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A Numerical Simulation of Hazardous Waste Destruction in a Three-Dimensional Dump Incinerator

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Abstract–A predictive model of carbon tetrachloride (CCl_4) incineration in a dump incinerator is described. An empirical model that incorporates the chemical kinetic aspects of CCl_4 destruction is developed to describe the flame inhibition characteristics of CCl_4, which is halogen compounds. Quantitative agreement is found between the predictions of the model and the measured values. Cavity hydrodynamics and flame structure studies are made in a dump incinerator proposed in this study. For the effective destruction of hazardous waste, the waste must injected in the recirculation region of high temperature with the condition of not disturbing the combustion cavity. The core flame has a significant impact on the structure of the recirculation region, in some cases completely changing the nature of the flow within the cavity. The dump incinerator has good characteristics for the destruction of hazardous waste. These characteristics should lead to a very compact device, one which is potentially transportable or usable in a dedicated manner by a small generator.

Key words: Incinerator, Dump, CFD, CCl_4, Nonequilibrium, Combustion

INTRODUCTION

Incineration is an attractive alternative for the treatment of several classes of toxic hazardous wastes. Particularly, dump incinerators located on the same site where the waste is generated usually have been considered because of less public opposition. A dump combustor (see Fig. 1) is characterized by the sudden expansion of a fuel-air mixture into a combustion cavity formed by a rearward facing step. This gives higher residence time in recirculation zone. Therefore it has enough reaction time for hazardous waste to be destroyed at high temperature. A major source of the hazardous waste generated is from chemical industries producing plastics, herbicides, pesticides and chlorinated solvents. All of these processes produce a class of hazardous waste termed the chlorinated hydrocarbons (CHCs), either directly or from undesirable side reactions. A number of studies have been reported on the CHCs combustion mechanism. In these studies, use has been made of shock tubes and small scale laboratory flames [Cundy et al., 1987; Morse et al., 1988]. These fundamental studies have proved that thermal destruction is indeed a viable method for satisfying the EPA (Environmental Protection Agency) regulations requiring hazardous waste destruction efficiencies to be greater than 99.99 percent [Oppelt, 1987].

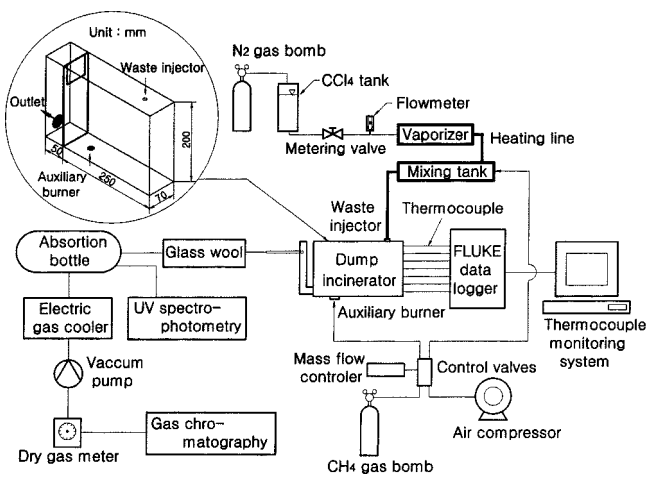

Fig. 1. The experimental dump incinerator system.

In addition to the fundamental studies, models have been developed to predict the performance of incineration processes [Silcox and Perching, 1988; McKenty et al., 1999]. However, these studies have made use of simplifying assumptions and do not provide detailed distribution of the turbulent flow field, temperature and species concentration in the incinerator. Even though conventional fast chemistry turbulent reaction models (for example, the conserved scalar method of Bilger and the eddy breakup models of Spalding and Magnussen and Hjertager) have been proposed, they do not describe the flame inhibition characteristics of halogen components [Bilger, 1976; Spalding, 1971; Magnussen and Hjertager, 1976].

Thus, the effect of nonequilibrium chemistry is as important as that of turbulent mixing, and an appropriate turbulent combustion model is to be used. Jang and Acharya used a fast chemistry turbulent reaction model for a premixed CH_4-CCl_4-air mixture [Jang and Acharya, 1988]. The basic concept of the model is that the destruction rate of CCl_4 is directly proportional to the reaction rate of CH_4 over a limited range of CCl_4 concentration. The CH_4 reaction rate is described by the phenomenological eddy breakup model recommended by [Magnussen and Hjertager, 1976]. However the model, which is essentially a fast chemistry model, does not directly

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incorporate the nonequilibrium effects in a C_3H_8-CCl_4-air flame. Given the complexity of the CHCs incineration process, a number of issues must be addressed before a practical incineration system can be put into operation. A reliable predictive methodology needs to be developed to guide the development of better incinerators.

In the current work, a more realistic calculation has been made for the C_3H_8-CCl_4-air reaction rate. To this end, use is made of the relation between the burning velocity and reaction rate from the thermal theory of flame propagation [Glassman, 1977]. The performance of the turbulent nonequilibrium reaction model developed in this study is compared with a dump incinerator. Also we present the construction of a steady three-dimensional model of the dump incinerator with nonequilibrium reaction model developed in this study, and its use in characterizing the structure of the flame front and recirculation zone and CCl_4 destruction to provide the basic data for the design and operation of dump incinerator.

EXPERIMENTAL APPARATUS AND PROCEDURE

A bench scale dump incinerator used in the present experiments (as shown in Fig. 1) is made of stainless steel insulated glass wool. Fuel (propane gas) and air are mixed and introduced into auxiliary burner and waste injector, respectively. Hazardous waste (CCl_4) is injected through the waste injector only. This location is chosen on the basis of numerical simulation [Chun, 1999]. The carbon tetrachloride is transported with the aid of a pumpless, "blow-case" system consisting of a pressurized liquid reservoir tank, a high precision flow regulation valve, and corresponding gauges for monitoring pressure and temperature [Bose and Senkan, 1983].

The carbon tetrachloride is injected into the heated gas at a heating unit. All the lines after the liquid injection are also heated to prevent condensation of the carbon tetrachloride. The combustion gases are continuously withdrawn from the dump incinerator and through the sample loop in a gas chromatograph (Shmadzu 14B) using a vacuum pump.

The gas analysis of C_3H_8, CO_2, O_2, N_2 is accomplished by using Porapak Q and molecular sieve 13X columns with the thermal conductivity detector of the gas chromatograph. The gas analysis of CCl_4 uses capillary DB-5 columns with the flame ionization detector. Absorptimetric Analyzer is used for HCl analysis. Temperature measurements are taken using 0.3 mm Pt/Pt-13% Rh thermocouples with Data Logger (Fluke 2625A).

MATHEMATICAL MODEL

Turbulence is modeled using the high Reynolds version of the two equation (k-ε) model [Launder and Spalding, 1972]. This requires the solution of the transport equations for kinetic energy of turbulence k and its dissipation rate ε. In this two-equation model, the "Boussinesq" gradient hypothesis is used for the second-order velocity fluctuation correlation term and a Prandtl-Kolmogorov relationship is used to correlate the turbulent viscosity to k and ε. As recommended by Launder and Spalding the presence of the near-wall viscous sublayer is resolved through the use of wall functions [Launder and Spalding, 1972].

Special attention is focused on the modeling of the turbulent reaction in a premixed C_3H_8-CCl_4-air flame. The reaction rate of this mixture is believed to be determined not only by turbulence mixing but also by chemical kinetics. This is particularly true since CCl_4 is incapable of a self-sustaining flame due to the low enthalpy of combustion and its flame inhibition. In order to resolve the nonequilibrium effects in C_3H_8-CCl_4-air flames, detailed chemical kinetic data is required. Efforts have been directed toward this end, but as yet, there is no well established chemical kinetic data available [Cundy et al., 1987; Morse et al., 1988]. Thus, a detailed consideration of the kinetic rates is not quite warranted at this stage. Rather, an empirical modeling approach is adopted in this study. Fast chemistry model is applied for turbulent reaction in premixed flame, and thermal theory and the concept of burning velocity are used to describe the flame inhibition characteristics of CCl_4 which is halogen compounds.

Based on the thermal theory of flame propagation, the reaction rate (RR) can be related to the flame burning velocity (S_u) by

$$S_u \sim (\alpha RR)^{1/2} \tag{1}$$

where α denotes the thermal diffusivity [Glassman, 1977]. Burning velocity is available as a function of R (molar concentration ratio of CCl_4 to C_3H_8) and ϕ (equivalence ratio) in a laboratory Bunsen flame study [Valeiras, 1982]. Utilizing Eq. (1) and the relationship between S_u vs. R, the reaction rate expression of C_3H_8-CCl_4-air mixture can be obtained as a function of R and ϕ as

$$\overline{RR}_{C_3H_8-CCl_4}\Big|_{at\ R,\phi} = \frac{\left(\frac{S_u^2}{\alpha}\right)_{R,\phi}}{\left(\frac{S_u^2}{\alpha}\right)_{R=0,\phi}} \times \overline{RR}_{C_3H_8}\Big|_{R=0,\phi} \tag{2}$$

In Eq. (2), $\overline{RR}_{C_3H_8}\Big|_{R=0,\phi}$ described fast chemistry model only represents the reaction rate of C_3H_8 in a pure C_3H_8-air reaction.

For any value of R between experimental data points, the corresponding burning velocity S_u is obtained by linear interpolation. Although another set of burning velocity data of C_3H_8-CCl_4-air mixture is also available for various R and ϕ values, this set of data is obtained in the water-cooled flat flame burner facility in which there are substantial amounts of heat extraction at the base compared to that in a Bunsen flame experiment [Morse, 1984]. Since the magnitude of heat extraction has a significant effect on flame temperature and burning velocity the flat flame burner data is excluded in this study.

The volumetric reaction rate of C_3H_8 ($\overline{RR}_{C_3H_8}$) in a C_3H_8-CCl_4-air mixture is given by the phenomenological eddy breakup model proposed by Magnussen and Hjertager, i.e.,

$$\overline{RR}_{C_3H_8} = \text{minimum of} \left| \bar{\rho} A \overline{m}_{fu} \frac{\varepsilon}{k}, \bar{\rho} A \frac{\overline{m}_{ox}}{s} \frac{\varepsilon}{k}, \rho A' \frac{\overline{m}_{pr}}{(1+s)} \frac{\varepsilon}{k} \right| \tag{3}$$

where $\bar{\rho}$ is the time-averaged density, s is the stoichiometric oxygen requirement by mass and A and A' are empirical constants given by Lockwood et al. [Lockwood et al., 1980].

In order to account for the C_3H_8 reaction rate in C_3H_8-CCl_4-air mixture, the following expressions are used for the species mass fractions appearing in Eq. (3).

$$\overline{m}_{fu} = \overline{m}_{C_3H_8} + \overline{m}_{CCl_4} \cdot \frac{M_C}{M_{CCl_4}},$$

$$\overline{m}_{ox} = \overline{m}_{O_2} + \overline{m}_{CCl_4} \cdot \frac{M_{Cl_4}}{M_{CCl_4}}, \text{ and}$$
$$\overline{m}_{pr} = \overline{m}_{CO_2} + \overline{m}_{H_2O} + \overline{m}_{HCl} \quad (4)$$

Once the C_3H_8 reaction rate is obtained, the individual species reaction rates can be calculated by using the stoichiometric reaction expression given by Eq. (5).

$$C_3H_8 + 2R\ CCl_4 + 5(O_2 + 3.76N_2) \rightarrow (3+2R)CO_2 + 8R\ HCl + 4(1-R)H_2O + (5\times 3.76)N_2 \quad (5)$$

In Eq. (5), as the R value increases the species mass fraction $\overline{m}_{C_3H_8}$ and $\overline{m}_{O_2}$ decreases, which results in a reduced reaction rate and finally the reaction will be quenched for large R values.

For example, CCl_4 reaction rate (RR_{CCl_4}) can be expressed as

$$\overline{RR}_{CCl_4} = \overline{RR}_{C_3H_8-CCl_4} \times \frac{R \cdot M_{CCl_4}}{M_{C_3H_8} + R \cdot M_{CCl_4}} \quad (6)$$

where M denotes the molecular weight.

Further, stoichiometric oxygen requirement (s) in Eq. (3) can be expressed as

$$s = \frac{5M_{O_2} + 4RM_{Cl_2}}{M_{C_3H_8} + 2RM_C} \quad (7)$$

The six flux model is employed for radiation heat transfer [Gosman and Lockwood, 1973; Spalding, 1980]. The products of gas combustion, such as CO_2 and H_2O, are strong selective absorbers and emitters, but they do not scatter radiation significantly. The absorptivities of N_2 and O_2 are so small that these gases are almost completely transparent to radiation. Absorption and scattering coefficient are used 1.45 m^{-1} and zero m^{-1}, respectively. The emissivity of stainless steel, which is the material of dump incinerator, is 0.6.

The composite radiation fluxes are defined as

$$\overline{R}_x = \frac{(I_x + J_x)}{2},\ \overline{R}_y = \frac{(K_y + L_y)}{2},\ \overline{R}_z = \frac{(M_z + N_z)}{2} \quad (8)$$

where I_x, J_x are radiation fluxes in positive and negative axial (x), K_y, L_y in positive and negative axial (y), M_z, N_z in positive and negative axial (z), respectively.

With these definitions, the RTEs (radiative transfer equations) are given as

$$\frac{d}{dx}\left(\frac{1}{a+s}\frac{d\overline{R}_x}{dx}\right) = a(\overline{R}_x - E) + \frac{s}{3}(2\overline{R}_x - \overline{R}_y - \overline{R}_z)$$
$$\frac{d}{dy}\left(\frac{1}{a+s}\frac{d\overline{R}_y}{dy}\right) = a(\overline{R}_y - E) + \frac{s}{3}(2\overline{R}_y - \overline{R}_x - \overline{R}_z)$$
$$\frac{d}{dz}\left(\frac{1}{a+s}\frac{d\overline{R}_z}{dz}\right) = a(\overline{R}_z - E) + \frac{s}{3}(2\overline{R}_z - \overline{R}_y - \overline{R}_x) \quad (9)$$

where a and s represent the absorption and scattering coefficient, respectively.

The E is the black-body emissive power as

$$E = S \times T^4 \quad (10)$$

where S represents the Stefan-Boltzmann constant (i.e., 5.6678E-8 W/m^2K^4) and T is absolute fluid temperature.

The contribution of radiative heat transfer to the energy equation is a source term involving the divergence of the radiative heat flux. The energy equation source term is given as Eq. (11).

$$S_{rad} = 2a[\overline{R}_x + \overline{R}_y + \overline{R}_y - 6E] \quad (11)$$

Local residence time, particularly in the recirculation region, is an important factor for the destruction of hazardous waste. Therefore it is required to calculate at any point within the calculation domain, the time taken for the injected fluid to reach that point. Local residence time, as a scalar variable ϕ in Eq. (13), is calculated. The source is given by:

$$S_\phi = \Delta t \sum_j \dot{m}_{inj} = \frac{\overline{\rho}\mathrm{Vol}}{\sum_j \dot{m}_{inj}} \sum_j \dot{m}_{inj} = \overline{\rho}\mathrm{Vol} \quad (12)$$

where Vol is the cell volume, and $\dot{m}_{inj}$ the mass inflow rate to the cell through a face j, where the summation is over all faces. All gas properties are calculated from the CHEMKIN thermodynamic data base [Kee and Jefferson, 1981].

CALCULATIONS

The nonuniform, orthogonal computational grid with physical dimensions is shown in Fig. 2. Inlet boundary condition is listed in Table 1. Coordinate stretching has been employed to increase the grid density near the dump and heat exchanger planes because we expect fluid dynamic effects to be important there. Grid compaction is employed in the core flow to accurately capture the flame. The grid size is 64×14×39. Calculations have been performed for a flame (see Table 1) selected by computing a series of cases.

The basic conservation equations for mass, momentum, energy,

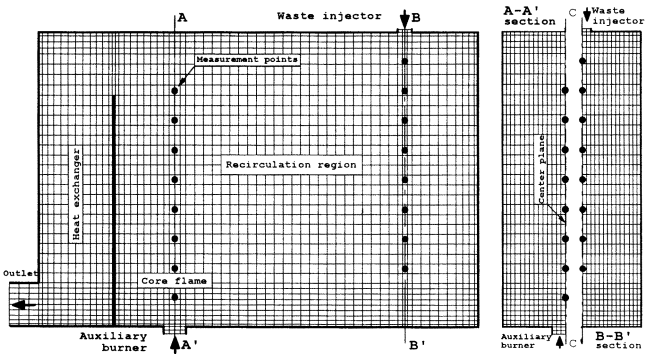

Fig. 2. Computational grid generation with measurement points and physical dimension.

Table 1. Inlet boundary condition

Auxiliary burner						Waste injector						
Q_{fm}	Q_{am}	T_m	ϕ_m	V_m	I_m	Q_{fw}	Q_{cw}	Q_{aw}	R	T_w	ϕ_w	V_w	I_w
0.8	19.1	353	1.0	1.87	5	0.2	1.2	15.2	0.6	353	1.0	3.51	5

List of symbols

Q_f : fuel flow rate (*l*/min)
Q_a : air flow rate (*l*/min)
T : mixture temperature (K)
V : axial velocity (m/s)
Q_c : hazardous waste flow rate (*l*/min)
R : molar concentration ratio of CCl_4 to C_3H_8
ϕ : equivalence ratio
I : turbulent intensity (%)

Subscripts

m : main burner
w : waste injector

turbulence quantities, radiation flux and species concentration can be expressed, in an Eulerian cartesian coordinate, as

$$\frac{\partial}{\partial x_i}(\rho \overline{u_i}\overline{\phi}) = \frac{\partial}{\partial x_i}\left(\Gamma_\phi \frac{\partial \overline{\phi}}{\partial x_i}\right) + S_\phi \tag{13}$$

in which ϕ denotes general dependent variables per unit mass. The dependent variables are the velocity components ($\bar{u}$, $\bar{v}$, $\bar{w}$), pressure ($\bar{p}$), turbulent kinetic energy ($\bar{k}$), dissipation rate ($\bar{\varepsilon}$), enthalpy ($\bar{h}$), composite radiation flux ($\bar{R}_x$, $\bar{R}_y$, $\bar{R}_z$), residence time ($\bar{t}$) and the mass fractions of chemical constituents ($\overline{m}_{C_3H_8}$, $\overline{m}_{CCl_4}$, $\overline{m}_{O_2}$, $\overline{m}_{CO_2}$, $\overline{m}_{HCl}$ and $\overline{m}_{H_2O}$). Γ_ϕ and S_ϕ represent the turbulent diffusion coefficient and source term, respectively. Expressions for the Γ_ϕ and S_ϕ are presented in Table 2 together with empirical constants for all species mass fractions and enthalpy, where σ denotes turbulent Prandtl/Schmidt number.

The solution of the Eulerian gas phase equations is done by control volume based finite difference procedure. A detailed description of this method is given by Patankar [Patankar, 1980]. In brief, the method requires the division of the computational domain into a number of control volumes, each associated with a grid print. The governing differential equations in each control volume profile are approximated in each coordinate direction in this study, power-law scheme is employed for the discretization of the convection term appeared in the governing Eq. (13).

A system of discretized linear equations is solved iteratively due to the nonlinear feature of the equation implicity imbedded in the coefficient of the discretized equation. The composite radiation fluxes in radiative transfer equations are solved by which the conduction term (i.e., first term) in Eq. (13) is omitted. The residence time must

Table 2. Expression for Γ_ϕ and S_ϕ for enthalpy and species mass fraction

ϕ	Γ_ϕ	S_ϕ
$\overline{m}_{C_3H_8}$	$\frac{\mu_{eff}}{\sigma_{C_3H_8}}$	$-\overline{RR}_{C_3H_8-CCl_4}\cdot\frac{M_{C_3H_8}}{M_{C_3H_8}+2R\cdot M_{CCl_4}}$
$\overline{m}_{CCl_4}$	$\frac{\mu_{eff}}{\sigma_{CCl_4}}$	$-\overline{RR}_{C_3H_8-CCl_4}\cdot\frac{2R\cdot M_{CCl_4}}{M_{C_3H_8}+2R\cdot M_{CCl_4}}$
$\overline{m}_{O_2}$	$\frac{\mu_{eff}}{\sigma_{O_2}}$	$-\overline{RR}_{C_3H_8-CCl_4}\cdot\frac{5M_{O_2}}{M_{C_3H_8}+2R\cdot M_{CCl_4}}$
$\overline{m}_{HCl}$	$\frac{\mu_{eff}}{\sigma_{HCl}}$	$\overline{RR}_{C_3H_8-CCl_4}\cdot\frac{8R\cdot M_{HCl}}{M_{C_3H_8}+2R\cdot M_{CCl_4}}$
$\overline{m}_{CO_2}$	$\frac{\mu_{eff}}{\sigma_{CO_2}}$	$(3+2R)\overline{RR}_{C_3H_8-CCl_4}\cdot\frac{M_{CO_2}}{M_{C_3H_8}+2R\cdot M_{CCl_4}}$
$\overline{m}_{H_2O}$	$\frac{\mu_{eff}}{\sigma_{H_2O}}$	$4(1-R)\overline{RR}_{C_3H_8-CCl_4}\cdot\frac{M_{H_2O}}{M_{C_3H_8}+2R\cdot M_{CCl_4}}$
$\overline{h}$	$\frac{\mu_{eff}}{\sigma_h}$	$\overline{RR}_{C_3H_8-CCl_4}\cdot H^*_{fu}-S^{**}_{rad}$

$^*H_{fu}=\frac{(20.4+1.73R)\cdot 10^8}{44+154\cdot 2R}$ [J/kg]

Constant in Combustion Models

$\sigma_{C_3H_8}=\sigma_{O_2}=\sigma_{HCl}=\sigma_{CO_2}=\sigma_{H_2O}=1$

$\sigma_{CCl_4}=\sigma_h=0.9$

$^{**}S_{rad}$ is in Eq. (8)

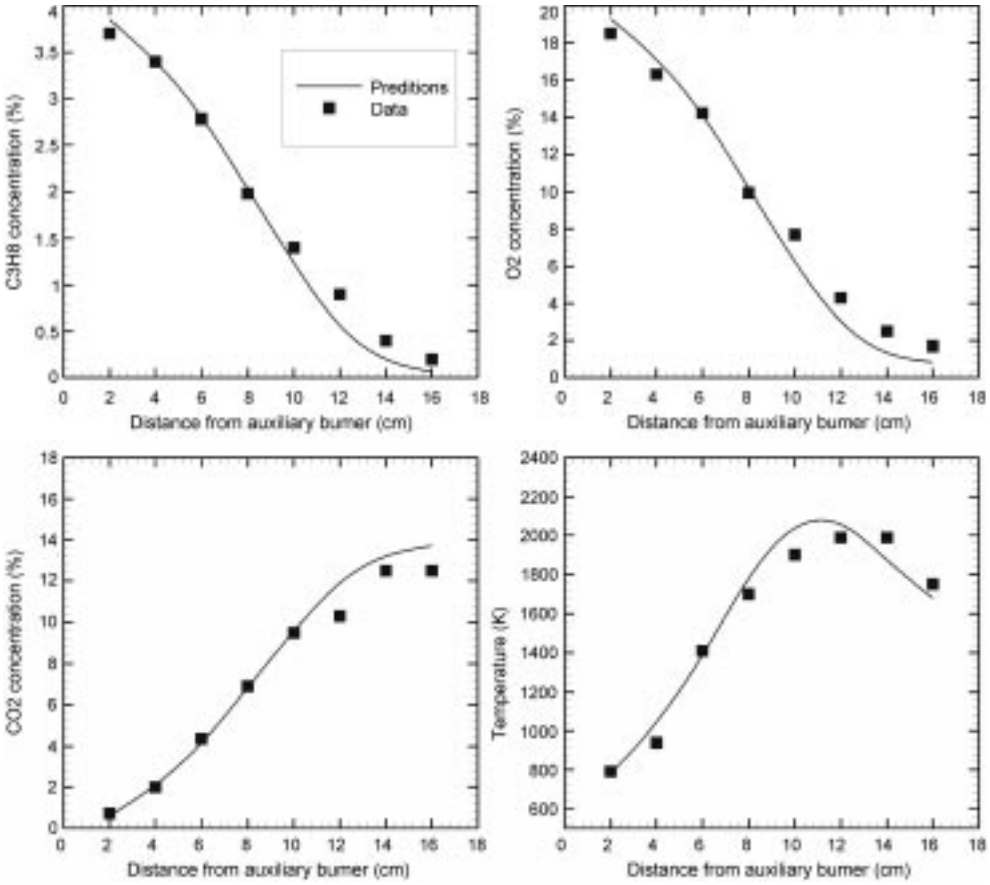

Fig. 3. Selected gas concentrations and temperature along a center line of the auxiliary burner plane.

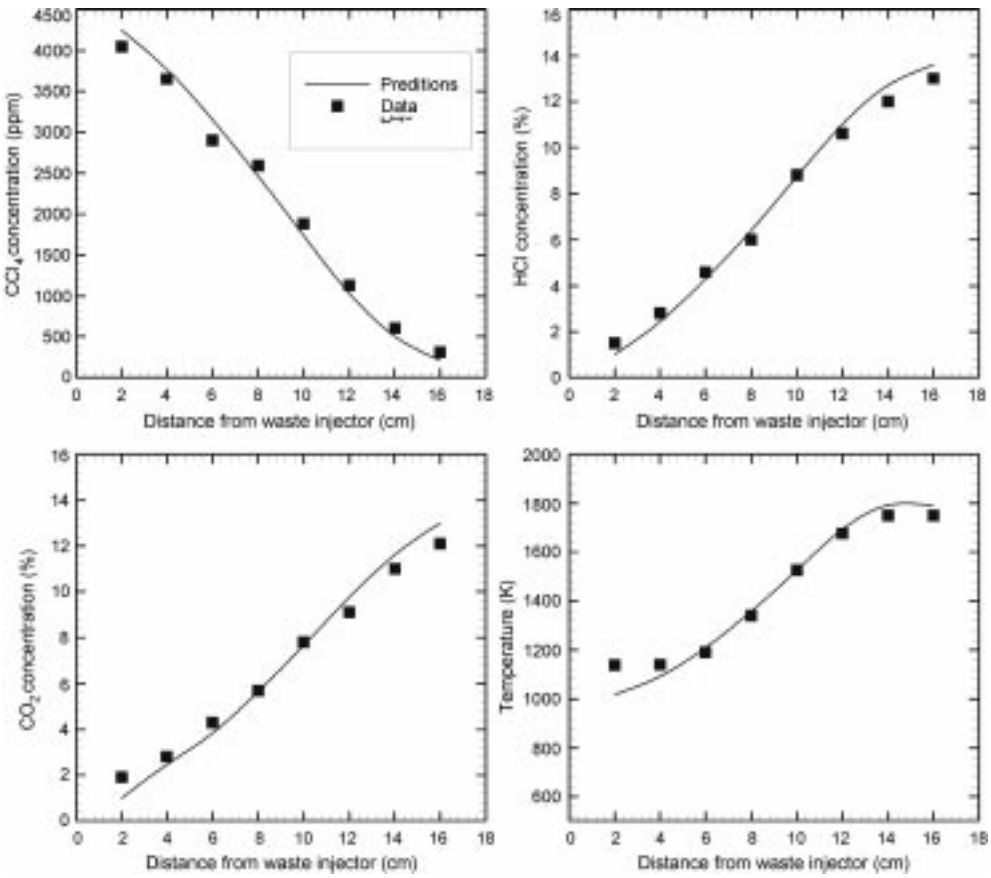

Fig. 4. Selected gas concentrations and temperature along a center line of the waste injector plane.

be only be convected by the fluid, so that the diffusion term must be deactivated. Numerical procedure for the differential equation is used by SIMPLEST (Semi-Implict Method for Pressure-Linked equations ShorTened) algorithm, which is a derivative of SIMPLE, to ensure rapid converge [Spalding, 1988].

RESULTS AND DISCUSSIONS

1. Comparison of Predictions and Measurements

Predictions of a dump incinerator include flow-velocity distribution, gas temperature and concentrations of major species (C_3H_8, CCl_4, O_2, CO_2, HCl etc). Detailed comparisons are made between selected model predictions and dump incinerator-probing measurements as dry basis.

Figs. 3 and 4 show selected gas concentrations and temperature at the centerline of section A-A' (referred as auxiliary burner plane) and section B-B' (referred as waste injector plane) in Fig. 2, respectively. The points are the data in all the figures. Corresponding selected gas concentrations and temperature profiles appear in Figs. 3 and 4, respectively.

Fig. 3 shows the comparisons along auxiliary burner plane. Measured C_3H_8 and O_2 consumptions are smaller than predicted, while measured CO_2 is lower than predicted in post flame region. This results because the reactions of both C_3H_8 and O_2 for experiment are slower than calculation. Therefore the overall flame length is larger than predicted as can be seen in the peak temperature in Fig. 3. That is why wall temperature boundary is not resonable, particularly in the baffle plate which affects the auxiliary burner flame. It would certainly be possible to apply more suitable boundary models but we have not pursued them [Peters and Weber, 1995].

Fig. 4 reveals that the agreement between the predictions and experimental data along a center line of waste injector plane is remarkably good. Particularly, agreement of CCl_4 and HCl means that the nonequilibrium reaction model developed in this study may be satisfied. Considering the complexity of that which is being modelled, the agreement between the predictions and data is on the whole excellent.

2. Cavity Hydrodynamics and Flame Structure

To study the cavity hydrodynamics and flame structure in a dump incinerator, proposed in this study, we selected a flame by computing a series of cases. We are evaluating the use of the recirculation region within the cavity as an oxidizing chemical reactor for the destruction of hazardous wastes by using the nonequilibrium reaction model developed in this study. Selected results at center plane, auxiliary burner and waste injector plane (see Fig. 2) are presented in Figs. 5-8.

Velocity fields and local residence time contours are shown in Fig. 5.

The arrows of velocity vectors indicate the direction of the flow and the length of the arrows are directly proportional to the magnitude of the velocity. When the mixtures at the auxiliary burner and surrogate injector respectively are introduced, large recirculation region is formed within the cavity behind the rearward facing step. The formation of recirculation region is important to have long re-

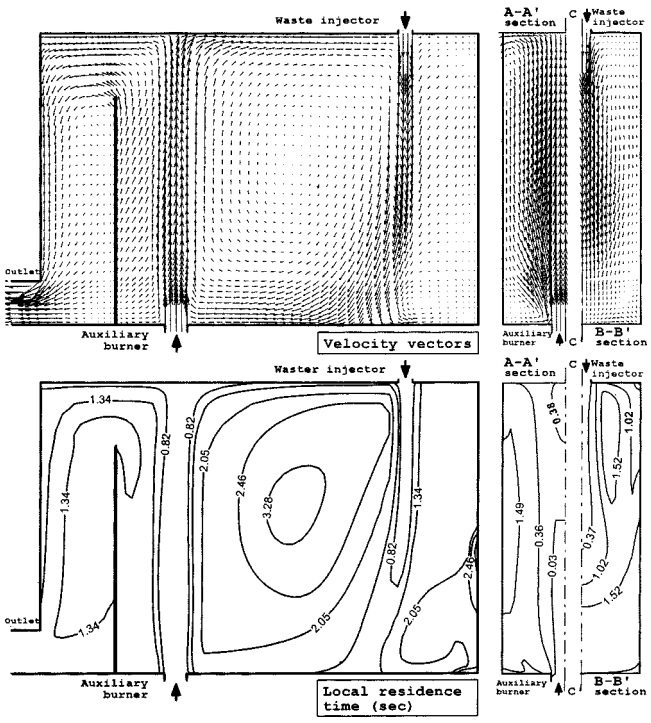

Fig. 5. Calculated vectors and local residence time contours.

sidence time at high temperature for the destruction of hazardous waste. Therefore the waste injector has been located at the point where recirculation region is not disturbed. The core flame has a very significant impact on the structure of recirculation region, in some cases completely changing the nature of the flow within the cavity.

Local residence time in recirculation region is more than 2 seconds. Provided that the recirculation region exists continuously in time, waste mixture injected into the recirculation zone will experience a relatively long residence time in a high temperature, potentially reactive environment in comparison with that in the core. In an incineration application, we make use of this by injecting waste directly into the recirculation region.

Fig. 6 depicts the temperature field and black-body power in Eq. (10) of six flux radiation model. The highest temperature and black-body power are found between the flame front and the streamline separating the core flow from the recirculation zone. Both counters show same shape nearly. It means that block-body power depends on the absolute temperature.

A lift and long core flame with low temperature is formed in waste injector because of the inhibiting effect of CCl_4. Therefore, most of the waste mixture burns in long flame-front and recirculation region. The inhibiting effect of halogens on the oxidation of hydrocarbon/air flames has been studied and defined by Westbrook and Dryer [1981] as the inhibitor provides competition for radical species, particularly H atoms. Regardless of inhibiting effect in waste injector,

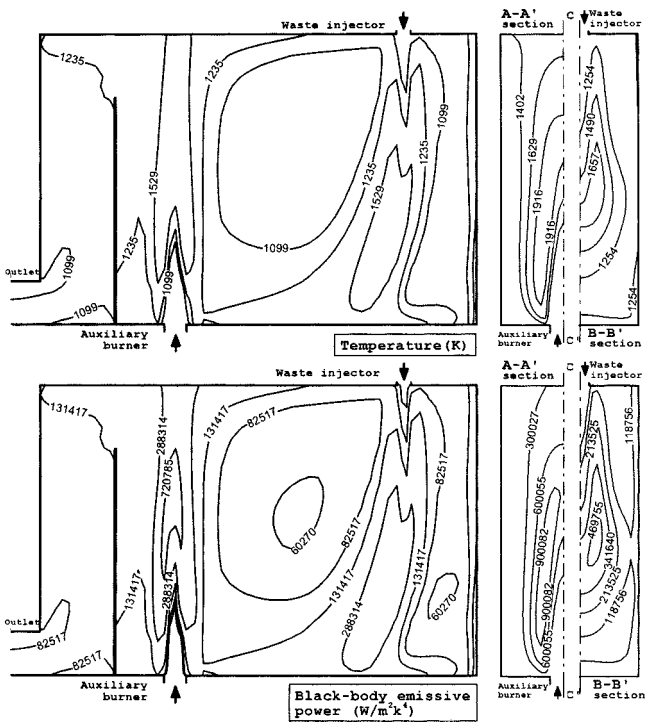

Fig. 6. Temperature and black-body emissive power contours.

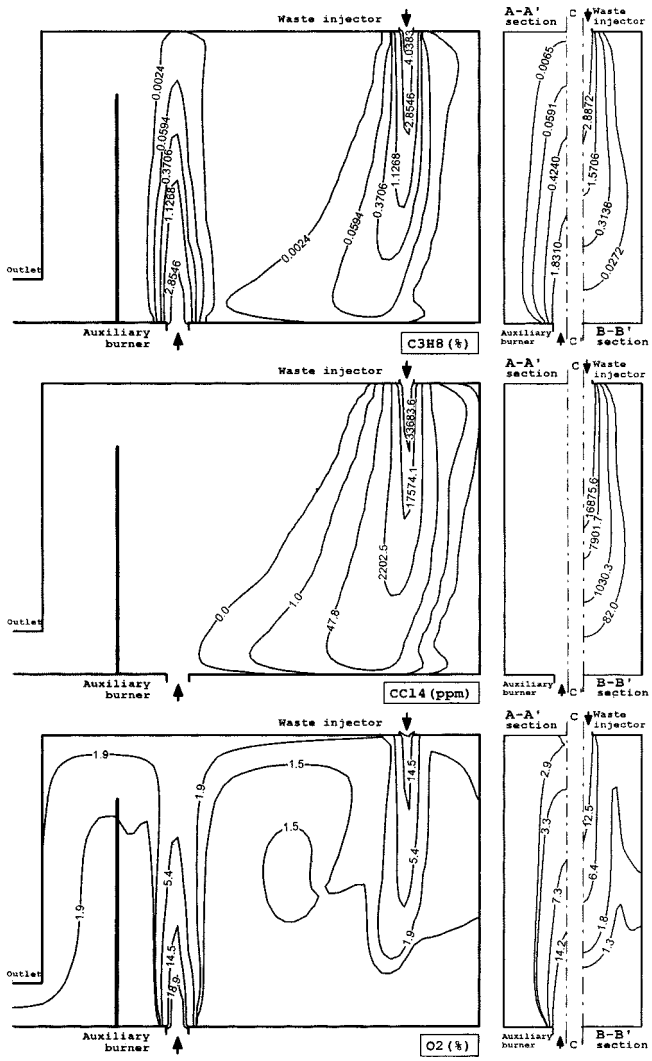

Fig. 7. C_3H_8, CCl_4, and O_2 concentrations.

the flame of the auxiliary burner burns stably. A higher temperature could be maintained (i.e., more than 1,000 K) in the recirculation region, which is particularly effective for the destruction of hazardous waste, and in the heat exchanger. High temperature in heat exchanger contributes to the complete destruction of CCl_4 which could not be destroyed in the recirculation region.

The dump incinerator designed in this study guarantees complete destruction, because most of the waste burn in the recirculation zone and complete burning is possible in the heat exchanger. Also the latent heat in heat exchanger transfers to dump to increase the reaction rate of mixture in auxiliary burner.

C_3H_8, CCl_4 and O_2 concentration plots are shown in Fig. 7.

C_3H_8 concentration contours near the auxiliary burner and waste injector have core shapes. The C_3H_8 concentration is decreased gradually up to flame-front at which exists high temperature. However because the mixture is consumed by burning, they decrease drastically from the rear of flame-front. The C_3H_8 concentration has been consumed at the exit completely.

The destruction of CCl_4 is achieved gradually at the core flame in the waste injector. CCl_4 destruction increases drastically through the flame-front which is high temperature. Remaining CCl_4 is destroyed completely through recirculation region.

Most of O_2 is consumed through core flame. Remaining O_2 enters either to recirculation to react with hazardous waste or to heat exchanger to react with remained combustible components. This oxidizing species must be supplied by diffusion across the flame-front separating the recirculation zone from core flow.

It is important to have sufficient oxygen in the recirculation zone, because the intermediates created by the burning of waste mixture could have a chance to burn out.

The contours of CO_2, HCl and H_2O concentrations are given in Fig. 8.

CO_2 is drastically increased at both flame-fronts, and is gradually increased in recirculation by reaction. H_2O is also increased drastically at both flame fronts. Higher H_2O concentration shows particularly at the upper of flame front in auxiliary burner. The reason is that CH_4 burns only at auxiliary burner. HCl is produced at long flame front in waste injector only due to the destruction of CCl_4. The lower concentration in auxiliary burner and heat exchanger stream is because the species produced in the flame front and recirculation region is diluted through this region.

Dump combustors are characterized by the sudden expansion of a fuel-air mixture into a combustion cavity. Recirculation zones are typically stabilized within the cavity by the sudden increase in cross-section at the point where the fuel-air mixture is introduced and the reactants are ignited. These zones contain mostly high temperature combustion products, and exchange mass and momentum relatively slowly with the surrounding gases. As a result, matter within the recirculation zone experiences a much longer residence time than that in the core flow. This means that waste through recirculation zone could be destroyed with high temperature.

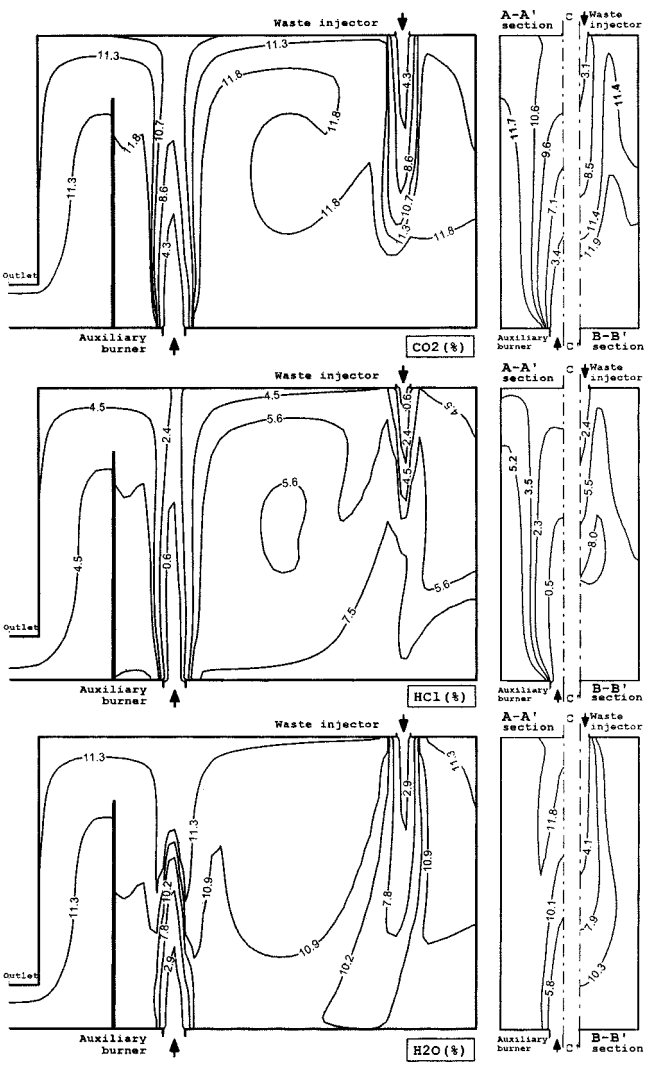

Fig. 8. CO_2, HCl and H_2O concentrations.

SUMMARY AND CONCLUSIONS

An empirical model that incorporates the chemical kinetic aspects of CCl_4 destruction is developed and model predictions are compared with experimental data. Comparisons of the predicted and measured value are reasonable. Results indicate that the flame inhibition feature of the halogen compounds and the associated kinetic effects must be incorporated, as in the empirical model in this paper, in order to obtain realistic predictions.

Cavity dynamics and flame structure are studied for a flame selected by computing a series of cases in the complex hydrodynamic environment of a dump incinerator designed in this study. For the good destruction of hazardous waste, it is effective that the waste is injected in the recirculation region of high temperature with the condition of not disturbing combustion cavity. The core flame has a significant impact on the structure of the recirculation region, in some cases completely changing the nature of the flow within the cavity.

The dump incinerator has several good characteristics in incineration application of hazardous waste, which is halogen compounds. It may guarantee the good destruction of hazardous waste due to a high degree of mixing within the recirculation region and high temperature in heat exchanger. In addition, this has relatively long residence time for hazardous wastes within the recirculation zone of high temperature and radical concentrations, or, equivalently, a relatively compact incinerator. These characteristics should lead to a

very compact device, one which is potentially transportable or usable in a dedicated manner by a small generator.

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REFERENCES

Bilger, R. W., "Turbulent Jet Diffusion Flames," *Prog. Energy Combustion Sci.*, **1**, 87 (1976).

Chun, Y. N., "Numerical Simulation of Dump Combustor with Auxiliary Fuel injection," *J. of KSME*, **13**(12), 948 (1999).

Cundy, V. A., Morse, J. S., Lester and Senser, D. W., "An Investigation of a Near-Stoichiometric CH_4/CCl_4/Air Premixed Flat Flame," *Chemosphere*, **6**, 989 (1987).

Bose, D. and Senkan, S. M., "On the Combustion of Chlorinated Hydrocarbons: I. Tichloroethylene," *Comb. Sci. and Tech.*, **35**, 187 (1983).

Glassman, I., "Combustion," Academic Press, New York, 118 (1977).

Gosman, A. D. and Lockwood, F. C., "Incorporation of a Flux Model for Radiation into a Finite-Difference Procedure for Furnace Calculations," 14th Symp. Combustion, 661 (1973).

Jang, D. S. and Acharya, "Two-Dimensional Modeling of Waste Combustion In A Kiln," presented at AIChE Spring National Meeting, New Orleans, La., March 6-10 (1988).

Kee, R. J. and Jefferson, T. H., "CHEMKIN: A General Purpose, Problem Independent, Transportable, Fortran Chemical Kinetics Code Package," Sandia National Laboratories Report SAND80-8003 (1981).

Launder, B. W. and Spalding, D. B., "Mathematical Models of Turbulence," Academic Press, New York (1972).

Lockwood, F. C., Salooja, A. P. and Syed, S. A., "A Prediction Method for Coal-Furnaces," *Combustion and Flame*, **38**, 1 (1980).

Magnussen, B. F. and Hjertager, H., "On Mathematical Modeling of Turbulent Combustion With Special Emphasis on Soot Formation and Combustion," 16th Symp. Combustion, The Combustion Institute, Pittsburgh, PA, 714 (1976).

McKenty, F., Gravel, L. and Camarero, R., "Numerical Simulation of Industrial Boiler," *Korean J. Chem. Eng.*, **16**, 4 (1999).

Morse, J. S., "Combustion of CCl_4 In A High Temperature Methane-Air Flame Environment," Ph. D. Dissertation, Department of Mechanical Engineering, Lousiana A Finite Difference Procedure for Furnace Calculation, 14th Symp. Combustion, L.A (1984).

Morse, J. S., Cundy, V. A. and Lester, T. W., "Thermal Destruction of Carbon Tetrachloride," presented at 1988 Spring Meeting, Western section, the Combustion Institute, Salt Lake City, Utah, March 21-22 (1988).

Oppelt, T., "Incineration of Hazardous Waste: A Critical Review," *J. Air Pollut. Control Assoc.*, **37**, 558 (1987).

Patankar, S. V., "Numerical Heat Transfer and Fluid Flows," Chemosphere, Washington, D.C. (1980).

Peters, A. A. F. and Weber, R., "Mathematical Modelling of a 2.25 MW_t Swirling Natural Gas Flame. Part 1: Eddy Break-up Concept for Turbulent Combustion: Probability Density Function Approach for Nitric Oxide Formation," *Combust. Sci. and Tech.*, **111**(110-111), 67 (1995).

Silcox, G. D. and Perching, D. W., "Heat Transfer Modeling In A Rotary Kiln for Hazardous Industrial Wastes," presented at AIChE Spring Nation Meeting, New Orleans, LA, March 6-10 (1988).

Spalding, D. B., "Mixing and Chemical Reaction In Steady Confined Turbulent Combustion," 13th Symp. Combustion, The Combustion Institute (1971).

Spalding, D. B., "PHOENICS Training Course Notes," CHAM TR/300 (1988).

Spalding, D. S., "Idealizations of Radiation," In mathematical Modelling of Fluid-mechanics, Heat Transfer and Chemical-reaction Process, Lecture 9, HTS/80/1, Imperial College, Mech. Engng., Dept., London (1980).

Valeiras, H. A., "Burning Velocities and Rates of Methane-chlorinated Hydrocarbon Flames," M.S. Thesis, Massachusetts Institute of Technology, Chemical Engineering (1982).

Westbrook, Charles, K. and Dryer, Fredrick, L., Eighteenth Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, 749 (1981).