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Modeling Aerosol Rainout

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ABSTRACT

The AIChE Center for Chemical Process Safety has coordinated research efforts aimed at characterizing and predicting the behavior of aerosols during accidental releases. Field tests designed to be used for validation of a predictive model (RELEASE) showed that aerosol rainout was a significant factor under the test conditions. In addition to summarizing the RELEASE model and the data from the field test, Woodward and Johnson (1999) corrected the measured aerosol rainout to account for the experimental conditions; their corrections rely on an initial estimate of the jet velocity that is not limited by choked flow conditions (sonic velocity). This paper discusses the jet expansion zone and considers how other models of the jet expansion zone influence the predicted aerosol rainout of the RELEASE model.

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The AIChE Center for Chemical Process Safety has coordinated research efforts aimed at characterizing and predicting the behavior of aerosols during accidental releases. Field tests designed to be used for validation of a predictive model (RELEASE) showed that aerosol rainout was a significant factor under the test conditions. In addition to summarizing the RELEASE model and the data from the field test, Woodward and Johnson (1999) corrected the measured aerosol rainout to account for the experimental conditions. Woodward and Johnson also calculated initial aerosol drop diameters which model predictions showed would be consistent with the corrected rainout estimates; their model predictions rely on an initial estimate of the jet velocity that fails to satisfy energy balance constraints. This paper discusses the jet expansion zone and considers how a different model of the jet expansion zone influences the predicted aerosol rainout of the RELEASE model.

BACKGROUND

Woodward and Johnson (1999) summarize the Center for Chemical Process Safety (CCPS) program to experimentally verify the RELEASE model originally developed by CREARE. Experimental programs were undertaken to measure the rainout for superheated releases of water and CFC-11 in the Oklahoma experimental program and chlorine, methylamine, and cyclohexane in the Nevada experimental program. In all of the data sets, evidence indicated that the liquid (rainout) capture system did not collect all of the rained out material. Results from some of the experiments were treated as unreliable, but various procedures were also developed to correct the rainout data to obtain the best estimate of the amount of material not carried downwind. In the water data set, temperature measurements of the rained out liquid showed that the liquid was at the ambient dew point indicating that droplet evaporation (mass transfer) had been limited by saturation conditions. This saturation limitation seems to be important because the rainout in the water experiments was significantly higher than that observed in the other data sets even after correction for ineffective liquid capture systems. Furthermore, this difference indicates that the other data sets showed that droplet evaporation may significantly influence rainout. Although the original version of RELEASE does not account for droplet evaporation, Johnson (1999) suggests an empirical approach to account for this mass transfer effect in RELEASE based on fitting model predictions to corrected rainout data (excluding the water data set); this version of RELEASE was not used herein.

In addition to difficulties with the experimental data, Woodward and Johnson also corrected the RELEASE model to properly determine the condensed phase mass. In order to compare experimental data, Woodward and Johnson used the Unified Dispersion Model (UDM) to get consistent drop size diameters from corrected rainout data because the UDM independently predicts rainout and droplet evaporation. Both RELEASE and UDM use the same procedure for estimating the velocity in the developing (depressurizing) jet.

MODELING THE JET EXPANSION (DEPRESSURIZATION) ZONE

Consider the diagram of the jet expansion zone shown in Figure 1. Plane 1 is assumed to be located where the pressure is the liquid storage pressure, and no vapor has yet formed (the fluid is liquid only); all of the test programs were designed to meet this condition. Plane 2 is assumed to be located where the pressure of the released fluid has just dropped to ambient pressure. The jet velocity at the end of the expansion zone, u_2, is modeled in RELEASE and the UDM as

$$u_2 = u_1 + \frac{\left(P_1 - P_a\right)}{G_1} \tag{1}$$

where G_1 is the mass flux at plane 1, u and P are the x-direction velocity and pressure at their respective locations, and P_2 is at ambient pressure (P_a). Note that air entrainment is considered

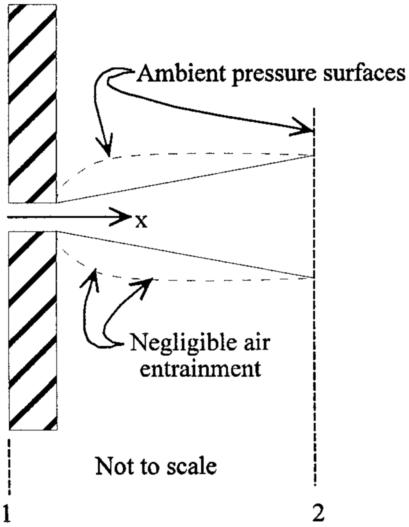


Figure 1. Schematic diagram of jet expansion (depressurization) zone

negligible in this zone, and all velocity profiles are assumed to be flat. Equation (1) is based on an x-direction momentum balance where the net force on the system is taken to be zero:

$$0 = mu_1 - mu_2 + P_1 A_1 + P_a(A_2 - A_1) - P_a A_2 \tag{2}$$

where m is the mass release rate. Such a momentum balance should apply for an incompressible fluid (so that no vapor is present at plane 2, depressurization occurs without vaporization, and the liquid phase is assumed to be incompressible) as well as for a fluid that vaporizes (flashes) between planes 1 and 2.

Consider now a mechanical energy balance between planes 1 and 2 for an incompressible fluid of density ρ:

$$\frac{1}{2}u_2^2 - \frac{1}{2}u_1^2 + \frac{1}{\rho}(P_a - P_1) + E_v = 0 \tag{3}$$

where E_v represents expansion losses; substituting Equation (1) into Equation (3) gives:

$$E_v = -\frac{1}{2}\left(\frac{P_1 - P_a}{G_1}\right)^2 < 0 \tag{4}$$

Since $E_v < 0$, Equation (1) violates energy balance constraints.

The x-direction momentum balance must be rewritten to include the force acting at plane 1 so that the balance becomes:

$$(P_1 - P_a)A_1 = mu_1 - mu_2 + P_1 A_1 + P_a(A_2 - A_1) - P_a A_2 \tag{5}$$

and therefore,

$$u_1 = u_2 \tag{6}$$

The left hand side of Equation (5) is the force that would propel a standard gas cylinder in the event the top valve is sheared off or the force that had to be accounted for in the design of the release apparatus used in the CCPS tests. Substituting Equation (6) into Equation (3) shows that $E_v = (P_1 - P_a)/\rho > 0$ for an incompressible fluid, and therefore, Equation (6) is consistent with energy balance constraints. This revised estimate of the expansion velocity is important, because it is used to calculate the (average) maximum drop size limited by aerodynamic breakup, d_{ave} using a Weber number criteria:

$$We = \frac{\rho_V d_{ave} u_2^2}{\sigma_L} \tag{7}$$

where ρ_V is the vapor phase density and σ_L is the liquid phase surface tension; RELEASE takes the critical Weber number to be 12. When comparing Equations (1) and (6), the differences in calculated parameters will be largest for the largest process pressure P_1; Table 1 summarizes the maximum difference in u_2 and d_{ave} for the test programs.

TABLE 1. COMPARISON OF MODELS FOR EXPANSION ZONE VELOCITY BASED ON MAXIMUM RELEASE PRESSURE

Test Program	u_2 from Equation (1) (m/s)	u_2 from Equation (6) (m/s)	$\frac{(u_2)_{EQN(6)}}{(u_2)_{EQN(1)}}$	$\frac{(d_{ave})_{EQN(6)}}{(d_{ave})_{EQN(1)}}$
water	96.2	35.7	0.37	7.2
CFC-11	37.6	16.0	0.43	5.5
chlorine	40.6	18.9	0.47	4.6
methylamine	42.2	19.6	0.47	4.6
cyclohexane	42.7	20.0	0.47	4.5

Equation (6) also agrees with experimental observations reported by Energy Analysts (1990): "Several water runs were made at 455°K (360°F) to determine the effects of increasing the liquid storage overpressure. ... The liquid capture results for these runs varied among themselves less than the standard deviation for the analyzed water data set (2.1 capture percent). For this series of runs, no effect of pressure on the liquid capture was found." RELEASE calculations are more sensitive to overpressure effects when Equation (1) is used to determine u_2.

Finally, note that the momentum balance in Equation (5) also applies when vaporization begins before depressurization is complete. Equation (6) shows that the kinetic energy terms cancel, and the energy balance becomes:

$$m\left(H_{L,1} - \left[(1 - \varphi)H_{L,2} + \varphi H_{V,2}\right)\right] + E_v = 0 \tag{8}$$

where φ is the flash fraction, $H_{L,1}$ and $H_{L,2}$ are the liquid-phase enthalpies at planes 1 and 2, respectively, and $H_{V,2}$ is the vapor-phase enthalpy at plane 2. Note that all properties are those of the released contaminant; air entrainment is neglected in this zone. Since E_v is typically taken to be zero here, the expansion is isenthalpic (but not reversible) as long as the vapor and liquid are in equilibrium at ambient pressure.

INFLUENCE ON RELEASE MODEL ESTIMATES

The RELEASE routine EXPAND.f was modified to set $u_1 = u_2$. (In addition to this change, a minor bug was found in EXPAND.f; the variable MDOTGO was misspelled as MODTGO, but this correction did not significantly affect calculations.)

Figure 2 compares RELEASE calculations based on the corrections of Woodward and Johnson and RELEASE calculations as proposed here with the normalized, corrected rainout data for the CFC-11, chlorine, methylamine (MMA), and cyclohexane tests. The RELEASE calculations are all straight lines indicating that (essentially) all (unflashed) liquid rains out (or, flash fraction plus rainout fraction equals 1). Note that in all of these data sets, it has been proposed that droplet evaporation could significantly reduce rainout by decreasing the droplet diameter during the evaporation process. Since RELEASE does not account for droplet evaporation, the RELEASE predictions should show greater rainout than observed, and with the approach discussed herein, the RELEASE calculations bound above the normalized rainout unless it is greater than 100%. The nucleation site density N_d recommended by CREARE was 10^{10} sites/m^3 (with a range from 10^6 to 10^{10} sites/m^3); for all of the cases in Figure 2, the RELEASE predictions were insensitive to the choice of N_d over the range of 10^6 to 10^{10} sites/m^3. This insensitivity to N_d is to be expected since all of the liquid phase is predicted to rain out.

Figure 3 compares RELEASE calculations as proposed here with the normalized, corrected rainout data for water. The RELEASE model predicts that all of the liquid phase rains out below about 440 K. As discussed above, the water data were taken under conditions that limited the importance of droplet evaporation. Since droplet evaporation was not considered in the original RELEASE code, the water test rainout data offer the best opportunity to assess the mechanisms that are included in RELEASE. As shown in Figure 3, the RELEASE calculations are sensitive to the choice of N_d above about 440 K; as expected, increasing N_d decreases the rainout. The lines for the RELEASE predictions are not smooth because the points used to make the calculations reflect different liquid orifice pressures. As discussed above, the water test program was designed to determine the effect of liquid orifice pressure on the rainout. As indicated in the figure, the RELEASE predictions are more sensitive to liquid orifice pressure than is supported by the data.

CONCLUSIONS

This paper has considered the jet expansion zone and how a different model of the jet expansion zone influences the predicted aerosol rainout of the RELEASE model. We conclude the following:

- At a vessel opening, the velocity of the decompressed fluid is (approximately) equal to the velocity of the liquid at process pressure if vaporization within the vessel is

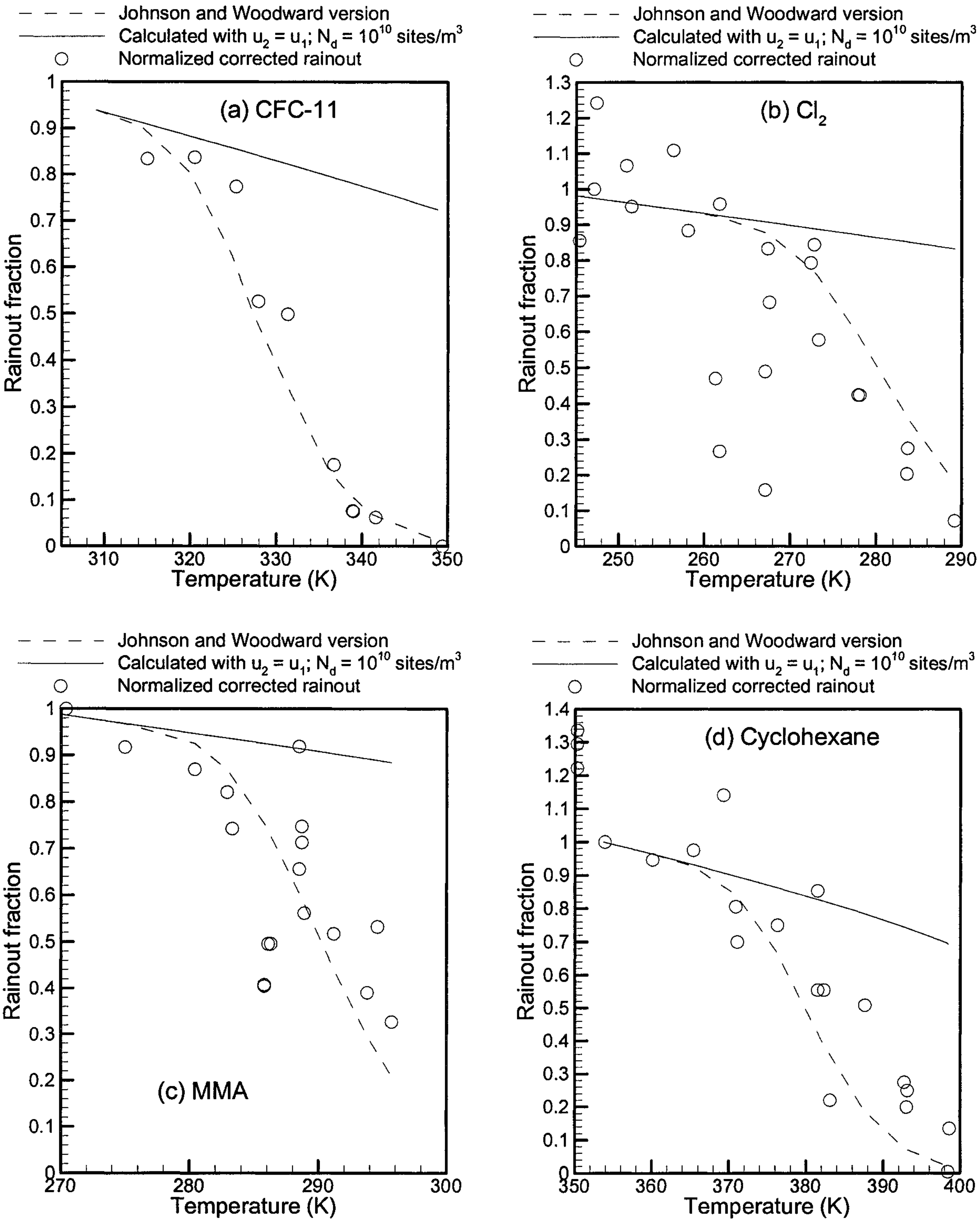
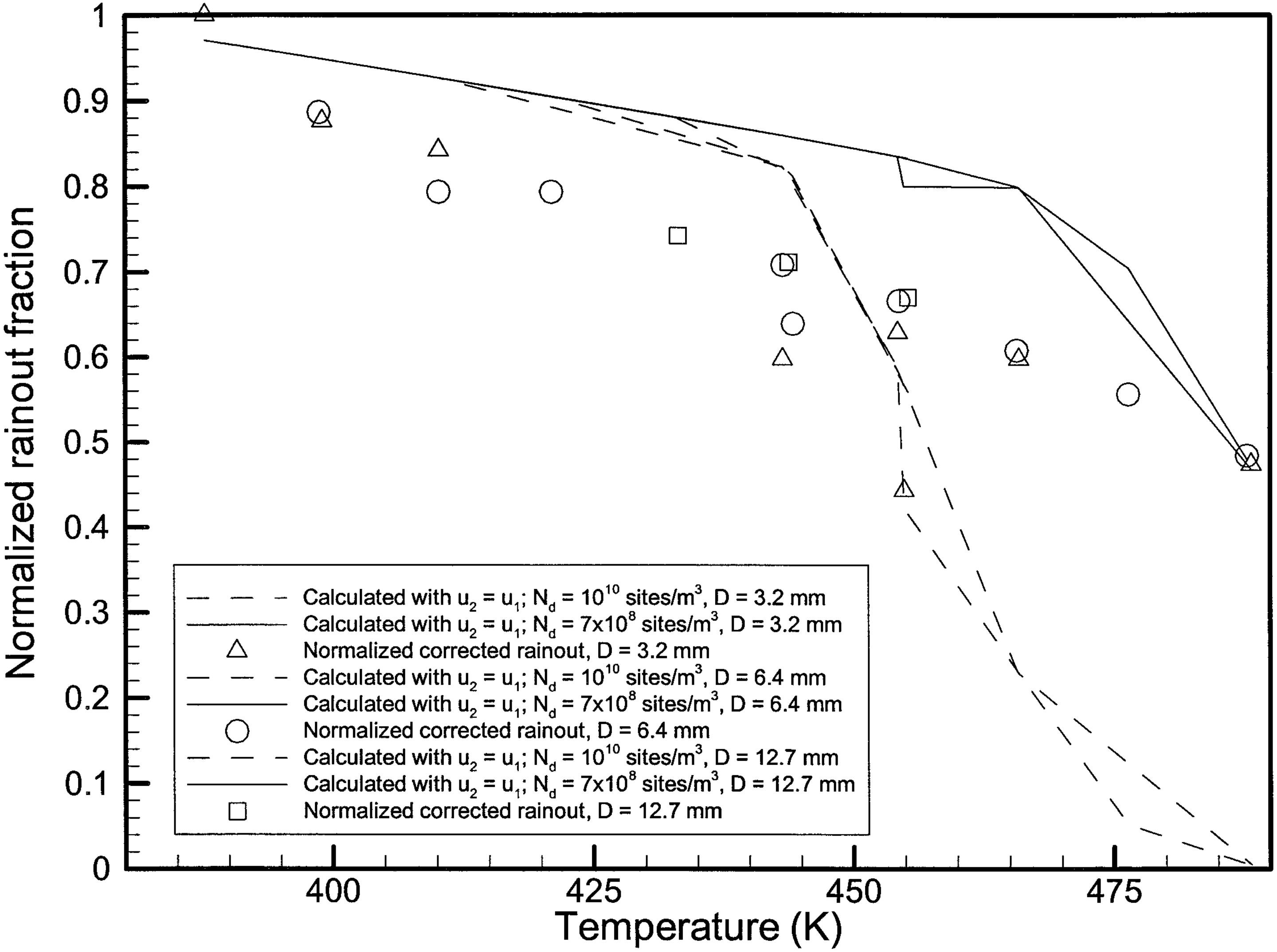


Figure 2. Comparison of RELEASE model predictions with normalized rainout data

Figure 3. Comparison of RELEASE model predictions with normalized rainout data for water test program



insignificant. Furthermore, if the liquid flashes during depressurization, the flashing process is essentially isenthalpic.

- Droplet evaporation significantly reduces rainout. When droplet evaporation is significant, RELEASE predictions bound above corrected, normalized observations of rainout (provided the maximum rainout is 100%).

- When droplet evaporation is less significant, RELEASE model predictions as described herein generally agree with observations of rainout in the water tests. For the water test data, the RELEASE model predictions are sensitive to the specification of the nucleation site density N_d.

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