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The effect of boundary layer flow on incinerator efficiency

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Abstract

Incinerators operating with excess air, a core temperature of about 1100 K, and a residence time of 1-2s should give essentially complete destruction of all organic pollutants exposed to these conditions. However, about 1% of the gas flows in the cooler boundary layer near the wall, where reaction occurs at a much lower rate. The decrease in reaction rate is partially offset by the lower velocity and by mass transfer of pollutant from the boundary layer to the core, but the overall effect is still a significant increase in the amount of unreacted pollutant. The effects of wall and core temperature and mass transfer from the boundary layer on incinerator efficiency were examined by computer simulation using toluene vapor in air as an example of a polluted stream.

Keywords: Incinerator; Organic pollutants; Efficiency; Boundary layer

1. Introduction

Thermal incineration is a common method for disposal of waste organic materials and for treating air contaminated with volatile organic pollutants. When treating dilute gaseous wastes, supplemental fuel is burned in a combustion chamber, and contaminated air fed to the chamber is heated to about 1000–1200 K by mixing with the combustion gases. The gases then pass through a secondary reaction zone (or a separate chamber) where the average residence time is one to several seconds, long enough to achieve nearly complete destruction of the pollutants. Liquid wastes may be sprayed into the combustion chamber and partially burned in the flame region, but additional time in the secondary reaction zone is needed for very high destruction efficiencies [1, 2]. Most incinerators for municipal solid wastes also have a primary combustion zone, where devolatilization and initial reactions occur, followed by a secondary zone where conversion is completed. This paper deals with the secondary reaction zone of an incinerator and not with reactions in flames or with

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Compound	Reference	$A (s^{-1})$	E (kcal/mol)	k at 1000 K (s ⁻¹)
Chlorobenzene	3	8 × 10 ⁴	23	0.8
Chlorobenzene	4	1.34×10^{17}	76.6	2.4
Toluene	4	2.28×10^{13}	56.5	10
Toluene	5	7.5×10^{11}	48	23
n-Hexane	4	6.02×10^{8}	34	20
<i>n</i> -Hexane	5	1.9×10^{11}	48	6
Methyl ethyl ketone	4	1.45×10^{14}	58.4	25
1,2-Dichloroethane	4	4.82×10^{11}	45.6	52

 Table 1

 Effective first-order rate constants for hydrocarbon oxidation

mixing patterns in the primary combustion chamber. Even if 99% conversion is obtained in the primary combustion zone, an additional 99% conversion of the remaining pollutant would have to be obtained in the secondary zone to get 99.99% destruction removal efficiency (DRE), the requirement for principal organic hazardous constituents (POHC) of a waste stream.

The extent of conversion in the secondary reaction zone depends on the temperature and residence time distribution and on the kinetics of the destruction reactions. Although hydrocarbon oxidations are complex chain reactions, first-order kinetics are sometimes assumed for simplified design calculations [3-5]. Effective rate constants for a few compounds are given in Table 1. For some compounds, frequency factors and activation energies from different sources vary widely, but the rate constants at the typical temperature of 1000 K generally differ by only 2- or 3fold. The oxygen concentration was not specified for these rate constants, but other studies [6] have shown only a slight increase in oxidation rate with oxygen concentration. Toluene was selected as a typical pollutant for this study because the rate constants [5] were in the middle of the range of values for E and k at 1000 K.

The ideal flow pattern in the secondary reactor is plug flow, since this gives the highest conversion for a first-order reaction and a given residence time:

$$x = 1 - \exp\left(-kt\right) \tag{1}$$

If the effective rate constant is 10 s^{-1} , a plug-flow reactor with t = 1 s gives a conversion x = 0.99995; at 1000 K, most organic compounds would react at least this rapidly. For unreactive material such as chlorobenzene or acetonitrile, 99.99% DRE could be met with an ideal reactor at 1100 K and 1-2 s residence time. However, the wall temperature in an incinerator is always lower than the center temperature, and gas flowing near the wall reacts more slowly than gas in the central region. For turbulent flow in a large diameter reactor at high Reynolds number, the gas flowing in the cool boundary layer is about 1% of the total flow; if the conversion for this gas is only 50%, the overall conversion can be no higher than 99.5% even if complete conversion is achieved in the central core region. Thus, the plug-flow model may be seriously in error when very high conversions are required, even though it might be satisfactory for conversions of 90–95%. (If only 90% conversion is needed, this could

be achieved with 91% in the core and nearly 0% in the boundary layer; only a 5% increase in rate constant or average residence time would be needed to offset the boundary layer effect.

The importance of boundary-layer flow on conversion in the post-flame region of a hazardous waste incinerator was discussed by Wolbach and Garman [1]. They proposed a model with up to 7 radial zones, with narrower zones near the wall, where the temperature and velocity profiles are steepest. A time-temperature history was developed for each zone and a flow-weighted average used to calculate the overall conversion. For destruction of carbon tetrachloride, their 3-zone model gave predicted overall conversions of 99–99.99%, and the effects of firing rate and excess air were similar to those measured for a pilot incinerator. However, the amount of unreacted hydrocarbon was overestimated by about an order of magnitude, perhaps because no allowance was made for mass transfer between zones.

In a similar work by Clark et al. [3], plug flow was assumed for the central zone of the incinerator, and zones near the wall were treated as laminar boundary layers with lower flow rates. Diffusional exchange between layers was included, but no details were given. The overall destruction efficiency was calculated by averaging the results from 10 000 flow-weighted random paths through the furnace. The model predicted lower conversions with increasing excess air or with heat removal (cold wall), in general agreement with experimental trends. However, the calculated conversion for the flow path along the wall was much higher than that for the central zone. The average residence time is higher in the boundary layer, but it seems unlikely that this would offset the lower rate constant near the wall, unless the activation energy was very low or the wall only slightly cooler than the gas in the center.

Detailed modeling of a rotary kiln incinerator by Worneck and Pershing [7] showed large radial variations in temperature and concentration near the wall at the kiln exit, which were due mainly to air leakage around the rim. Their model included effective exchange coefficients between fluid elements based on laminar and turbulent diffusion, but the contribution of mass transfer near the wall was not brought out. Other recent studies [8, 9] have used 2-D and 3-D models to predict detailed mixing patterns and temperature profiles, in incinerators, but the effects of mass transfer and reaction in the boundary layer were not included. The purpose of this study is to illustrate the importance of reaction and mass transfer in the cool boundary layer by using a relatively simple model that could be incorporated into the complex 3-D models used to study commercial incinerators.

2. Model development

In the simplest 2-zone model for the secondary combustion chamber, the pollutant conversion in the wall region is based on the average temperature and residence time in the boundary layer, and this is combined with the conversion in the core region using a flow-weighted average. The average residence time for the boundary layer is about twice that for the core zone, but the lower temperature can make the rate constant an order of magnitude lower, which would more than offset the greater residence time.



Fig. 1. Thermal and velocity boundary layers.

An improved 2-zone model allows for mass transfer of reactant from the boundary layer, where the reactant concentration is relatively high, to the central core. This increases the pollutant conversion in the boundary layer zone and increases the overall destruction efficiency. In multizone models, the temperature boundary layer is subdivided to account more accurately for the change in reaction rate constant, and mass transfer takes place between the sublayers as well as from the inner layer to the core. Both 2-zone and multizone models were used in this study with and without allowance for mass transfer between zones.

The model calculations were carried out for a large cylindrical incinerator operating with fully developed turbulent flow and no temperature change along the length of the reactor. For an incinerator 3.6 m in diameter and an average gas velocity of 4.0 m/s at 1100 K, the Reynolds number is 1.0×10^5 . A portion of the velocity profile calculated from the universal velocity distribution equation [10] is shown in Fig. 1. The complete profile would show a gradual increase in velocity in the turbulent core to a maximum of 500 cm/s at the center (R = 180 cm). For all models, plug flow of gas was assumed for the central core with a velocity equal to the average velocity $\overline{V} = 4.0 \text{ m/s}$.

The thickness of the boundary layer zone for the 2-zone and multizone models was chosen to be the effective thickness of the thermal boundary layer, which was calculated from the thermal conductivity of air at 900 K and the convective heat transfer coefficient given by the Dittus–Boelter equation [11]:

$$\frac{hD}{k_{\rm g}} = 0.023 \left(\frac{DG}{\mu}\right)^{0.8} \left(\frac{C_p \mu}{k_{\rm g}}\right)^{1/3},\tag{2}$$

$$z = \frac{k_{\rm g}}{h}.\tag{3}$$

As shown in Fig. 1, the thermal boundary layer is slightly smaller than the viscous sublayer plus the buffer layer. The wall temperature was found after calculating the combined resistance of the steel shell plus 10 cm of brick lining and then estimating the external heat transfer coefficient from correlations for natural convection plus radiation [12]. A linear gradient was assumed from the wall to the inner edge of the thermal boundary layer. The actual temperature gradient is curved and extends into the turbulent core, but the linear assumption is adequate for this study.

For the 2-zone model, the velocity and temperature at the center of the thermal boundary layer are used to determine the rate constant and residence time for gas flowing in this layer. The rest of the gas is assumed to be at the center temperature and have a residence time equal to the nominal residence time, $t = L/\overline{V}$. For $\overline{V} = 4.0 \text{ m/s}$, the thermal boundary layer has a thickness of 1.75 cm and a cross-sectional area 1.93% of the total area. The flow through this zone is 0.81% of the total gas flow. For larger diameter units, the boundary layer is somewhat thicker, since h varies with $D^{-0.2}$, but flow through the boundary layer is a smaller faction of the total flow. When testing the multizone models, the thermal boundary layer is divided into 2 to 5 sublayers of equal thickness. The velocity at the midpoint of each sublayer is used to calculate the average residence time and the gas flow rate in that layer. Fig. 2 shows the 3-zone model with the thickness of the sublayers exaggerated for clarity.

Because of differences in reaction rate and residence time, radial concentrating gradients develop near the wall of the incinerator. Usually, the reactant conversion is lowest near the wall, and mass transfer of reactant from the boundary layer towards the center increases the average conversion in the boundary layer. The mass transfer coefficient for transfer between zones is based on k_c , the normal coefficient for transfer from the wall to the bulk fluid [13].

$$\frac{k_{\rm c}D}{D_{\rm AB}} = 0.023 \left(\frac{DG}{\mu}\right)^{0.8} \left(\frac{\mu}{\rho D_{\rm AB}}\right)^{1/3}.$$
(4)

For the 2-zone model, the average diffusion distance is half the thickness of the boundary layer, so the effective coefficient is twice the normal value:

$$K = 2k_{\rm c}.$$
(5)

For the multizone model with n sublayers in the boundary layer, the coefficient for mass transfer between layers is proportional to n,

 $K_n = nk_c. (6)$

For transfer from the innermost layer to the core, the diffusion distance is only half as great as that between layers, and the coefficient is twice as large,

$$K_1 = 2nk_c. \tag{7}$$



Fig. 2. Multizone model.

In this study, the difference between the thermal and concentration boundary layers is not rigorously accounted for. Because the Schmidt number is about 2.2 and the Prandtl number is 0.7, the effective thickness of the concentration boundary layer is 30% less than that of the thermal boundary layer. Basing the mass transfer coefficient on k_c therefore gives higher rates of mass transfer between zones than if based solely on molecular diffusion. However, the layer thicknesses and flows in each zone are still based on the thermal boundary layer.

The first-order rate constant for toluene removal was taken from published values and an activation energy of 48.1 kcal/mol [5],

$$k = 7.535 \times 10^{11} \exp\left(\frac{-24.220}{T}\right) \mathrm{s}^{-1}.$$
 (8)

For the 2-zone and multizone models the incremental conversion in each zone was computed by material balance allowing for the axial concentration change due to reaction and mass transfer into and out of the zone:

$$V_{n}A_{Rn} \frac{\Delta C_{n}}{\Delta l} = -k_{n}A_{Rn} \left(C_{n} + \frac{\Delta C_{n}}{2} \right) + K_{n+1}A_{1,n+1} \left(C_{n+1} + \frac{\Delta C_{n+1}}{2} - C_{n} - \frac{\Delta C_{n}}{2} \right) - K_{n}A_{ln} \left(C_{n} + \frac{\Delta C_{n}}{2} - C_{n-1} - \frac{\Delta C_{n-1}}{2} \right).$$
(9)



Fig. 3. Effect of number of sublayers on fraction unconverted.

Eq. 9 was solved by iteration using a zone length $\Delta l = 0.1$ cm, which gives less than a 5% change in concentration across each element for runs at 1100 K.

3. Results

The effect of the number of sublayers on (1 - x), the average fraction unconverted, is shown in Fig. 3 for 1100 K and t = 1 s. With only one zone in the boundary layer, the fraction unconverted is 0.0022, but (1 - x) drops to about 0.0002 for two or more sublayers. The 10-fold decrease in (1 - x) is due mainly to the change in rate constant. For a single layer, k is 0.24 s^{-1} at the midpoint temperature, and the boundary layer conversion is about 60%. With two zones in the boundary layer, the rate constants are 0.0013 s^{-1} for the outer zone and 11.1 s^{-1} for the inner zone. The reaction rate is negligible in the outer zone, but there is a decrease in reactant concentration due to mass transfer. The inner zone has a very high conversion and about 2/3 of the boundary layer flow, and these factors contribute to a much lower calculated value of (1 - x).

To show the importance of diffusion, some of the computations were repeated without the mass transfer terms, and the results are plotted in Fig. 4. With a single boundary layer, the average (1 - x) is 0.0066, about 3 times greater than when diffusion is allowed for. The core conversion is essentially complete for both cases, and the boundary layer has about 0.8% of the total flow. The boundary layer value of (1 - x) is about 0.81 without diffusion and 0.27 when mass transfer is allowed for. With 2, 3, or 4 sublayers in the boundary layer, mass transfer has a greater effect, lowering the overall (1 - x) from 0.003 to 0.0002. With several sublayers, the



Fig. 4. Fraction unconverted in absence of mass transfer.



Fig. 5. Comparison of ideal and non-ideal reactors.

reaction rate is negligible in the layers nearest the wall, and concentration changes in these layers are due almost entirely to mass transfer.

The model should improve as the number of sublayers is increased, but there was little change from n = 4 to n = 5, and further computations were done with 5 sublayers and a total of 6 zones. For other cases with a smaller difference between the

core and wall temperatures or a low activation energy, a model with only 2 or 3 zones might be satisfactory.

The conversion in the non-ideal reactor with a cool boundary layer is compared with that for an ideal plug-flow reactor in Fig. 5. For the plug-flow reactor, $\ln(1 - x)$ is proportional to the residence time, and 99.9999% conversion is obtained in 0.6 s at 1000 K. For the non-ideal reactor, the plot is almost the same up to 95% conversion, and then the conversion increases much less rapidly, as if a slower reaction was taking place. However, the slow change in (1 - x) is limited by the rate of mass transfer from zones near the wall to zones near the core, where the temperature is high enough for fast reaction.

In the high conversion region, raising the core temperature increases the overall conversion much less for the non-ideal reactor than for the plug-flow reactor. Table 2 shows that a 200 K increase in core temperature gives a 20-fold reduction in (1 - x), but this corresponds to only a 40% increase in the effective rate constant or an apparent activation energy of 4 kcal/mol. The real rate constant increases by a factor of 57 for the same temperature change. Table 2 also shows the effect of changing the wall temperature by changing the insulation thickness. At a constant core temperature of 1100 K, an increase in wall temperature of 134 K lowers (1 - x) only 4-fold. Changing wall temperature has less effect than changing center temperature, because there is hardly any reaction in the outermost zone, and raising the temperature of the inner zones, where appreciable reaction does occur, is more beneficial.

For pollutants other than toluenc, results similar to Fig. 5 would be expected, even if the Arrhenius equation and first-order kinetics are not strictly followed. Compounds with a lower activation energy would give less difference between rate constants at the center and at the wall, and the difference in conversion between plug-flow and the boundary layer models would be smaller. For an incinerator with water-cooled walls, the much lower wall temperature would accentuate the conversion differential predicted because of boundary layer flow.

The results presented here show the compensating effects of mass transfer and reaction in the boundary layer, and this part of the multizone boundary layer model could be used with a more complete fluid-mechanics model for detailed incinerator studies. The model predictions have not been checked with experiments, and other approaches to mass transfer in the boundary could be considered. However, the film

Temperature (K)		1-x	k_{app}	k_{center}
Center	Wall		(s ⁻¹)	(s^{-1})
1000	560	5.5×10^{-4}	7.5	22.8
1100	584	1.6×10^{-4}	8.7	206
1200	606	0.26×10^{-4}	10.6	1293
1100	528	2.4×10^{-4}	8.3	206
1100	662	0.6×10^{-4}	9.7	206

Effect of wall temperature and core temperature on conversion for a non-ideal reactor with a cool boundary layer

Table 2

mass transfer coefficient varies with $D_{AB}^{2/3}$, and a model based on molecular diffusion and $D_{AB}^{1,0}$ would be unrealistic. Mass transfer in the boundary layer is really an unsteady-state process caused by random eddies coming close to the wall, and this process leads to a fractional exponent for D_{AB} [14].

One way to improve the incinerator efficiency is to promote mixing of boundary layer gas with gas in the core. Some mixing can be achieved by using wall jets or by adding baffles at the wall. If the gas in the boundary layer is completely mixed with core gas part way along the reactor, much higher efficiencies could be obtained. Using the 1000 K results as an example, Fig. 3 shows the fraction that is unconverted at t = 0.5 s to be 2×10^{-3} . If complete mixing of core and boundary layer gas is achieved at this point, and a new boundary layer forms, the next 0.5 s would convert 99.8% of the remaining material for an overall conversion of 99.9996% $(1 - x = (2 \times 10^{-3})^2)$. However, if only part of the boundary layer gas is mixed with the bulk gas, the increase in conversion will not be as great, and more elaborate models of the system would be needed to predict the performance.

4. Conclusions

(1) An incinerator operating with a wall temperature significantly lower than the core temperature may have a fraction unreacted that is up to several orders of magnitude greater than that for an ideal plug-flow reactor.

(2) For an incinerator with a cool wall, mass transfer from the boundary layer to the core region greatly improves the overall conversion.

(3) Devices to promote mixing of gas in the boundary layer with gas in the central core should lead to much higher destruction efficiencies.

5. Nomenclature

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$A_{\rm R}$	cross-section	ial area for g	gas now	
	0		•. •	. 1

 $A_{\rm I}$ area for mass transfer per unit length of reactor

c

- *C* concentration of pollutant
- $C_{\rm p}$ heat capacity of gas
- *D* reactor diameter
- D_{AB} binary gas diffusivity
- G mass velocity
- *h* heat transfer coefficient for gas film
- k reaction rate constant
- $k_{\rm g}$ thermal conductivity of gas
- $k_{\rm c}$ mass transfer coefficient, wall to bulk gas
- K mass transfer coefficient for boundary layer models
- L length
- *n* number of sublayers in the boundary layer
- t time

- T temperature (K)
- *x* fraction converted
- V gas velocity
- *z* effective film thickness
- μ viscosity of gas
- ρ gas density

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