**Short description of the B&M and Gaussian model approaches to the JR III MWG model comparison exercise using three Desert Tortoise trials and three FLADIS trials**

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**1. Britter and McQuaid (B&M) model overview**

The Britter and McQuaid (B&M, 1988) Workbook for Dense Gas Modeling uses principles of basic physics and thermodynamics to develop simplified nomograms for calculating dense gas dispersion, involving dimensionless combinations of the fundamental variables and parameters. There is one nomogram for instantaneous releases, and another for continuous releases. The major output from the nomograms is the maximum dimensionless plume centerline concentration, C/Co, as a function of downwind distance, x. Co is the concentration in the initial cloud. The B&M nomograms were applied to three Desert Tortoise ammonia release trials (1, 2, and 4) and three FLADIS ammonia release trials (9, 16, and 24), which are being used for a current multi-model comparison. The exercise is being led by the JR III Modeling Working group (MWG). The B&M model can be considered as a baseline against which other, more sophisticated models, could be compared.

The B&M model is valid for distances beyond the point, xo, where all of the TIC aerosol has evaporated, using heat provided by the entrained ambient air. The xo values listed by Chang and Gant (2021, 2022) were used for our MWG study. For comparison, the B&M handbook has a simple basic thermodynamics method to calculate the volume and initial density (at xo) of a cloud released as a two-phase pure mixture. These B&M – calculated parameters were within 10 or 20% of those produced by the Chang and Gant methodology.

Separate nomograms for continuous plume and for instantaneous puff releases are presented in the B&M 1988 Workbook. For Desert Tortoise (DT), the continuous plume nomogram was used because the release duration exceeded the travel time to the most distant sampling arc (at x = 800 m). For FLADIS the release duration greatly exceeded (by more than an order of magnitude) the travel time, so our initial B&M model applications to the FLADIS data also used the continuous plume B&M nomogram.

As explained in section 3, since the critical Richardson number, Ric, was not exceeded for the FLADIS field experiment trials, the B&M nomograms were not appropriate and, instead, a Gaussian plume model (see section 2), valid for passive neutral gases, was used for the FLADIS trials.

The B&M nomogram for continuous plumes contains curves (for C/Co = 0.002, 0.005, 0.01, 0.02, 0.05, and 0.1) that are based on observations from several field and laboratory experiments. B&M state that the curves are valid only for the ranges of cloud stability and downwind distance that encompass the available experiments. The relative concentrations curve at the small distance limit represents C/Co = 0.1. For the three DT trials, this curve passes through normalized downwind distances varying from about 30 to 65 x/Di, where Di is a distance scale that depends on cloud excess density, volume flux, and wind speed. For smaller x/Di, Hanna, Chang and Strimaitis (1993) suggested an interpolation formula for C/Co that was based on B&M’s asymptotic formula and matched the B&M curve at about x/Di of 30. In reality, though, depending on the cloud stability parameter (go’2qo)0.2/U used as the abscissa of the B&M nomogram, the C/Co = 0.1 curve starts out at about x/Di = 55 at the passive limit, increases to a maximum of about x/Di = 65, and then decreases monotonically to values of about x/Di = 30 at the most stable edge of the nomogram domain. The key parameters go’, qo, and U are defined below.

g’o = g(ρpo – ρa)/ρa (m/s2) (1)

where g is the acceleration of gravity (9.8 m/s2), ρpo is initial plume density (at position xo) and ρa is ambient air density. In addition, qo is the continuous volume flow rate (m3/s) at position xo, and U is mean wind speed (at z = 10 m),

To produce the current B&M model predictions, and trying to account for the curvature of the C/Co = 0.1 line in the nomogram, the Hanna et al (1993) interpolation formula was used, but its “constant” was adjusted to agree with the B&M nomogram C/Co = 0.1 curve for each DT trial, at the nomogram abscissa value for that trial (go’2qo)0.2/U. Thus, the interpolation formulas used for the three DT trials (1, 2, and 4) are.

DT1 (for which (go’2qo)0.2/U = 0.8) C/Co = 513(x/Di)2/(1 + 513(x/Di)2) (2)

DT2 (for which (go’2qo)0.2/U = 1.0) C/Co = 427(x/Di)2/(1 + 427(x/Di)2) (3)

DT4 (for which (go’2qo)0.2/U = 1.2) C/Co = 400(x/Di)2/(1 + 400(x/Di)2) (4)

The above interpolation formulas are used for small normalized distances x/Di where C/Co > 0.1, and the B&M nomogram is used for larger normalized distances where C/Co < 0.1. Note that, at small x, C/Co approaches 1.0 (i.e., C approaches Co)

For the three DT trials, the B&M equation on p 43 of the Workbook is used for the growth of cloud width W, accounting for the fact that the initial width is Wo at the point, xo, where all liquid has evaporated. B&M define a scaling length, lb, as go’qo/U3. Then the total W is:

W = Wo + 2.5lb1/3x2/3 (4)

To convert from W to σy, the identity σy = W/(12)1/2 = 0289W is used, which is valid for a top-hat concentration distribution (i.e., constant C across the plume width W)

**2. Gaussian plume model overview**

For a ground level source, with the receptor also at ground level, the Gaussian plume model states that the plume centerline concentration, C, is:

C/qou = 1/(πσyσz) (5)

where σy = σyo + σyt and σz = σzo+ σzt. It is assumed that σyo = σzo are the initial values (at a downwind distance of 4 or 5 m for the FLADIS trials) as provided by Chang and Gant in their guidance documents. Since they provided the “cloud width W and depth H”, here, the standard assumption is made that σy = 0.289W.

Subscript t in the σy andσz definitions refers to the turbulent dispersion coefficient, which is calculated at a distance of x-xo. For FLADIS, Briggs’ simple analytical formulas for σyt and σzt for rural class D conditions are used (Hanna et al., 1982). The total σy and σy are:

σy = σyo+ 0.08(x-xo) (6)

σz = σzo + 0.06(x-xo)/(1+0.0015(x-xo))1/2 (7)

**3. Deviations from the prescribed model input conditions**

The MWG provided descriptions of various model inputs that all modelers were to use. A 22 page document was distributed in December 2021 (Chang and Gant, 2021) and updated on 30 March 2022. Chang and Gant provided additional guidance in email messages dated 12 and 26 January 2022 and 30 March 2022.

Joseph Chang provided, on 23 February 2022, calculations of ambient air density for each of the six trials.

Simon Gant sent an email message on 27 February, confirming that the total release mass equaled the given mass emission rate times the given release duration.

The B&M model was initially applied to all six DT and FLADIS release trials. However, the initial relative density flux for the FLADIS trials was much smaller than that for the DT trials. This is because the mass release rate in FLADIS was about a factor of 200 less than that at DT. The critical Richardson number, Rc, was calculated using the formula in the B&M Workbook for continuous sources:

Ric = (go’qo)/(LU3), (8)

L is the initial cloud distance scale at distance xo. The B&M Workbook states that the cloud is behaving as a dense cloud if Ric > 0.15.

For DT and FLADIS, it was assumed that L was the cloud width W. The initial (at distance xo) cloud densities and sizes were as prescribed by the MWG. For DT, average values were go’ = 4 m/s2, W = 25 m, U = 6 m/s and qo = 800 m3/s. For FLADIS, go’ = 4 m/s2, W = 0.8 m, U = 5 m/s and qo = 3 m3/s. It is calculated that Ric = 0.6 for DT and 0.12 for FLADIS. This suggests that the DT release plume can be considered to be behaving as a dense cloud, while the FLADIS release plume is behaving as a passive (neutral density) cloud.

So, for the FLADIS simulations, a simple Gaussian continuous plume model for neutral density clouds was used, as described in section 2. The calculated concentration, C, is at the plume centerline.

All predicted C’s are vapor concentrations, since it is assumed that all aerosols have evaporated by distance x­o.

**4. Deviations from prescribed model outputs**

In the revised predictions dated 1 April, B&M model calculations of concentration and cloud width W were made at 10 locations within the requested distance range from 50 to 1000 m. The distances used were 50, 100, 200, 300, 400, 500, 600, 700, 800, and 1000 m.

Gaussian model calculations of concentration and σy were made at 10 locations within the requested distance range from 10 to 250 m. The distances used were 10, 20, 30, 50, 70, 100, 150, 200, 240, and 250 m.

**References**

Britter, R.E., McQuaid, J., 1988. Workbook on the Dispersion of Dense Gases. HSE Contract report No 17/1988. UK Health and Safety Executive, 160 pp.

Chang, J.C., Gant, S.E., 2021. JRIII Modelers Working Group Initial Modeling Exercise (version 2.3 21 Dec 2021), 22 pp.

Hanna, S.R., 2020. Britter and McQuaid 1988 Workbook nomograms for dense gas modeling applied to the Jack Rabbit II chlorine release trials. *Atmos. Environ.* 232, <https://doi.org/10.1016/j.atmosenv.2020.117539>

Hanna, S.R., G.A. Briggs and R.P. Hosker, 1982. *Handbook on Atmospheric Diffusion*. DOE/TIC‑11223, Department of Energy, 102 pp.

Hanna, S.R., Chang, J.C, Strimaitis, D.G., 1993. Hazardous gas model evaluation with field observations. *Atmos. Environ.* 27A: 2265-2285.

Hanna, S.R., Strimaitis, D.G., Chang, J.C., 1991. Evaluation of 14 hazardous gas models with ammonia and hydrogen fluoride field data. *J. Haz. Mat.* 26: 127-158.