Modeling Analysis for Dioxin Formation in a Pilot Fluidized-bed Combustor

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Introduction

Mathematical modeling is a widely used method in chemical process design and analysis; models of various complexities for different types of reactors have been developed in the past (1). Combustor models having considered the kinetics of pollutant formation such as NO_x, SO_x and particulate matter are also available; however, there are only a few attempts to model PCDD/F formation in combustors, *int. al.* (2). We report in this paper a work of modeling PCDD/Fs in a pilot-scale fluidized-bed combustor; the operating parameters and PCDD/F measurements of this combustor have been documented previously (3,4).

Modeling Methods

1. Entrainment of ash particles from the fluidized bed

The condition for fly ash entrainment from a fluidized bed is that the terminal velocity (U_t) of the ash particle is equal to or smaller than the gas fluidization velocity (U_g). The nomial gas flow rate in this combustor is: V = 2.5 Nm^3/h; at the freeboard of the fluidized bed the temperature is 700°C and the gas flow rate is: V_g = 2.5x(700+273)/(25+273) = 8.16 m^3/h; the freeboard has diameter 0.2 m and cross sectional area A_f = 0.0314 m^2; thus the gas velocity is: $U_g = V_g/(3600 \times A_f)$ = 8.16/(3600x0.0314) = 0.07 m/s. The entrained particles have $U_t = U_g$ = 0.07 m/s; and the particle diameter (d_p) can be calculated using the Stokes law:

$$U_t = g(\rho_p - \rho_g)d_p^2/18u_g$$

where, g = 9.81 m/s^2; particle density ρ_p = 2000 kg/m^3; gas density ρ_g = 0.363 kg/m^3 and gas viscosity $u_g = 4.876 \times 10^{-5}$ kg/ms both at 700°C. Substitute these figures and U_t into the above equation, then obtain: d_p = 56 um. The entrainment rate constant (K^*) of particles of different sizes in a fluidized bed is given by

$$K^*/\rho_g U_g = 23.7 \exp\{-5.4\, U_t/U_g\}$$

For d_p = 56 um, K^* is calculated from the above to be $2.7x10^{-3}$ kg/m^2s. The fluidized bed has diameter 0.1 m and cross sectional area A_b = 0.0078 m^2. The entrainment rate is: $R = K^*A_b = 2.7x10^{-3}x0.0078 = 2.12x10^{-5}$ kg/s. The fly ash loading is: M = R/V = $2.12x10^{-5}/(2.5/3600)$ = 30.5 g/Nm^3. At STP the gas density is: ρ_g = 1.186 kg/Nm^3, so the fly ash loading can be expressed as: M^* = 0.0257 kg/kg-gas.

2. Gas-solid two-phase flow in the cooling section

In the horizontal pipes of the cooling section following this pilot combustor, fly ashes may settle down on the surface of the pipes when the gas velocity is too low and/or the particle size is too large. The critical saltation velocity (U_s) is the gas velocity at which particle sedimentation or saltation begins and can be estimated using the correlation:

$$M^* = \{1/10^{1.44dp+1.96}\} \{U_s/(gD_t)^{0.5}\}^{1.1dp+2.5}$$

The pipe diameter D_t = 0.035 m, and other parameters have been given in the previous section. From the above equation it can be calculated that the critical saltation velocity U_s = 0.89 m/s. At the exit of the cooling pipes the temperature is ca. 200°C; the gas flow rate is: V_g = 2.5 x (200+273)/(25+273) = 3.968 m^3/h; the cross sectional area of the pipe is: $A_t = 9.62x10^{-4}$ m^2; so the gas velocity is: $U_g = V_g/(3600xA_t) = 3.968/(3600x9.62x10^{-4})$ = 1.15 m/s. This gas velocity is larger than the critical saltation velocity, therefore the gas-solid two-phase flow in the cooling section of this pilot combustor is likely to have full suspension of solid particles in the gas stream. Still, the solid phase residence time should be longer than the gas phase residence time in horizontal pipe flow; some correlations are available (5), but difficult to use for the present case. Depending on the temperature profile of the cooling section the gas phase residence time has previously been calculated to be 2 - 8 sec. A typical solid phase residence time of 5 sec is assumed in the following calculation.

3. PCDD/F formation levels

For PCDD/F formation from carbon degradation pathway an optimal PCDD/F formation rate of 0.034 ug/g min based on the weight of fly ash and solid phase residence time has been recommended (6). It is known that PCDD/F formation rates vary with the reaction temperature, gas composition, and fly ash carbon and metal concentrations. But a rate expression incorporating these influecing factors has not yet been developed. For PCDD formation from aromatic dimerization pathway the PCDD formation rates measured at the high aromatic concentrations in laboratory are difficult to apply to the low aromatic concentration (10 - 150 ug/Nm^3) conditions in this pilot combustor. We therefore use only PCDD/F formation rate k = 0.034 ug/gmin and calculate the PCDD/F formation level (D) from the fly ash loading (M) and solid phase residence time (t):

$$D = kMt = 0.034x30.5x5/60 = 86.4 \text{ ng/Nm}^3$$

Assuming 50 ng total PCDD/F = 1 ng I-TEQ as in (6), D is converted to 17.3 ng-TEQ/Nm^3. Measured flue gas TE output from this pilot combustor are in the range 2 - 60 ng-TEQ/Nm^3.

Discussion

The physical aspects of fluidized-bed reactors such as fluidization phenomena, particle elutriation, heat and mass transfer, and hydrodynamics of two-phase flow are fairly well understood from a chemical reaction engineering perspective. The global combustion behaviour can also be modeled using material and energy balance and the kinetics of solid fuel pyrolysis, hydrocarbon combustion, and carbon burnout. A limiting factor in modeling PCDD/F formation in fluidized-bed combustor is the lack of kinetic correlation of the PCDD/F formation rates measured in laboratory; because of this, it may not be worthwhile to go into further details of the physical and combustion aspects of fluidized-bed combustors at present. In this modeling work, the variations of PCDD/F formation rates with other parameters have been neglected and a typical formation rate of 0.034 ug/g min has been used in the calculation; the predicted PCDD/F formation level is 17.3 ng-TEQ/Nm^3, which is winthin the range of the flue gas PCDD/F concentrations (2 - 60 ng-TEQ/Nm^3) measured at this pilot combustor. This seems to suggest that PCDD/F formation rate data measured in laboratory experiments can be used to predict PCDD/F formation levels in combustors under some circumstances. If the variations of PCDD/F formation rates with temperature can also be considered in the model, an analysis of the influence of the temperature profile in the cooling section on PCDD/Fs should be possible. In real municipal waste incinerators the geometry and flow patterns in the boiler and air pollution control devices are much more complex, so greater efforts are needed to develop mathematical models for process analysis and optimization purposes.

References

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