



SPREADSHEET MODEL TO DESIGN OF HAZARDOUS WASTE INCINERATORS

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ABSTRACT:

Introduction: Expanding a spreadsheet model which is used for key engineering calculations for hazardous waste incinerations (HWI) is the most important task in the management of hazardous wastes. The objectives of this study were to develop rigorous calculation procedures for the design and analysis of the incinerator, and incorporate these procedures into an easy-to-use computer program.

Findings: In this study, an innovative spreadsheet model application for the HWI is presented in order to provide a convenient method for calculation of flue gas and incinerator design data based on the thermodynamic and the stoichiometric calculations.

Conclusions: HWI program was organized into three parts in MS Excel: input data, calculations, and output of the results. A conceptual dataset was used to show the performance of this model using different criteria parameters. The model proved to be an efficient tool to help to engineering calculations for HWI.

INTRODUCTION

Urbanization and the growth of cities lead to the large amount of municipal solid waste (MSW) production as a major problem in current societies. Appropriate management in MSW collection, transportation and processing as well as leachate and gas control is crucial. Three important options which are considered as MSW processing

measures consist of: thermal treatment, biological treatment and landfilling. Reducing volume and weight and toxicity of wastes in thermal processes like incinerators are useful advantages of these methods [1]. Due to overpopulation, energy demand is increasing as well as its price and fossil fuel sources deficiencies. All mentioned challenges in addition of environmental problems like

global warming and greenhouse gas emissions urged us to apply waste heat recovery systems [2, 3]. In spite of incinerators of the main goal as treating wastes, currently MSW incinerators have been operating as waste to energy (WtE) converters in more developed countries such as Japan, Germany, Sweden, The Netherland, Denmark and the United Kingdom [1, 2].

Renewable energy sources, WtE systems are the new concept of incinerators regarding to lower rate of discharged hazardous pollutants in new facilities which is suitable for both biodegradable and non-biodegradable materials [4]. CO_2 , NO_2 , NH_3 and organic carbon are main emissions of MSW incinerators. Temperature, demanding air and the gases emitting in disposal process is under control in incinerators [5] but calculating the quantity of these pollutants deserve paramount importance. Quality and quantity of pollutants dramatically will be changed based on the waste volume and combustion conditions. Chemistry and thermodynamic calculations of burning process and emitting pollutants without appropriate software is very complicated and time consuming. Therefore, a suitable model in this area could be a key to measure various pollutants in the case of an incinerator. This study aimed to provide an applicable and convenient method regarding of hazardous waste emissions in the incinerators based on: 1) thermodynamic calculations, which related operating incinerator temperature, excess air, and feed (including not only waste but also possible fuel requirements) heating value; 2) stoichiometric calculations, which yield the composition and flow rate of gaseous emissions from incinerators burning hazardous waste; 3) incinerator design including pollutant emission calculations and physical design criteria. By using this model, operator can find sufficient information about the quality and quantity of output pollutants for proper judgments.

Different softwares are introduced to design of incinerators, including Enviropak for combustion calculation and incinerator design and estimation of NO_x and So_x components and incineration ef-

iciency; CYCOM is another computer program for the design and simulation of incineration plants; W2E software is a supporting tool for incineration process simulation. Suggested model is available for user in Excel with simple preliminary data. Using this program in addition to flue gas composition, data of flue gas including mass and molar flow rate, temperature, and gaseous pollutants concentration can be achieved. Also, design criteria such as volume, diameter, length, and residence time will be calculated.

SOFTWARE DESCRIPTION

Usage of spreadsheet model

In this study, user-friendly model has been developed according to the concept of thermodynamic and stoichiometric to make the computation of the HWI simple. This can be effectively used to design of the incinerator, pollutants emission data and physical design criteria according to the preliminary data.

Methods and equations

Hazardous waste incinerator program has been set up in MS Excel based on thermodynamic and stoichiometric equations [6]. The structure of variables, mathematical relationships, and specific features of the HWI presented in this study are described in this section. Fig.1 illustrates a flow diagram of calculation stages. Various variables are necessary as preliminary data in the first stage, including waste loading rate, percent of excess air, flue gas superficial velocity, and waste composition.

This model is practical for estimation of waste composition as elemental (atom and mass basis) and componential (mole and mass basis). Since mass basis of elemental composition can be specified by x-ray fluorescence (XRF) test, we develop a model which enables users to apply mass basis of elemental composition. This program accepts the following element symbols: C (CO_2), H (H_2O), O (O_2), S (SO_2), N (N_2), Cl (HCl), F (HF), Br (Br_2), and I (I_2) Water and ash may

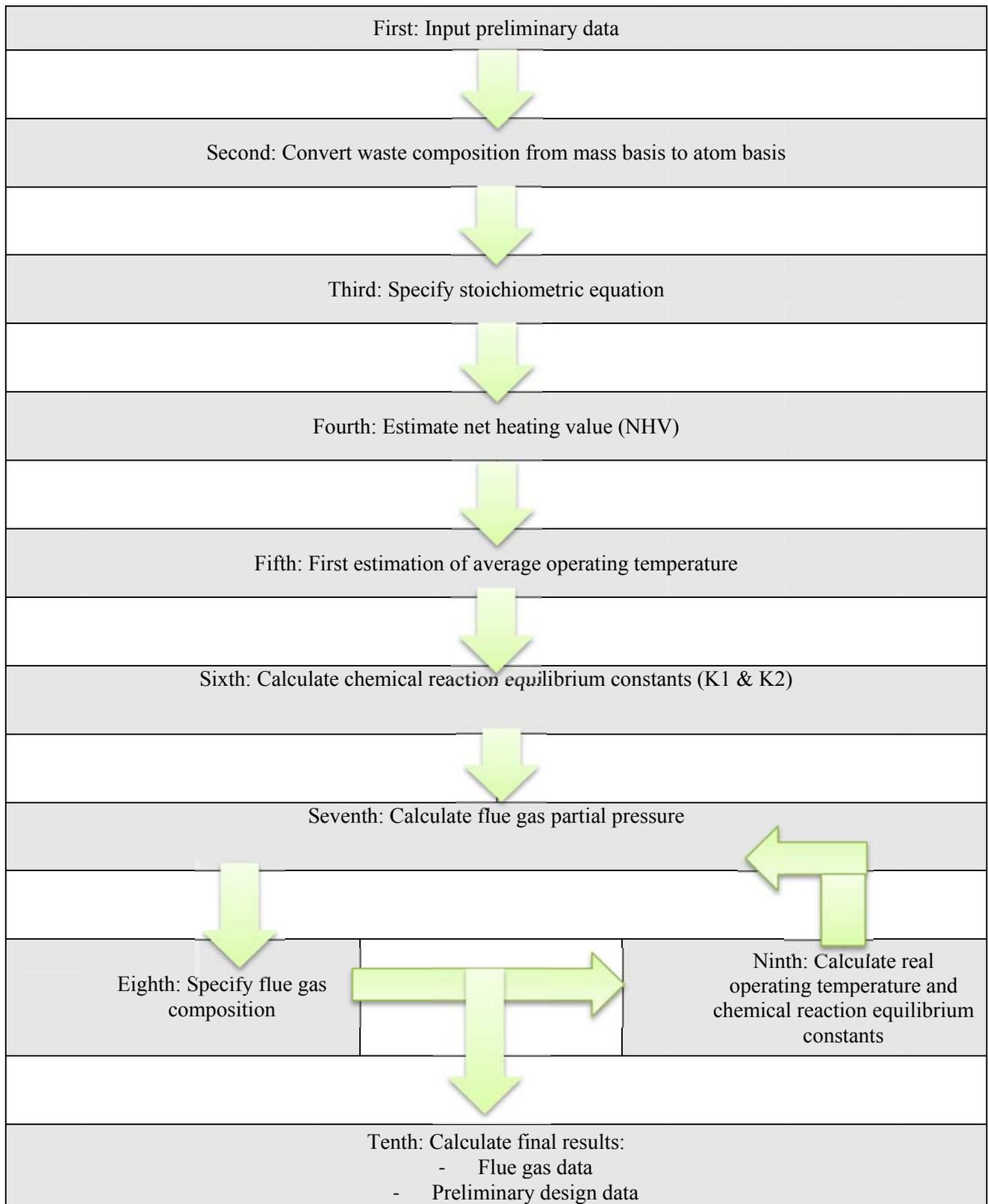
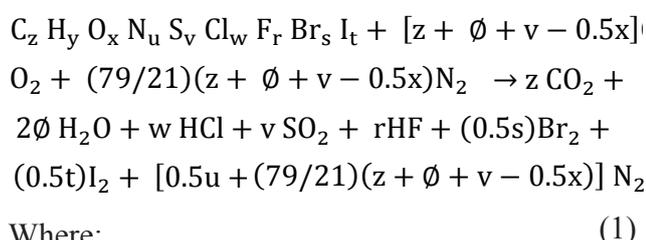


Fig.1. Flow diagram of calculation stages

be treated as “elements” if desired, by using the symbols: WA and AS, respectively.

In the second stage, the elemental analysis of the waste is converted to an atom basis based on percent of elements, flow rate, and atomic weight of elements.

In the third stage stoichiometric equation is written using Eq.(1), (2) and (3) that indices (z, y, x, u, v, w, r, s, t) are obtained from the initial compositions in the second stage.



Where:

$$\phi = \frac{y-w-r}{4} \text{ if } y > (w + r) \quad (2)$$

$$\phi = 0 \text{ if } y \leq (w + r) \quad (3)$$

In the fourth stage, Dulong's method, Eq. (4), is used to estimate the net heating value (NHV) based on the mass percent of elements.

$$NHV_{Btu/lb} = 14000 m_C + 45000 (m_H - 0.125 m_O) - 760 m_{Cl} + 4500 m_S \quad (4)$$

Where m_C , m_H , m_O , m_{Cl} , and m_S are the mass percent of elements in the preliminary data.

In the fifth stage, to obtain a first estimation of the average operating temperature ($^{\circ}F$), Eq. (5) is applied.

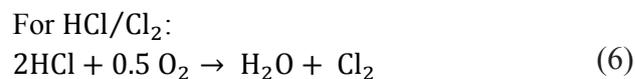
$$T = 60 + (NHV/0.3) / [1 + (1 + EA)(7.5 \times 10^{-4})(NHV)] \quad (5)$$

Where ϕ is net heating value as ϕ from the fourth stage and EA is percent of excess air in the preliminary data.

In the sixth stage, chemical reaction equilibrium constants are calculated from Eq.(7) and (9) as

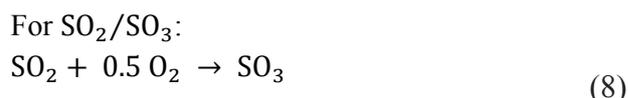
for the ϕ and ϕ , respectively at initial operating temperature.

For:



$$\ln K_1 = (7048.7/T) + (0.0151 \ln T) - (9.06 * 10^{-5}T) - (2.714 * 10^4 T^{-2}) - 8.09 \quad (7)$$

For :



$$\ln K_2 = (11996/T) - (0.362 \ln T) + (9.36 * 10^{-4}T) - (2.969 * 10^5 T^{-2}) - 9.88 \quad (9)$$

Where ϕ is as ϕ and T is initial operating temperature as $^{\circ}K$.

In the seventh stage, flue gas partial pressure can be calculated using the coefficients in the reaction stoichiometric equation, Eq. (1) considering the percent of excess air. Afterwards, initial flue gas partial pressure is corrected using equilibrium constants in the previous stage and Eq.(10) and (11).

$$K_1 = \frac{P(Cl_2) P(H_2O)}{P(HCl)^2 P(O_2)^{1/2}} \quad (10)$$

$$K_2 = \frac{P(SO_3)}{P(SO_2) P(O_2)^{1/2}} \quad (11)$$

In the eighth stage, initial flue gas composition is obtained based on the partial pressure and coefficients in the reaction stoichiometric equation.

In the ninth stage, a more accurate operating temperature is calculated. This temperature is determined by an enthalpy balance. In order to calculate the enthalpy, change that occurs when the flue gases are heated from the 60 $^{\circ}F$ reference temperature to the adiabatic flame (incinerator) temperature, the heat capacity as a function of temperature is required. Equilibrium constants must be recalculated at this revised temperature. Then, the calculation stages are repeated from seventh stage and the partial pressure of the flue gas components is recalculated using the revised

equilibrium constants. Next, final flue gas composition is generated.

In the final stage, flue gas and preliminary design data are calculated. Flue gas data are comprised of flow rate (mass, molar, volumetric), HCl mass flow rate, sulfur trioxide and chlorine concentration. Preliminary design data are included heat release rate, incinerator volume, diameter, length, and residence time.

Advantages and limitations

This model is available for user in Excel with simple preliminary data. Using this program in addition to flue gas composition, data of flue gas including mass and molar flow rate, temperature, and gaseous pollutants concentration can be achieved. Also, design criteria such as volume, diameter, length, and residence time will be calculated.

This model is practical for waste composition estimation as elemental (atom and mass basis) and

compositional (mole and mass basis). Since mass basis of elemental composition can be specified by XRF test, we only developed model based on the mass basis of elemental composition.

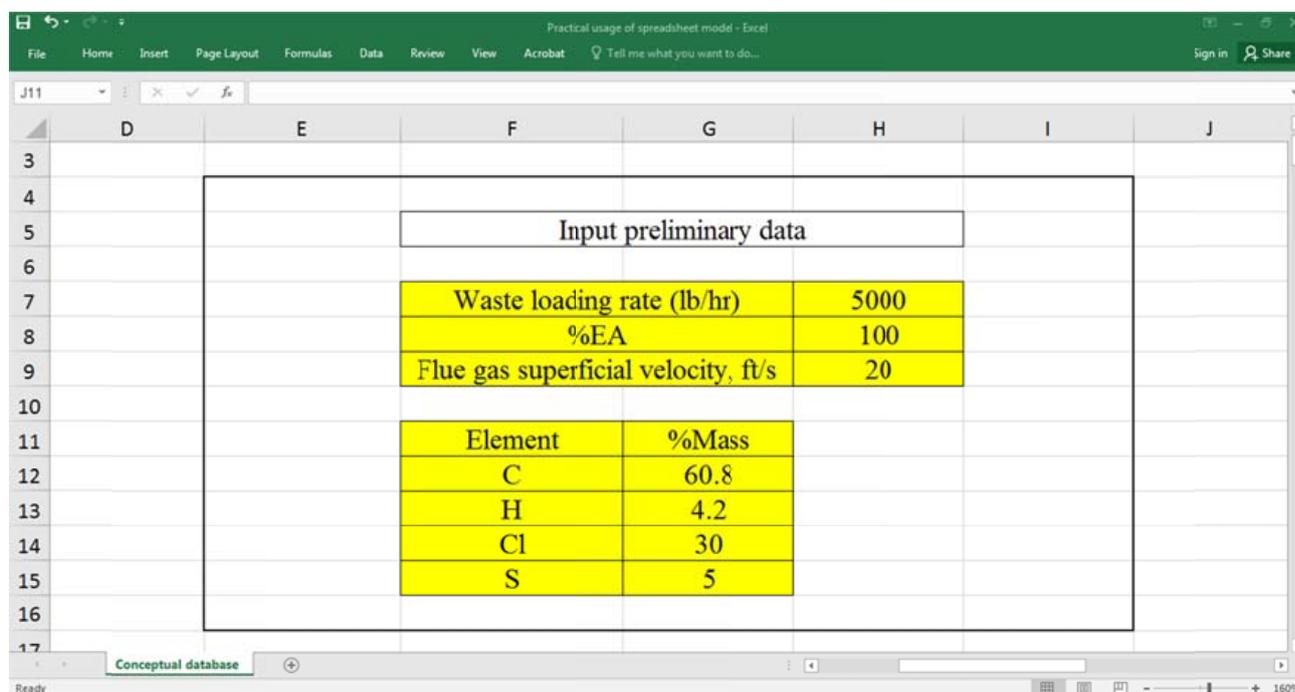
Practical usage of spreadsheet model

Preliminary data

In this study, we tested the performance of the HWI model on a conceptual database, including a hazardous waste contains - on an elemental basis – carbon, hydrogen, chlorine, and sulfur. The waste is a 95% (by mass) chlorobenzene/sulfur mixture. Preliminary data of waste bulk are shown in Fig.2

Convert waste composition from mass basis to atom basis

Based on the mass percent of elements and waste loading rate, the elemental analysis of the waste is converted to an atom basis, as shown in Fig.3.



Input preliminary data	
Waste loading rate (lb/hr)	5000
%EA	100
Flue gas superficial velocity, ft/s	20

Element	%Mass
C	60.8
H	4.2
Cl	30
S	5

Fig.2. Preliminary data

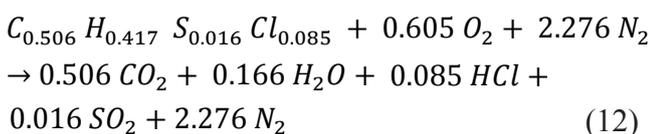
Waste componential composition						
Element	%w/w	lb/hr	Aw	lb-Atom*	%Atom	
C	60.80	3040	12.01	5.06	49.48	
H	4.20	210	1.01	4.17	40.72	
Cl	30.00	1500	35.45	0.85	8.27	
S	5.00	250	32.06	0.16	1.52	
O	0.00	0	16.00	0.00	0.00	
N	0.00	0	14.00	0.00	0.00	
F	0.00	0	19.00	0.00	0.00	
Br	0.00	0	79.90	0.00	0.00	
I	0.00	0	126.90	0.00	0.00	
Total		5000		10.23	100.00	

* Basis: 100 lb waste

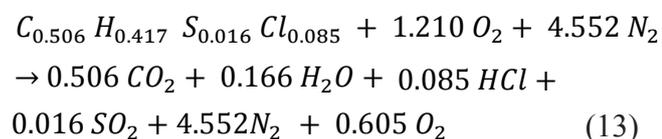
Fig.3. Waste componential composition

Specify stoichiometric equation

The stoichiometric equation is written using Eq.(1). The constants in this equation are in the fifth column in Fig.3 and when one lb mole of waste is used as a basis, constants are $z=0.505$, $y=0.417$, $x=0.0$, $u=0.0$, $v=0.016$, and $w=0.085$. Then and Eq.(12) becomes:



With 100% excess air, the oxygen and nitrogen in the stoichiometric equation are doubled. Therefore, Eq.(13) becomes:



Estimate net heating value (NHV)

Since heat data of combustion is not given and the waste contains only carbon, hydrogen, chlorine, and sulfur, Dulong's method, Eq.(4), is used to estimate the NHV.

Where m_C , m_H , m_O , m_{Cl} , and m_S are the mass per-

cent of elements in the Fig.2. Accordingly, NHV is equal to 10400 Btu/lb (5777 cal/g).

First estimate of average operating temperature

Eq.(5) is used to obtain a first estimation of the average operating temperature in the incinerator. Based on NHV as Btu/lb and percent of excess air, first estimation of the average temperature for this conceptual data is 2148 °F (1449 °K, 1176 °C).

Calculate chemical reaction equilibrium constants (K_1 & K_2)

Chemical reaction equilibrium constants (K_1 & K_2) at first estimation of the average temperature equal to 1449 °K are now obtained from Eq.(7) and (9), that for HCl/Cl_2 (K_1) and SO_2/SO_3 (K_2) is $0.038 \text{ atm}^{-1/2}$ $0.048 \text{ atm}^{-1/2}$, respectively.

Calculate flue gas partial pressure

The partial pressure of the components can be calculated based on the coefficients in the stoichiometric equation with excess air, Eq.(13). According to this equation, the total number of moles in the flue gas per lb mole of waste mixture is 5.928 lb mole. For an incinerator operating at 1 atm, the partial pressure is equal to mole fractions. For example:

Initial flue gas partial pressures		
Component	No. of moles	Pi (atm)
CO ₂	0.506	0.085
H ₂ O	0.166	0.028
HCl	0.085	0.014
O ₂	0.605	0.102
N ₂	4.551	0.768
SO ₂	0.016	0.003
HF	0.000	0.000
Br ₂	0.000	0.000
I ₂	0.000	0.000
Cl ₂	0.000	0.000
SO ₃	0.000	0.000
Total	5.928	1.000

Fig.4. Initial flue gas partial pressure

The partial pressure calculated for other components is provided in Fig.4.

Considering the equilibrium reactions, Eq.(6) and (8), the partial pressure is corrected as shown in Table 1. In this table, z and y represent the number of moles of and in equilibrium conditions, also N represents the total number of moles in the flue gas at equilibrium which starts with one mole of flue gas originally. Note that N is the sum of column 2 and is equal to $1-0.5z-0.5y$. Substituting these partial pressure and the values of the equilibrium constants found in Eq.(7) and (9) into Eq.(10) and (11) yields:

$$P(\text{CO}_2) = 0.506 / 5.928 = 0.085 \quad (14)$$

and

$$0.04872 = (y) / ((0.003-y)(0.102 - 0.5z - 0.5y)^{0.5} N^{0.5}) \quad (15)$$

where

$$N = 1 - 0.5z - 0.5y \quad (16)$$

Basis: 1 mole of flue gas before equilibrium reactions occur

Eq.(14) and (15) must be solved simultaneously to determine the values of z and y. These equations will be simplified due to the small value of z and y in comparison to the original partial pressure. So, they change to:

$$0.03839 = (z)(0.028+z) / (0.014 - 2z)^2 \cdot (0.102 - 0.5z - 0.5y)^{0.5} \quad (17)$$

and

$$0.04872 = (y) / (0.003-y)(0.102 - 0.5z - 0.5y)^{0.5} \quad (18)$$

Z and y can be calculated by trial – and – error using goal seek menu in Excel. The response of solving Eq.(17) and (18) yield values of z and y equal to 8.59* and 4.11*atm, respectively. Further correction leads to revised partial pressure shown in Fig.5. Also, the flue gas composition in Fig.6 is based on the partial pressure shown in Fig.5.

Partial pressure obtains by dividing the number of moles to N. Due to the small value of z and y, the value of N equals to 1. Therefore, partial pressure will be equal to the number of moles for each

Table 1. Corrected flue gas partial pressure

Component	No. of moles	Partial pressure (atm)
CO_2	0.085	$(0.085)/N$
H_2O	$0.028 + z$	$(0.028 + z)/N$
HCl	$0.014 - 2z$	$(0.014 - 2z)/N$
O_2	$0.102 - 0.5z - 0.5y$	$(0.102 - 0.5z - 0.5y)/N$
N_2	0.768	$(0.768)/N$
SO_2	$0.003 - y$	$(0.003 - y)/N$
HF	0	0
Br_2	0	0
I_2	0	0
Cl_2	z	z/N
SO_3	y	y/N
Total	$1-0.5z-0.5y$	1

Practical usage of spreadsheet model - Excel

Corrected flue gas partial pressure		
Component	No. of moles	Partial Pressure (atm)
CO_2	0.085	0.085
H_2O	0.028	0.028
HCl	0.014	0.014
O_2	0.102	0.102
N_2	0.768	0.768
SO_2	0.003	0.003
HF	0.000	0.000
Br_2	0.000	0.000
I_2	0.000	0.000
Cl_2	8.592E-05	0.000
SO_3	4.110E-05	0.000
Total	1.000	1.000

Fig.5. Corrected flue gas partial pressure

component and corrected flue gas partial pressure is equal to initial flue gas partial pressure.

Specify flue gas composition

The flue gas composition, Fig.6, can be specified based on constants in the stoichiometric equation and the partial pressure shown in Fig.5. Note that this composition does not represent the final flue gas composition since these results are based on an incinerator approximate temperature (2148 °F).

Calculate real operating temperature and chemical reaction equilibrium constants

Real operating temperature can be calculated using the heat capacity of each component (Fig.7). The second column is based on one gram of the waste-fuel mixture in Fig.6. The heat capacity as a function of temperature are taken from molar heat capacities and the units on the heat capacity is cal/gmol-K [7].

The screenshot shows an Excel spreadsheet with a table titled "Flue gas composition". The table has 7 columns: Component, %Mole, lbmole*, Mw, lb*, and %Mass. The rows list various chemical species and their properties.

Component	%Mole	lbmole*	Mw	lb*	%Mass
CO ₂	8.54	5.06	44.01	222.80	12.65
H ₂ O	2.82	1.66	18.02	29.91	1.70
HCl	1.41	0.85	36.46	30.85	1.75
O ₂	10.20	6.05	32.00	193.55	10.99
N ₂	76.77	45.51	28.00	1274.22	72.33
SO ₂	0.26	0.16	64.06	9.99	0.57
HF	0.00	0.00	20.01	0.00	0.00
Br ₂	0.00	0.00	159.81	0.00	0.00
I ₂	0.00	0.00	253.80	0.00	0.00
Cl ₂	0.01	0.00	70.90	0.30	0.02
SO ₃	0.00	0.00	80.06	0.12	0.01
Total	100.01	59.29		1761.75	100.00

*Basis: 100 lb waste-fuel mixture.

Fig.6. Flue gas composition

The screenshot shows an Excel spreadsheet with a table titled "Heat capacity calculations". The table has 9 columns: Component, gmole per, a, b*10⁻³, c*10⁻⁵, Δa, Δb, and Δc. The rows list various chemical species and their heat capacity parameters.

Component	gmole per	a	b*10 ⁻³	c*10 ⁻⁵	Δa	Δb	Δc
CO ₂	5.06E-02	10.57	2.10	-2.06	0.535	0.0001	-10428.643
H ₂ O	1.66E-02	7.30	2.46	0.00	0.121	0.000	0.000
HCl	8.46E-03	6.27	1.24	0.30	0.053	0.000	253.879
O ₂	6.05E-02	7.16	1.00	-0.40	0.433	0.000	-2419.403
N ₂	4.55E-01	6.83	0.90	-0.12	3.108	0.000	-5460.937
SO ₂	1.56E-03	11.04	1.88	-1.84	0.017	0.000	-286.962
HF	0.00E+00	0.00	0.00	0.00	0.000	0.000	0.000
Br ₂	0.00E+00	8.92	0.12	-0.30	0.000	0.000	0.000
I ₂	0.00E+00	0.00	0.00	0.00	0.000	0.000	0.000
Cl ₂	4.23E-05	8.85	0.16	-1.80	0.000	0.000	-7.616
SO ₃	1.56E-05	13.90	6.10	-3.22	0.000	0.000	-5.022
Total					4.268	0.001	-18354.704

Fig.7. Heat capacity calculations

If, by definition:

$$\Delta a = \sum_i (gmol_i)(a_i). \text{ etc ...} \quad (19)$$

Then, for this system:

$$\Delta a = 4.26$$

$$\Delta b = 6.00 \cdot 10^{-4}$$

$$\Delta c = -1.83 \cdot 10^4$$

The Eq.(20) will be used to evaluate real operating temperature because following prerequisite exist: 1) waste, auxiliary fuel (when used) and air are assumed to be close to ambient temperature; 2) the combustion condition is assumed to be adiabatic.

$$NHV(cal/g) + \Delta a (T - 298) + (\Delta b/2) (T^2 - 298^2) - \Delta c [(1/T) - (1/298)] = 0 \quad (20)$$

Note that the NHV term must be negative (-5771 cal/g mol) because the system is releasing energy during the combustion steps.

Solving of Eq.(20) by trial – and – error results in:

$$T = 1501^\circ k = 2243^\circ F = 2702^\circ R$$

Equilibrium constants must be recalculated at this revised temperature in Eq.(7) and (9). The results are:

$$K_1 = 0.032 \text{ atm}^{-1/2}$$

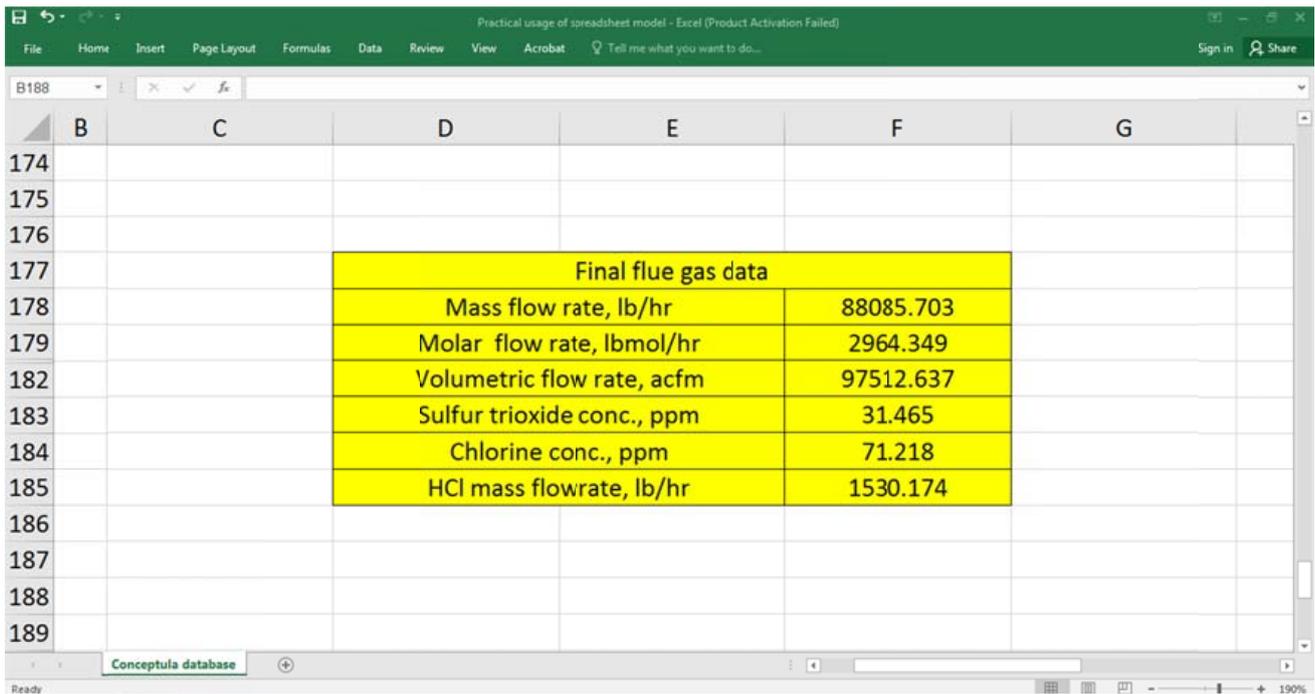
$$K_2 = 0.038 \text{ atm}^{-1/2}$$

The partial pressure of the flue gas components is recalculated using the more accurate equilibrium constants. The final flue gas composition is shown in Fig.8. Note that, for more accuracy, the process just described could be repeated. The results in Fig.8 could be used with a new enthalpy balance to calculate a new incinerator temperature; revised values of and based on this new temperature could be determined; and a new composition is generated. Although the results would not differ much from those shown in Fig.8.

Component	%Mole	lbmole*	Mw	lb*	%Mass
CO ₂	8.54	5.06	44.01	222.83	12.65
H ₂ O	2.81	1.67	18.02	30.07	1.71
HCl	1.42	0.84	36.46	30.60	1.74
O ₂	10.20	6.05	32.00	193.48	10.98
N ₂	76.77	45.51	28.00	1274.41	72.34
SO ₂	0.26	0.15	64.06	9.87	0.56
HF	0.00	0.00	20.01	0.00	0.00
Br ₂	0.00	0.00	159.81	0.00	0.00
I ₂	0.00	0.00	253.80	0.00	0.00
Cl ₂	0.01	0.004	70.90	0.30	0.02
SO ₃	0.00	0.002	80.06	0.15	0.01
Total	100.01	59.29		1761.71	100.00

*Basis: 100 lb waste-fuel mixture.

Fig.8. Final flue gas composition



Final flue gas data	
Mass flow rate, lb/hr	88085.703
Molar flow rate, lbmol/hr	2964.349
Volumetric flow rate, acfm	97512.637
Sulfur trioxide conc., ppm	31.465
Chlorine conc., ppm	71.218
HCl mass flowrate, lb/hr	1530.174

Fig.9. Final flue gas data

Final results

-Flue gas data

In the final gas data as shown in Fig.9, the mass and molar flow rates of the flue gas are calculated from the results in Fig.8. Volumetric flow rate is calculated using the ideal gas law ($P=1$ atm).

- Preliminary design data

In the preliminary design data as shown in Fig.10, the volume of the incinerator is calculated from Eq.(21) and (22):

$$V = q/q_H \quad (21)$$

$$q = (NHV)(m') \quad (22)$$

Where q is heat rate generated by the combustion at 60°F as , is the heat release rate equal to 25,000 , and is waste loading rate as lb/hr, and NHV is net heating value as .

The approximate physical dimensions of the incinerator are based on a superficial velocity of 20 ft/sec. These dimensions yield an L/D ratio lower than 3, which is a reasonable value. Residence time is 1.28 s and the values lower than 0.75 s is unacceptable.

AVAILABILITY AND REQUIREMENTS

This program is entitled as hazardous waste incinerator (HWI). Access link to this program is via: (<http://tums.ac.ir/ajaxplorer/data/public/21515a1de72ee65dc2c3633f11ed1e3b.php?lang=en>).

FINANCIAL SUPPORTS

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COMPETING INTERESTS

The authors confirm that there is not any competing interest in publishing the results of the study.

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ETHICAL CONSIDERATIONS

Ethical issues (including plagiarism, informed consent, misconduct, data fabrication and/or falsification, double publication and/or submission, redundancy, etc) have been completely observed by the authors.

Preliminary design data	
Heat release rate, Btu/hr	51995000
Incinerator volume, ft ³	2079.80
Incinerator area, ft ²	81.26
D,ft	10.17
L,ft	25.59
L/D	2.52
Residence time, Sec	1.28

Fig.10. Preliminary design data

CONVESION FACTORS

$$1 \text{ lb} = 0.45 \text{ kg}$$

$$1 \text{ ft} = 0.30 \text{ m}$$

$$1 \text{ }^{\circ}\text{F} = 1.8T \text{ (}^{\circ}\text{C)} + 32$$

$$1 \text{ }^{\circ}\text{K} = 273.15 + T \text{ (}^{\circ}\text{C)}$$

$$1 \text{ }^{\circ}\text{K} = (\text{ }^{\circ}\text{F} - 32) \times 5/9 + 273.15$$

$$1 \text{ ft/s} = 0.3048 \text{ m/s}$$

$$1 \text{ lb/h} = 0.000126 \text{ kg/s}$$

$$1 \text{ BTU/lb} = 0.55 \text{ Cal/g}$$

$$1 \text{ Btu/h.ft}^3 = 10.343 \text{ W/m}^3$$

$$1 \text{ ft}^3/\text{min} = 4.72 \times 10^{-4} \text{ m}^3/\text{s}$$

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