibangunkan.

Adalah dicadangkan untuk memasukkan persamaan tenaga ke dalam aturcara komputer yang telah dibangunkan dari mana suhu adiabatik boleh dikira. Bagi ketepatan aturcara komputer, sebatian lain boleh ditambah contohnya H, OH, HO_2,

N_2O, HNO_2, H_2O_2, SO, N, O dan CH_4. Di samping itu kelembapan dalam udara perlu diambil kira. Subrutin tambahan boleh dimasukkan dalam aturcara komputer bagi mengira parameter termodinamik dan kandungan bahan api tambahan dalam kes di mana sisa pepejal mengandungi nilai haba yang tidak mencukupi. Reka bentuk relau dan peralatan tambah bagi penunuan tersebut boleh dimasukkan juga.

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LIST OF ABBREVIATIONS

$\propto$	Probability at which, the Null Hypothesis H_o is rejected.
ε	Error tolerated when using the Newton's Method.
A/F	Air Fuel Ratio.
Act	Actual Condition.
A(i,j)	Matrix which contains Partial derivatives (Jacobi Matrix).
CARS	Coherent Anti-stokes Raman Scattering.
CE	Combustion Efficiency.
df	Degree of Freedom used in Statistics.
E_j	Elemental Composition of Element j.
Eqs	Equation (s).
%EX	Percentage Excess Air.
f_i	Mole Fraction of element i.
F_j	Function which contains equation j.
$\partial F_j/\partial X_i$	Partial Derivative of Function F_j with respect to X_i.
$\partial \mathbf{F}/\partial \mathbf{X}$	Jacobi Matrix incorporated in A(i,j).
ΔG^o	Free Energy Change.
H_o	Null Hypothesis used in Statistics.
H_A	Alternative Hypothesis used in Statistics.
ΔH^o	Standard Heat of Reaction.
ΔH_T	Standard Enthalpy Change.
INS	Institute of Nuclear Science.
K	Chemical Equilibrium Constant / Degree in Kelvin.
K_P	Equilibrium Constant based on Partial Pressure.

KP_i	Equilibrium Constant for element i.
LIF	Laser-Induced Fluorescence.
M_i	Mass Fraction of Element i in the Reactants.
m_i	Mass Fraction of Element i in the Products of Combustion.
MF_i	Mass Fraction of Molecule i.
MSW	Municipal Solid Waste.
MW_i	Molecular Weight of Element i in Reactants.
mw_i	Molecular Weight of Element i in Products of Combustion.
MWF_i	Average Molecular Weight of Molecule i.
N	Total mole in Products / Nitrogen Atom.
N_i	Moles of Element i in Reactants.
n_i	Moles of Element i in Products of Combustion.
Nc_i	Number of Carbon Atom in the Molecule i.
Ncl_i	Number of Chlorine Atom in the Molecule i.
Nh_i	Number of Hydrogen Atom in the Molecule i.
N_{ji}	Number of element j in the Molecule i.
No_i	Number of Oxygen Atom in the Molecule i.
P	Absolute Pressure.
P_i	Partial Pressure of element i in Products.
ppmv	Part Per Million by Volume.
P_{tot}, R	Total Pressure (1 atm) and Gas Constant respectively.
RP and RC	Results obtained from Program and INS respectively.
S_1, S_2	Standard Deviations from INS and Program respectively.
S_e	Standard Error.
S_p^2	Pooled Variance Estimate.

st	Stoichiometric Condition (% EX=0).
T	Temperature of the Products of Combustion.
T-test	Test used to compare two Means in Statistics (Student's t distribution).
T_{cal}	T-test Calculated.
T_{crit}	T-test taken from Statistical Table.
X_i	Mole fraction as Y_i used after reducing the number of unknowns.
X^{it}	Solution obtained at iteration it.
ΔX	Difference between solution at it and it+1.
Y_i	Mole fraction of component i in the products.

CHAPTER I

INTRODUCTION

For thousands of years the value of burning wastes has been recognized, both to reduce the quantity of surplus materials generated by households, trades, and agricultural practices, and to provide fuel for heating or cooking. Recognition of the potential environmental problems generated by burning solid wastes also has a long history.

According to Brunner (1984), the specific benefits of incineration include:

- The volume and weight of the waste is reduced to a fraction of its original size.
- Waste reduction is immediate; it does not require landfill or holding pond.
- Waste can be incinerated on-site, without having to be carted to a distant area.
- Air discharges can be effectively controlled for minimal impact on the atmospheric environment.
- The ash residue is usually non-putrescible, or sterile.
- Technology exists to completely destroy even the most hazardous of materials in a complete and effective manner.
- Incineration requires a relatively small disposal area, not the acres and acres required for lagoons or land burial.
- Using heat recovery techniques the cost of operation can often be reduced or offset by the use of or sale of energy.

Incineration will not solve all waste problems (Brunner, 1984), it has some disadvantages which include:

- High capital cost.
- Skilled operators are required.
- Not all materials are incinerable.
- Some materials require supplemental fuel to attain mandated efficiency of destruction.

1.1 Background of the Study

In the combustion of municipal solid waste [MSW], it is necessary first to understand the fundamentals of solid fuels and combustion issues. Those issues recognize that solid waste is not a single fuel. Rather, it is a heterogeneous mixture of widely dissimilar organic and inorganic materials which are thrown into a single combustion chamber. The process of combustion (Tillman et al.,1989) is manipulated through mechanical method, fuel blending and separation, physical operation, and accomplished by careful attention to the chemistry of solid waste oxidation. This last point is the main concern of this research.

It is necessary to develop a computer program which can compute the product of combustion at several excesses of air and temperatures, so that it can be seen clearly how each product reacts when some parameters are manipulated. The products of combustion under study include CO_2, CO, H_2O, H_2, SO_2, SO_3, HCl, Cl_2, N_2, O_2, NO, and NO_2. Since we have 12 unknowns it is necessary that 12 equations

be solved analytically or numerically, depending on the complexity of the equations used.

This study is divided into two parts; part one is concerned with chemical analysis such as chemical reaction (combustion) analysis and the other is concerned with chemical equilibrium analysis. In chemical reaction analysis we are concerned with computing the stoichiometric air used for the combustion of solid fuels and relating this amount of air by adding additional air. Therefore the stochiometric of each element in the reactant is known, so that a mass balance or atom balance around each element can be made. For the chemical equilibrium analysis, it includes six chemical equilibrium reactions due to dissociation of CO_2, H_2O, SO_3, NO, NO_2 and H_2O+Cl_2 and their reverse reactions due to oxidation of CO, H_2, SO_2, N_2, NO, HCl respectively.

1.2 Statement of Problem

In this research, many variables are used and many unknowns exist. It is preferable to specify those variables and unknowns for the clarity of the problem. The variables used include:

- Waste composition (mass fractions).
- Excess air introduced.
- Temperature of the products.

The developed program can simulate combustion process for different temperatures and percentage of excess air. The varied values of excess air are presented in Table 1.1, while the varied temperatures is given below.

Varied Temperature:

T(°C)	527	727	927	1125	1327	1427
T(K)	800	1000	1200	1400	1600	1700

Table 1.1 Varied Percentage Excess Air used

VAR N_o	Percentage Excess Air [% EX]							
VAR 1	0	10	20	30	50	100	150	200
VAR 2	0	1	2	3	5	7	8	10
VAR 3	10	12	13	14	15	17	18	20
VAR 4	20	22	23	24	25	27	28	30
VAR 5	30	32	33	34	35	37	38	40
VAR 6	40	42	43	44	45	47	48	50
VAR 7	50	55	60	65	70	80	90	100
VAR 8	150	155	160	165	170	180	190	200

Twelve unknowns (concentration of combustion product) are considered and they are:

- CO_2: Carbon dioxide.
- CO : Carbon monoxide.
- H_2O: Water.
- H_2 : Hydrogen.