DAHLGREN DIVISION
NAVAL SURFACE WARFARE CENTER
Dahlgren, Virginia 22448-5100

NSWCDD/TR-14/489

MODEL VALIDATION AGAINST THE MODELERS' DATA ARCHIVE

BY DAVID A. BAKER
TIMOTHY J. BAUER

ASYMMETRIC SYSTEMS DEPARTMENT

AUGUST 2014

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
	August 2014	Final

4. TITLE AND SUBTITLE

MODEL VALIDATION AGAINST THE MODELERS' DATA ARCHIVE

5. FUNDING NUMBERS

6. AUTHOR(s)

David A. Baker and Timothy J. Bauer

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

Naval Surface Warfare Center, Dahlgren Division
CBR Analysis, Testing, and Systems Engineering Branch (Code Z24)
4045 Higley Road, Suite 344
Dahlgren, VA 22448-5162

8. PERFORMING ORGANIZATION REPORT NUMBER

NSWCDD/TR-14/489

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION/AVAILABILITY STATEMENT

DISTRIBUTION STATEMENT A – Approved for public release; distribution is unlimited.

12b. DISTRIBUTION CODE

13. ABSTRACT (Maximum 200 words)

The Modelers' Data Archive (MDA) was used to validate the RAILCAR toxic industrial chemical (TIC) source characterization model and the Vapor, Liquid, and Solid Tracking (VLSTRACK) atmospheric transport and dispersion (ATD) model for dense gas releases. The source term predictions from RAILCAR were compared to the field trial descriptions in the MDA report. The RAILCAR source parameters were input into VLSTRACK, and the downwind plume results were statistically compared to the MDA data. The RAILCAR-VLSTRACK model proves to be a viable model for the release of TICs into the environment, although the bias and accuracy were not as good as some other ATD models. VLSTRACK was designed to simulate an attack, whereas the field trials in the MDA were highly controlled releases mostly leading to large area vapor sources. The greatest source of error is likely due to the inability of VLSTRACK to simulate an area vapor source. RAILCAR is being integrated into two other ATD models as part of this project, and validation results are expected to show significant improvement.

14. SUBJECT TERMS	15. NUMBER OF PAGES
toxic industrial chemical, RAILCAR program, VLSTRACK program, Modelers' Data Archive, atmospheric transport and dispersion	70
	16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORTS	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UL

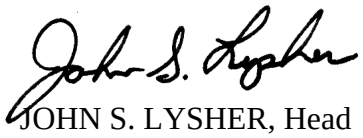
FOREWORD

This paper describes the use of the Modelers' Data Archive (MDA) to validate the RAILCAR toxic industrial chemical (TIC) source characterization model and the Vapor, Liquid, and Solid Tracking (VLSTRACK) atmospheric transport and dispersion (ATD) model for dense gas releases. The source term predictions from RAILCAR were compared to the field trial descriptions in the MDA report. The RAILCAR source parameters were input into VLSTRACK, and the downwind plume results were statistically compared to the MDA data.

The RAILCAR-VLSTRACK model proves to be a viable model for the release of TICs into the environment, although the bias and accuracy were not as good as some other ATD models. VLSTRACK was designed to simulate an attack, whereas the field trials in the MDA were highly controlled releases mostly leading to large-area vapor sources. The greatest source of error is likely due to the inability of VLSTRACK to simulate an area vapor source. RAILCAR is being integrated into two ATD models designed to simulate area vapor sources. This validation effort will be repeated with those coupled models, and the statistical results are expected to be better than those documented here.

This report has been reviewed by Gaurang R. Davë, Head, CBR Analysis, Testing, and Systems Engineering Branch (Code Z24), and Michael Pompeii, Acting Head, CBR Defense Division.

Approved by:



JOHN S. LYSHER, Head
Asymmetric Systems Department

CONTENTS

CONTENTS (Continued)

ILLUSTRATIONS

TABLES

GLOSSARY

ATD	Atmospheric Transport and Dispersion
CBR	Chemical/Biological/Radiological
DHS	Department of Homeland Security
DoD	Department of Defense
DOT	Department of Transportation
GUI	Graphical User Interface
HF	Hydrogen Fluoride
LNG	Liquefied Natural Gas
LPG	Liquefied Propane Gas
MDA	Modelers' Data Archive
NSWCDD	Naval Surface Warfare Center, Dahlgren Division
TIC	Toxic Industrial Chemical
TIM	Toxic Industrial Material
TSA	Transportation Security Administration
VLSTRACK	(Chemical and Biological Agent) Vapor, Liquid, and Solid Tracking

1.0 INTRODUCTION

Current fiscal year 2014 (FY14) Transportation Security Administration (TSA) tasking includes validating the toxic industrial chemical (TIC) source and atmospheric transport and dispersion (ATD) models developed and used for this project against existing field trial data, pending completion of the planned Jack Rabbit 2 field trials. The relevant task for the effort addressed here is Task 4 of the current Interagency Agreement, as detailed below.

> Task 4. Validate the Coupled RAILCAR-ATD Models
> Although additional field trials forming mist pools or stationary clouds would be preferable for RAILCAR validation, such data will not be available until at least FY16. In the meantime, there is a need to do some validation of RAILCAR and also to validate its operation with ATD models. A database of dense gas field trials that has been used to validate ATD models exists; current models developed to simulate releases of chemicals forming dense gases include DEGADIS, HGSYSTEM, PHAST, TRACE, SLAB, ALOHA, and SCIPUFF. The Modelers' Data Archive (MDA) was developed specifically for use by modelers in validating their models and participating in model comparisons. The data associated with six sets of field trials have been extracted and converted into model input and output parameters. The MDA is hosted by the George Mason University data archives and contains data from the following field trials: Desert Tortoise – NH_3 jets; Goldfish – HF jets; Burro – liquefied natural gas (LNG) area sources; Coyote – LNG area sources; Maplin Sands – LNG area sources; and Thorney Island – Freon instantaneous releases. This task will use RAILCAR to simulate each source and provide inputs to the ALOHA, QUIC, and VLSTRACK models. Reasonable agreement with downwind concentration data will thus validate the coupled RAILCAR-ATD modeling capabilities.
>
> RAILCAR also includes methodology to define the source for TICs not stored as pressurized liquids. These TICs range from chemicals like hydrogen cyanide, having boiling temperatures close to ambient, to low volatility chemicals such as sulfuric acid. A limited number of field trials have been conducted involving large releases of some of these TICs. An archive of such data does not exist, but subject matter experts, who have previously supported and are currently supporting Department of Homeland Security (DHS), can help locate relevant field trial reports. This task will include using the coupled RAILCAR-ATD models to simulate these field trials as well as the dense gas ones listed above. This task will begin as soon as the RAILCAR-ALOHA and RAILCAR-QUIC integration tasks are completed.

This paper describes the use of the MDA to validate the RAILCAR[1] TIC source characterization model and the Vapor, Liquid, and Solid Tracking (VLSTRACK)[2] ATD model

for dense gas releases. The source term predictions from RAILCAR will be compared to the field trial descriptions in the MDA report:[3]

> S. R. Hanna, D. G. Strimaitis, and J. C. Chang, *Hazard Response Modeling Uncertainty (A Quantitative Method), Volume II, Evaluation of Commonly Used Hazardous Gas Dispersion Models*, Sigma Research Corporation, Westford, MA, September 1991.

The RAILCAR source parameters will be input into VLSTRACK, and the downwind plume results will be statistically compared to the MDA data. When this effort proceeds to validate RAILCAR-ALOHA and RAILCAR-QUIC, the RAILCAR source terms will be passed directly to the respective ATD model.

1.1 Modelers' Data Archive

The MDA includes reduced data from six dense gas field trial campaigns:

1) Burro: Eight trials; 1- to 3-min releases of liquefied natural gas (LNG, ~90% methane) forming a boiling liquid pool on a water surface. Molecular weight and liquid density are adjusted for the LNG composition.

2) Coyote: Three trials; 1- to 1.5-min releases of LNG (~90% methane) forming a boiling liquid pool on a water surface. Molecular weight and liquid density are adjusted for the LNG composition.

3) Desert Tortoise: Four trials; 2- to 6-min releases of pressurized liquid anhydrous ammonia from a horizontal pipe oriented in the downwind direction forming a two-phase plume.

4) Goldfish: Three trials; 2- to 6-min releases of pressurized liquid hydrogen fluoride from a horizontal pipe oriented in the downwind direction forming a two-phase plume.

5) Maplin Sands: a) Four trials; 1.5- to 4-min releases of LNG (~90% methane) forming a boiling liquid pool on a water surface. Molecular weight and liquid density are adjusted for the LNG composition. b) Eight trials; 1.5- to 6-min releases of liquefied propane gas (LPG) forming a boiling liquid pool on a water surface. Molecular weight and liquid density are adjusted for the LPG composition.

6) Thorney Island: a) Two trials; 7- to 8-min Freon-12 (dichlorodifluoromethane) in nitrogen (32% by volume) releases from a ground area source forming a vapor plume. b) Nine trials; instantaneous Freon-12 in nitrogen mixture releases at ground level forming a vapor puff. Molecular weight is adjusted for Freon-12 volume fraction.

The source for each release has been defined in terms of type of release, phase, temperature, height, mass, duration, and diameter. When relevant, release pressure or concentration is provided. Physical properties for the chemical are provided; molecular weight, liquid density, and concentration are also provided for the mixtures where relevant. Environmental conditions include date and time, geographic location, surface pressure and

temperature, relative humidity, wind speed (at 2-m height), ground temperature, surface roughness length, friction velocity, inverse Monin-Obukhov length, cloud cover, and Pasquill stability category (plus a few additional parameters not needed for this effort). Measurement locations are represented by downwind distance and height. Field trial results have been converted to peak concentration and averaging time, maximum concentration and averaging time, and lateral sigma for maximum concentration at each downwind distance.

The MDA also includes reduced data from two neutrally buoyant particle and gas field trial campaigns:

7) Hanford: a) Five trials; 15- to 20-min Krypton-85 tracer releases from a horizontal pipe oriented in the downwind direction forming a particle plume. b) Six trials; instantaneous Krypton-85 tracer releases at ground level forming a particle puff.

8) Prairie Grass: Forty-four trials; 10-min releases of sulfur dioxide from a horizontal pipe oriented in the downwind direction forming a vapor plume.

The same set of parameters is provided for these field trials as for the dense gas field trials.

For the six dense gas field trial campaigns, RAILCAR will be set up to match the defined release conditions. The resulting area vapor flux or horizontal vapor jet source terms will then be converted into VLSTRACK input parameters. For the two neutrally buoyant particle/gas field trial campaigns, the MDA source terms will be converted to VLSTRACK input parameters without executing RAILCAR.

1.2 RAILCAR Parameter File Records

The Toxic Industrial Chemical (TIC) thermodynamic property file, RAILCAR.PAR, contains all of the physical properties (obtained from reputable literature sources or estimated from the best literature equations) for each chemical addressed by RAILCAR. The records for each TIC consist of the following:

Line	Parameter(s)
1	character string for the TIC name (25-character limit)
2	freezing temperature (°C)
	critical temperature (°C)
3	molecular weight (g/mole)
	liquid viscosity at 20 °C (cp)
	liquid heat capacity (specific heat) at boiling temperature (kJ/kg-K)
	vapor heat capacity (specific heat) at boiling temperature (kJ/kg-K)
	liquid surface tension at boiling temperature (dynes/cm)
	vapor diffusivity at 20 °C (cm^2/s)
4	liquid density at boiling temperature (kg/m^3)
	liquid density rate of change with temperature (kg/m^3-K)
5	Antoine constants A, B, and C for temperature in °C and pressure in atmospheres
6	heat of vaporization at boiling temperature (kJ/kg)
	heat of vaporization rate of change with temperature (kJ/kg-K)

RAILCAR.PAR did not include entries for LNG, LPG, or Freon-12, so physical properties for each of these chemicals were obtained from the National Institute of Standards and Technology website or MDA field trial summaries. Liquid density and heat of vaporization are assumed constant with temperature, and values for liquid viscosity, liquid surface tension, and vapor diffusivity are from TICs having similar molecular weights (ammonia for methane, nitrogen dioxide for propane, and fluorotrichloromethane for Freon-12). The RAILCAR entries relevant to the MDA dense gas field trials are:

```
ammonia
 -78.20   132.40
 17.03    0.14 4.44 2.29 26.4 0.153
 681.0    -1.232
 4.8689   1113.93   262.741
 1372.00  -2.890
Freon-12
 -157.95  96.85
 120.91   0.42 0.97 0.61 18.4 0.058
 1520.0   0.000
 3.8111   782.072   235.377
 165.00   0.000
hydrogen fluoride
 -83.20   188.00
 20.01    0.11 4.05 1.46 18.5 0.155
 1002.0   -2.700
 4.9148   1556.56   297.349
 1403.90  -3.000
methane (LNG)
 -182.55  -82.55
 16.04    0.14 3.35 2.24 26.4 0.153
 431.2    0.000
 3.9895   443.028   272.660
 511.90   0.000
propane (LPG)
 -187.65  96.75
 43.93    0.42 2.52 1.68 36.2 0.127
 500.9    0.000
 3.9829   819.296   248.733
 425.74   0.000
```

1.3 VLSTRACK Chemical/Biological Agent Parameter File Records

The chemical/biological agent parameter file, VLSAGN.PAR, contains all of the physical properties for each CBR material addressed by VLSTRACK. The records for each TIC consist of the following (in Figures 1 through 3):

```
Chemical/Biological Agent Definition:
 1 = agent name (12 characters)
 2 = agent abbreviation (3 characters)
 3 = agent type category
 4 = liquid density (g/cm3)
 5 = dissemination efficiency (%)
 6 = boiling temperature (°C)
 7 = ATP-45 NBC message agent term (4 characters)
```

Figure 1. First Line of a Chemical/Biological Agent Parameter Description

```
 Physical Properties:
 2 = volatility at 20 deg C (g/cm3)
 5 = heat of vaporization (cm2/s2 = cal/g*4.184e7)
```

Figure 2. Second Line of a Chemical/Biological Agent Parameter Description

```
Toxicity Values:
 1 = median lethal dosage (mg-min/m3)
 2 = lethal dosage probit slope
 3 = median severe incapacitation dosage (mg-min/m3)
 4 = severe incapacitation dosage probit slope
 5 = median threshold effects dosage (mg-min/m3)
 6 = threshold effects dosage probit slope
 7 = median lethal dose (mg)
 8 = lethal dose probit slope
 9 = median severe incapacitation dose (mg)
10 = severe incapacitation dose probit slope
```

Figure 3. Third Line of a Chemical/Biological Agent Parameter Description

VLSAGN.PAR did include entries for LNG, LPG, or Freon-12, so the physical properties defined for RAILCAR of each of these chemicals were adapted for the VLSTRACK parameters. Krypton-85 is a radioisotope released as a tracer material. It is characterized by its radiological activity rather than mass. For simulating a tracer release, the compound and mass are not important as long as the bulk behavior has no dense gas effects. For the VLSTRACK record, Krypton-85 is assigned the physical properties of hydrogen cyanide, since the molecular weight of that TIC is almost the same as that of air and will not contribute to any dense gas effects. For the VLSTRACK simulations associated with the MDA field trials, the release will be characterized as 100% vapor. Dense vapor effects associated with the molecular weight will be included in the ATD computations, but there will be no liquid phase or cooling from aerosol evaporation for any of the releases. Those processes are accounted for by RAILCAR in defining the vapor flux from the source area. The VLSTRACK entries relevant to the MDA field trials are the following:

```
'Methane(LNG)' 'LNG'   3      0.43    70.0    -162.0  '    '
         0.199                5.12e+009
10000.0 12.0  1000.0  12.0  100.0      5.0   10000.0  5.0   5000.0 5.0
'Ammonia     ' 'NH3'   3      0.61    70.0     -33.0  '    '
         0.0067               1.37e+010
139000. 17.0 17400.0  17.0 1560.0      5.0   10000.0  5.0   5000.0 5.0
'HF          ' 'HF '   3      1.00    70.0      20.0  '    '
         0.000911             1.40e+010
28600.0 12.0  4470.0  12.0  790.0      5.0   10000.0  5.0   5000.0 5.0
'Propane(LPG)' 'LPG'   3      0.50    70.0     -42.0  '    '
         0.016                4.26e+009
10000.0 12.0  1000.0  12.0  100.0      5.0   10000.0  5.0   5000.0 5.0
'Freon-12    ' 'F12'   3      1.52    70.0     -30.0  '    '
         0.028                1.65e+009
10000.0 12.0  1000.0  12.0  100.0      5.0   10000.0  5.0   5000.0 5.0
'Krypton-85  ' 'K85'   3      0.70    70.0      26.0  '    '
         0.000982             5.46e+009
10000.0 12.0  1000.0  12.0  100.0      5.0   10000.0  5.0   5000.0 5.0
'SO2         ' 'SO2'   3      1.38    70.0     -10.0  '    '
         0.0093               3.89e+009
40400.0 12.0  6190.0  12.0   20.0      5.0   10000.0  5.0   5000.0 5.0
```

Since output will not be in terms of percent toxicity, generic values have been assigned to LNG, LPG, Freon-12, and Krypton-85 for the entries in the third line of those records.

2.0 FIELD TRIAL SIMULATIONS

As stated above, for validating RAILCAR and VLSTRACK against each of the six dense gas field trials, the source was first simulated by RAILCAR. Then, transportation and dispersion were simulated by VLSTRACK. The two neutrally buoyant gases were modeled by VLSTRACK alone. Because every trial had unique settings and characteristics, the approach was slightly different for each one. This section will detail how each type of field trial was modeled.

2.1 RAILCAR Input Parameters

For each dense gas field trial, each parameter in the RAILCAR input file, RAILCALC.DAT, must be defined according to either a value from the MDA or a recommended value. Recommended values are defined in the *RAILCAR 4.1 Software User's Manual*, and the most appropriate values for the type of release are selected. Although the MDA includes records for all of the environmental parameters contained in RAILCALC.DAT, all values are not always provided. METPROPS is a program created to use the available MDA values to compute the remaining values. METPROPS uses VLSTRACK atmospheric methodology; environmental parameters computed using METPROPS are then consistent with those computed by VLSTRACK. There are four combinations of environmental parameters that can be entered into METPROPS:

```
1 = friction velocity and 2-m wind speed
2 = friction velocity, 10-m wind speed, and surface type
3 = 2-m wind speed, surface type, and stability
4 = 10-m wind speed, surface type, and stability
```

File METPROPS.OUT is set up to generate the 2nd and 3rd last lines in RAILCALC.DAT, so it also asks the user for the entrainment factor and sheltering factor. The MDA does not always report soil temperature, so the third line in METPROPS.OUT provides ground temperature, again based on VLSTRACK methodology.

Since the RAILCAR input parameters for each dense gas trial are similar, they will only be outlined once. Any necessary modifications to the input parameters for specific trials will be noted in the specific trial section. The RAILCAR parameters – in the order in which they appear in the Graphical User Interface (GUI) and their source or recommended values – are as follows (MDA parameter titles are in [ ]):

- TIC name: name as it appears in RAILCAR.PAR (or as it appears in the dropdown list)
- mass input type: tank mass
- initial tank mass: [spill/evaporation rate (kg/s)]×[spill duration (s)] or [total released (kg)]
- remaining mass: 0

- tank temperature: [source temperature (K)] – 273.15
- tank pressure: 0 atm
- tank thickness input type: 0 = user input
- tank thickness: 0.005 m
- ullage volume fraction: 0.1
- calculate tank pressure: checked
- liquid head pressure: 0
- inert gas pressure: [exit pressure (atm)] – [TIC vapor pressure] or (0 for instantaneous releases; adjust to match spill/evaporation rate for refrigerated liquids)
- surface type: know roughness length
- surface roughness length: [roughness length z0 (m)]
- entrainment factor: enhanced for jets and pools, normal for instantaneous
- sheltering factor: 3
- air temperature: [ambient temperature #1-lower (K)] – 273.15
- ground temperature: [soil temperature (K)] – 273.15 (otherwise, from METPROPS)
- relative humidity: [relative humidity (%)]
- wind speed height: [measurement ht for domain-avg wind data (m)]
- wind speed: [domain-avg wind speed (m/s)]
- friction velocity: [friction velocity u-star (m/s)] (otherwise, from METPROPS)
- terrain elevation type: surface pressure
- surface height or pressure: [ambient pressure (atm)] (otherwise, 1)
- hole/pipe parameter type: diameter
- orifice type: unrestricted
- equivalent hole/pipe diameter: [source diameter (m)]/(0.0254) for pressurized liquids], (12.00 for instantaneous releases, 6.00 for refrigerated liquids)
- orifice diameter: 0
- hole area: 0
- orifice area: 0
- aerosol fraction rained out due to impaction: 0
- liquid foaming flag: no
- liquid mass fraction becoming foam: 0
- minimum vaporization mass fraction: 0.005 or (adjust to match spill/evaporation rate for pressurized liquids)
- pool mass fraction absorbing into ground: 0
- liquid pool depth: 0.8 or (adjust to match source diameter for refrigerated liquids)
- entrainment ratio: 180 for pure compounds; computed for mixtures (Thorney Island trials)
- cloud height: 4 m

All releases must be configured in terms of a mass flowing through a hole in a tank. Plumes are characterized by a constant spill/evaporation rate and spill duration. These values represent the mass flow rate and the duration for the release but do not necessarily represent the duration of vapor flux from the release area as either a stationary cloud or a boiling liquid pool. The tank for the RAILCAR runs is configured with the hole at the bottom, so that the release

mass equals the initial mass. The average jet mass flow rate must then match the field trial constant jet mass flow rate to have the same release duration. For the liquid pool releases, the pool depth can be adjusted to match the MDA source diameter.

RAILCAR will characterize each source as either a horizontal plume vapor source or an area vapor source. For area vapor sources, if the tank empty time is more than $1/5^{th}$ of the time it takes for all of the liquid to evaporate, RAILCAR will characterize the area source as growing. Otherwise, it will be a constant area vapor source.

2.2 VLSTRACK Input Parameters

For each dense gas field trial, each source parameter in the VLSTRACK input file, VLSTRACK.DAT, was defined according to the RAILCAR-defined vapor area or plume source or values from the MDA. For each neutrally buoyant particle/gas field trial, each parameter in VLSTRACK.DAT was defined according to a value from the MDA. The VLSTRACK input parameters that define a horizontal plume are significantly different than those that define an area vapor source. Area vapor sources will result from MDA field trials resulting in either boiling liquid pools or instantaneous dense gas releases. The instantaneous Krypton-85 releases in the Hanford field trials form single puffs and also have unique input parameter sets. Each of these three source types are addressed separately in this section.

2.2.1 Horizontal Plume

The Desert Tortoise, Goldfish, and Thorney Island continuous dense gas field trials and the Hanford continuous and Prairie Grass neutrally buoyant gas trials all generated a horizontal plume. As discussed below, RAILCAR predicted a horizontal plume would be generated rather than a stationary vapor cloud for all trials of this type.

The VLSTRACK parameters, in the order in which they appear in the input windows, and their source or recommended values are as follows (MDA parameter titles are in [ ]):

- munition: Sprayer
- chem/bio agent: name as it appears in VLSAGN.PAR
- date: [day] [month] [year]
- local attack time: [hour] [minute]
- attack location: 36.7000N 116.0000W
- ground surface type: user-defined
- map scale: user-defined at 13000:1
- output type: dosage
- hazard contour type: Mass Units (mg-min/m^3)
- output mode: cumulative
- probability output: normal
- detonation coordinates: Gaussian
- wind measurement height: [measurement height for domain-avg wind data (m)]

- averaging time: [averaging time for averaged concentration (s)], [averaging time for peak concentration (s)]
- meteorology mode: time variable
- detector alarm mode: passive
- output grid size: 111 by 101
- grid sizing mode: fixed
- lower left location: 36.6978N 116.0012W
- upper right location: 36.7022N 115.9889W
- contour levels: 1E5×A, 1E4×A, 1E3×A, 1E2×A (A = conversion from ppm to mg/m^3)
- contour levels: 100.00 10.00 1.000 0.1000 mg/m^2
- contour levels: 10000.00 1000.00 100.000 10.0000 mg/m^3
- dosage output height: [suggested receptor height for modeling (m)]
- output frequency: 600.000 s
- plot pause mode: normal
- Gaussian plume mode: stationary sprayer
- sprayer duration: [spill duration (s)]
- random number seed: 349875
- wind meander seed: 863005
- grid output mode: end of run
- number of munitions: 100
- rate of fire: 1000 (simultaneous bursts)
- height of release: [source elevation (m)]
- fill weight: [spill/evaporation rate (kg/s)]×[spill duration (s)]/100
- lateral sigma = (RAILCAR plume diameter)/4
- downrange target sigma: 0.00 m
- crossrange target sigma: 0.00 m
- droplet MMD: 20. microns
- geo droplet dist sigma: 1.0
- dissemination efficiency: 100.00%
- Pasquill stability category: [Pasquill-Gifford stability class (A=1;D=4;F=6)]
- wind bearing: 270.0 DTN
- wind speed: [domain-avg wind speed (m/s)]
- forecast time: 0000
- cloud cover: [cloud cover (%)] (converted into thirds as clear, partly cloudy, overcast)
- air temperature: [ambient temperature #1-lower (K)] – 273.15]
- relative humidity: [relative humidity (%)]

Since the attack location doesn't affect computations, the Nevada Test Site latitude and longitude were used for all field trials. This enabled the same coordinates to be used for the fixed grid corners and detector locations. Dosage output type was selected, as both dosage and concentration are output at each time step at the detector locations. The lateral plume sigma was assumed to equal $1/4^{th}$ the plume diameter defined by RAILCAR. Since averaging times were different for the peak and average concentration values, two VLSTRACK runs were completed for each field trial. The grid was sized so that the downwind direction extended from -100 m to

+1000 m, and the crosswind direction extended from -250 m to +250 m. Downwind grid spacing was 10 m, and crosswind grid spacing was 5 m. The dosage contour levels are in multiples of 10, with the lowest contour level representing 100 ppm-min. The MDA includes soil temperature, and VLSTRACK uses ground temperature to compute surface evaporation for liquid deposited onto the ground surface; however, RAILCAR had already converted each dense vapor source into an all-vapor flux. The neutrally buoyant releases didn't involve liquid deposition. MDA soil temperature was thus not used for the VLSTRACK simulations.

Three parameters in OVERWRTE.PAR were also changed from the default values:

- initial vapor mass set to 100%: 'PV' 100
- time step set to 1.0 s: 'TS' 1
- roughness length set to MDA value: 'RF' 1E6×[roughness length z0 (m)]

Nine detectors were defined at distances directly downwind from the release location from 100 m to 900 m at 100-m spacing. These distances covered the downwind sensor distances used in most of the field trials. The detector positions were adjusted for the field trials with different distances. Measurement height was set to 1 m above ground (adjusted for alternate MDA heights), and the threshold concentration value was set to 10 mg/m^3. Recording time was set to 60 min. Each detector recorded concentration and dosage every time step from when the concentration at the location first exceeded the threshold value to when it later decreased below that value. The output frequency was therefore 1 s for as long as the cloud took to pass by each detector.

2.2.2 Area Vapor Source

The Burro, Coyote, and Maplin Sands field trials generated a boiling liquid pool, and Thorney Island Instantaneous field trials generated a stationary vapor cloud. RAILCAR simulated the liquid and dense gas physical processes and characterized each release as an area vapor source from ground level and the top of the cloud, respectively. The same set of VLSTRACK parameters is used for both of these release types.

VLSTRACK simulates all releases as a series of Gaussian puffs and cannot represent an area vapor source of uniform vapor flux. In order to best approximate this type of release, multiple small and flat puffs are generated at random locations within the circular release area over the release duration. In order to avoid the normal concentration distribution for a single puff extending beyond the circular release area, the target diameter is set to 80% of the release diameter, and the puff lateral sigma is set to 10% of that value. The vertical sigma is set to 1 m for a liquid pool and 50% of the cloud height for a stationary vapor cloud. If RAILCAR determines the tank empty time to be less than $1/5^{th}$ the total pool evaporation time, then it is classified as a constant area vapor source. The VLSTRACK parameters for constant area vapor sources – in the order in which they appear in the input windows – and their source or recommended values are as follows (MDA parameter titles are in [ ]):

- munition: User-Defined
- chem/bio agent: name as it appears in VLSAGN.PAR
- date: [month] [day] [year]
- local attack time: [hour] [minute]
- attack location: 36.7000N 116.0000W
- trajectory angle: 90.0 DTN
- ground surface type: user-defined
- output type: dosage
- hazard contour type: mass units (mg-min/m^3)
- output mode: cumulative
- probability output flag: normal output
- map scale: user-defined at 13000:1
- detonation coordinates: uniform elliptical
- munition density: 999.0000 rds/hectare
- downrange target size: 0.8×[source diameter (m)]
- crossrange target size: 0.8×[source diameter (m)]
- wind measurement height: [measurement height for domain-avg wind data (m)]
- averaging time: [averaging time for averaged concentration (s)], [averaging time for peak concentration (s)]
- meteorology mode: time variable
- detector alarm mode: passive
- output grid size: 111 by 101
- grid sizing mode: fixed
- lower left location: 36.6978N 116.0012W
- upper right location: 36.7022N 115.9889W
- contour levels: 1E5×A, 1E4×A, 1E3×A, 1E2×A (A = conversion from ppm to mg/m^3)
- contour levels: 100.00 10.00 1.000 0.1000 mg/m^2
- contour levels: 10000.00 1000.00 100.000 10.0000 mg/m^3
- dosage output height: [suggested receptor height for modeling (m)]
- output frequency: 600.000 s
- plot pause mode: normal
- random number seed: 349875
- wind meander seed: 863005
- grid output mode: end of run
- source type: point
- rate of fire: 60×(number of munitions)/(RAILCAR vapor source duration)
- height of release: 0.00 m for liquid pools, RAILCAR height for stationary vapor clouds
- fill weight: [spill/evaporation rate (kg/s)]×[spill duration (s)]/(number of munitions)
- lateral sigma: 0.1×[source diameter (m)]
- vertical sigma: 1.000 m for liquid pools, (RAILCAR height)/2 for stationary vapor clouds
- droplet MMD: 20. microns
- geo droplet dist sigma: 1.0
- dissemination efficiency: 100.00%

- Pasquill stability category: [Pasquill-Gifford stability class (A=1;D=4;F=6)]
- wind bearing: 270.0 DTN
- wind speed: [domain-avg wind speed (m/s)]
- forecast time: 0000
- cloud cover: [cloud cover (%)] (converted into thirds as clear, partly cloudy, overcast)
- air temperature: [ambient temperature #1-lower (K)] – 273.15]
- relative humidity: [relative humidity (%)]

When RAILCAR determined the release was a growing area vapor source, VLSTRACK was first run using a constant area and vapor mass rate. The resulting munition coordinates randomly generated within the release area were then converted using program FILEGEN to a growing area source. This program takes the initial coordinates and adjusts those that occur while the pool or cloud is growing and scales the coordinates to fit within the circular release area for the puff formation time. After FILEGEN was run, VLSTRACK was run again with the adjusted source terms. VLSTRACK input parameters were the same as for a constant area vapor source except for the following parameters:

- source type: line
- detonation coordinates: puff property read
- property input file: (file generated from FILEGEN)

The same three parameters in OVERWRTE.PAR were changed from the default values:

- initial vapor mass set to 100%: 'PV' 100
- time step set to 1.0 s: 'TS' 1
- roughness length set to MDA value: 'RF' 1E6×[roughness length z0 (m)]

2.2.3 Single Puff

The Hanford Instantaneous field trials generated a single, neutrally buoyant puff containing Krypton-85 particles. RAILCAR was not used for neutrally buoyant releases, and the source parameters were entered directly into the VLSTRACK simulations. The VLSTRACK parameters – in the order in which they appear in the input windows – and their source or recommended values are as follows (MDA parameter titles are in [ ]):

- munition: User-Defined
- chem/bio agent: name as it appears in VLSAGN.PAR
- date: [month] [day] [year]
- local attack time: [hour] [minute]
- attack location: 36.7000N 116.0000W
- ground surface type: user-defined
- output type: dosage
- hazard contour type: mg-min/m^3
- output mode: cumulative

- probability output flag: normal output
- map scale: user-defined at 13000:1
- detonation coordinates: Gaussian
- wind measurement height: [measurement height for domain-avg wind data (m)]
- averaging time: [averaging time for averaged concentration (s)], [averaging time for peak concentration (s)]
- meteorology mode: time variable
- detector alarm mode: passive
- output grid size: 111 by 101
- grid sizing mode: fixed
- lower left location: 36.6978N 116.0012W
- upper right location: 36.7022N 115.9889W
- contour levels: 1E5×A, 1E4×A, 1E3×A, 1E2×A (A = conversion from ppm to mg/m^3)
- contour levels: 100.00 10.00 1.000 0.1000 mg/m^2
- contour levels: 10000.00 1000.00 100.000 10.0000 mg/m^3
- dosage output height: [suggested receptor height for modeling (m)]
- output frequency: 600.000 s
- plot pause mode: normal
- wind meander seed: 863005
- grid output mode: end of run
- source type: point
- number of munitions: 1
- height of release: 0.00 m
- fill weight: 0.100 kg
- lateral sigma: 2.000 m
- vertical sigma: 2.000 m
- droplet MMD: 20. microns
- geo droplet dist sigma: 1.0
- dissemination efficiency: 100.00%
- Pasquill stability category: [Pasquill-Gifford stability class (A=1;D=4;F=6)]
- wind bearing: 270.0 DTN
- wind speed: [domain-avg wind speed (m/s)]
- forecast time: 0000
- cloud cover: [cloud cover (%)] (converted into thirds as clear, partly cloudy, overcast)
- air temperature: [ambient temperature #1-lower (K)] – 273.15]
- relative humidity: [relative humidity (%)]

3.0 INDIVIDUAL MDA FIELD TRIAL SIMULATIONS

This section explains in greater detail the method and input parameters that were used when simulating the individual field trials from the MDA. Both RAILCAR and VLSTRACK were designed to model an attack, but the MDA field trials were completed in a highly controlled and structured manner. Because there is this fundamental difference, RAILCAR and VLSTRACK input parameters were manipulated to best model the controlled field trials. Simulation procedures and default parameter values for each set of MDA trials are defined in this section, along with detailing a test case for each trial. Since detector location varied by trial, a spreadsheet was created to calculate the longitude for corresponding distances downwind.

3.1 Burro Trials

The eight Burro trials consisted of 1- to 3-min releases of liquefied natural gas (LNG, ~90% methane) forming a boiling liquid pool on a water surface. RAILCAR defined Burro trials 4, 5, 6, 7, and 9 as growing area vapor sources and Burro trials 2, 3, and 8 as constant area vapor sources. Burro 9 will be the test case. The procedure for a constant area vapor source was the same as the first part of a growing area vapor source. The RAILCAR input parameters mapped to the MDA records were:

- initial tank mass = (135.98 kg/s)×(79 s) = 10742 kg
- tank temperature = -162.6 C
- inert gas pressure = 7.00 atm
- surface roughness length = 0.0002 m
- air temperature = 308.52 K – 273.15 = 35.4 C
- ground temperature = 35.4 + 0.0 = 35.4 C
- wind speed at 2-m height = 5.7 m/s
- relative humidity = 14.4 %
- friction velocity = 0.250 m/s
- surface height or pressure = 0.928 atm
- equivalent hole/pipe diameter = 6.00 in (refrigerated liquid)
- liquid pool depth = 1.38 cm

In order for the LNG to be all liquid, the tank temperature was adjusted to just below the boiling temperature of -162.51 C (computed by RAILCAR for the MDA ambient pressure of 0.928 atmospheres). The MDA does not include ground temperature for this field trial so it was determined using METPROPS. The inert gas pressure was adjusted to result in the liquid empty time matching the 79-s spill duration. The liquid pool depth was adjusted to match the source diameter of 45.13 m. RAILCAR characterizes this release as a growing area vapor source:

```
Growing Area Vapor Source Properties:
final diameter=           45.15 m
growth duration=           78.9 s
total duration=           390.0 s
vapor mass rate=        30.6299 kg/s
height=                    0.00 m
```

RAILCAR predicted that the boiling liquid pool would grow linearly in area to a diameter of 45 m during the 79-s tank empty time. Vapor mass rate increased linearly from 0 kg/s to 30.63 kg/s over that duration and then remained at that rate for an additional 311 s. The boiling liquid pool thus took just under five times as long as the jet duration to evaporate. The average vapor mass rate of 27.54 kg/s was thus $1/5^{th}$ the reported MDA spill/evaporation rate. The VLSTRACK parameters for the initial run of this field trial were:

- chem/bio agent = Methane (LNG)
- date = September 17, 1980
- local attack time = 1837 (0237Z) day
- downrange target size = 0.8×45.13 = 36.10 m
- crossrange target size = 0.8×45.13 = 36.10 m
- wind measurement height = 2.000 m
- averaging time = 1.000 s
- contour levels = 67000.00 6700.00 670.000 67.0000 mg-min/m^3
- dosage output height = 1.00 m
- number of munitions = 102 (determined by VLSTRACK from munition density and target size)
- rate of fire = 60×102/390 = 15.7 rds/min
- height of release = 0.00 m
- fill weight = (135.98 kg/s)×(79 s)/102 = 105.310 kg
- lateral sigma = 0.1×45.13 = 4.510 m
- vertical sigma = 1.000 m
- Pasquill stability category = D (Neutral)
- wind speed = 5.7 m/s
- air temperature = 35.0 C
- relative humidity = 10% (VLSTRACK truncates to multiples of 10)
- cloud cover = clear (from MDA value of 15%)

If this were a constant area vapor source, VLSTRACK would be run in this manner twice, for the short and long averaging times, and the trail would be complete. However, this trial was a growing area vapor source, so FILEGEN was run. The FILEGEN parameters of this trial were:

- file type to generate: 1 = property input
- time varying source type: 2 = growing liquid pool
- munition coordinate file name = (VLSTRACK output file prefix).POS

- number of munitions = number of munitions from VLSTRACK munition property window
- release mass = (135.98 kg/s)×(79 s) = 10742 kg
- transient vapor mass: 0.5 × 30.63 × 79 = 1210 kg (0.5 × vapor mass rate × tank empty time)
- final vapor mass rate = 30.63 kg/s
- tank empty time = 78.9 s
- final time = 390.0 s
- final pool diameter = 45.15 m

VLSTRACK was run again with the following changes:

- averaging time: 1.000 s and 50.000 s (two runs)
- source type: line
- detonation coordinates: puff property read
- property input file: (file generated from FILEGEN)

To ensure the detectors were placed at the correct locations downwind, the output file was checked. The unit conversion for methane is 0.67 mg/ppm-m^3.

3.2 Coyote Trials

Similar to the Burro trials, the three Coyote trials consisted of 1- to 1.5-min releases of LNG (~90% methane) forming a boiling liquid pool on a water surface. RAILCAR classified Coyote trials 3 and 5 as growing area vapor sources and Coyote trial 6 as a constant area vapor source. Since the procedures and default values are the same as for the Burro trials, no test case will be shown. The test case in Section 3.1 can be used for reference.

3.3 Desert Tortoise Trials

The four Desert Tortoise trials consist of 2- to 6-min releases of pressurized liquid anhydrous ammonia from a horizontal pipe oriented in the downwind direction forming a two-phase plume. RAILCAR characterized the trials as horizontal plume vapor sources. Desert Tortoise 1 will be the test case. The RAILCAR input parameters mapped to the MDA records were:

- initial tank mass = (79.7 kg/s)×(126 s) = 10042 kg
- tank temperature = 294.7 K – 273.15 = 21.6 C
- inert gas head pressure = 10.0 atm – 8.94 atm = 1.06 atm
- surface roughness length = 0.003 m
- air temperature = 302.03 K – 273.15 = 28.9 C
- ground temperature = 304.8 K – 273.15 = 31.7 C
- relative humidity = 13 %

- wind speed at 2-m height = 7.4 m/s
- surface height or pressure = 0.897 atm
- equivalent hole/pipe diameter = (0.081 m)/(0.0254) = 3.19 in

To match the liquid empty time to the 126-s spill duration, the minimum vaporization mass fraction was adjusted to 0.006. The MDA does not include a friction velocity u-star for this field trial, so domain-avg wind speed at 2-m measurement height, roughness length z0, and Pasquill-Gifford stability class (A=1;D=4;F=6) were entered into METPROPS and resulted in a friction velocity of 0.4552 m/s. RAILCAR characterized this release as a plume:

```
Horizontal Plume Vapor Source Properties:
diameter=                10.12 m
duration=                146.1 s
vapor mass rate=        68.6335 kg/s
height=                   2.00 m
```

This characterization, though, includes the vapor mass and duration for tank depressurization. Since the field trial did not involve tank depressurization, the duration and vapor mass rate were reset to match the MDA values of 126 s and 79.7 kg/s, respectively. RAILCAR also assigns a default 2-m height for any plume source type. The MDA source elevation, which was needed for the VLSTRACK input parameters, is 0.79 m. Since there was a large mass released, 100 stationary sprayers were used to simulate the release the ammonia. The VLSTRACK parameters for this field trial were:

- chem/bio agent = Ammonia
- date = August 24, 1983
- local attack time = 1637 (0037Z) day
- wind measurement height = 2.000 m
- averaging time = 1.000 s and 80.000 s (two simulations)
- contour levels = 71000.00 7100.00 710.000 71.0000 mg-min/m^3
- dosage output height = 1.00 m
- sprayer duration = 126.000 s
- height of release = 0.79 m
- fill weight = (79.7 kg/s)×(126 s)/100 = 100.420 kg
- lateral sigma = 2.530 m
- Pasquill stability category = D (Neutral)
- wind speed = 7.5 m/s
- air temperature = 29.0 C
- relative humidity = 10%
- cloud cover = clear (from MDA value of 1%)

The unit conversion for ammonia is 0.71 mg/ppm-m^3.

3.4 Goldfish Trials

The three Goldfish trials consisted of 2- to 6-min releases of pressurized liquid hydrogen fluoride from a horizontal pipe oriented in the downwind direction forming a two-phase plume. Like the Desert Tortoise trials, RAILCAR characterized the trials as horizontal plume vapor sources. Goldfish 1 will be the test case. The RAILCAR input parameters mapped to the MDA records were:

- initial tank mass = (27.67 kg/s)×(125 s) = 3458.75 kg
- tank temperature = 313.2 K – 273.15 = 40.05 C
- inert gas head pressure = 14.0 atm
- surface roughness length = 0.003 m
- air temperature = 310.4 K – 273.15 = 37.25 C
- ground temperature = 310.4 K – 273.15 = 37.25 C (from METPROPS)
- relative humidity = 4.9 %
- wind speed at 2-m height = 5.6 m/s
- surface height or pressure = 0.893 atm
- equivalent hole/pipe diameter = (0.0419 m)/(0.0254) = 1.650 in
- minimum vaporization fraction = 0

Minimum vaporization fraction was set to 0 to increase jet flow rate. Since hydrogen fluoride has a low volatility, a higher inert gas head pressure than reported in the MDA was necessary to achieve the liquid empty time and jet flow rate needed to match the spill duration and spill evaporation time. RAILCAR characterized this release as a plume:

```
Horizontal Plume Vapor Source Properties:
diameter=                  4.78 m
duration=                139.6 s
vapor mass rate=       24.7792 kg/s
height=                    2.00 m
```

This characterization, though, includes the vapor mass and duration for tank depressurization. Since the field trial did not involve tank depressurization, the duration and vapor mass rate were reset to match the MDA values of 125 s and 27.67 kg/s, respectively. The source elevation of 1 m was also used. This set of trials had detectors at a long downwind distance. As a result, map scale and grid size were changed. The VLSTRACK parameters for this field trial were:

- chem/bio agent = HF
- date = 01 August 1986
- local attack time = 1815 (0215Z) day
- map scale = 40000:1
- wind measurement height = 2.000 m
- averaging time = 67.000 s and 88.000 s (two simulations)
- upper right grid location = 36.7022, 115.9662

- contour levels = 183000.00 18300.00 1830.000 183.0000 mg-min/m^3
- dosage output height = 1.00 m
- sprayer duration = 125.000 s
- height of release = 1.0 m
- fill weight = (27.67 kg/s)×(125 s)/100 = 34.588 kg
- lateral sigma = 1.195 m
- Pasquill stability category = D (Neutral)
- wind speed = 5.6 m/s
- air temperature = 37.0 C
- relative humidity = 0%
- cloud cover = clear (not given so assumed to be clear)

The unit conversion of hydrogen fluoride is 0.83 mg/ppm-m^3.

3.5 Maplin Sands Trials

The first four Maplin Sands trials consist of 1.5- to 4-min releases of LNG (~90% methane) forming a boiling liquid pool on a water surface. The other eight Maplin Sands trials consist of 1.5- to 6-min releases of liquefied propane gas (LPG) forming a boiling liquid pool on a water surface. Of the four LNG trials, RAILCAR only characterized Maplin Sands 27 as a constant area vapor source. The other three trials, Maplin Sands 29, 34, 35, were growing area vapor sources. Of the eight LPG trials, RAILCAR characterized Maplin Sands 42, 43, 47, 49, 54 as constant area vapor sources, and Maplin Sands 46, 50, 52 were growing area vapor sources. Maplin Sands 43 will be the test case. The RAILCAR input parameters mapped to the MDA records were:

- initial tank mass = (19.2 kg/s)×(330 s) = 6336 kg
- tank temperature = -43.10 C (set below boiling point of -43.03 C)
- inert gas pressure = 0.0589 atm
- surface roughness length = 0.0003 m
- air temperature = 290.2 K – 273.15 = 17.05 C
- ground temperature = 292.1 K – 273.15 = 18.95 C
- wind speed at 10-m height = 5.8 m/s
- relative humidity = 72 %
- friction velocity = 0.2477 m/s (from METPROPS)
- surface height or pressure = 1 atm
- equivalent hole/pipe diameter = 6.00 in (It is a refrigerated liquid.)
- liquid pool depth = 7.02 cm

The MDA does not provide friction velocity u-star or Pasquill stability class for this set of trials. In order to run METPROPS, an estimation of the Pasquill stability class was necessary. C (slightly unstable) stability was estimated for this trial, while D (neutral) stability was estimated for the rest of the trials. Ambient pressure and relative humidity are not given in the MDA so values of 1 atm and 72% were used, respectively. Inert gas pressure was adjusted to

0.0589 atm to match liquid empty time to spill duration, and liquid pool depth was adjusted to 7.02 cm to match pool diameter to source diameter in the MDA. RAILCAR characterized this release as a constant area vapor source:

```
Constant Area Vapor Source Properties:
 diameter=                14.30 m
 duration=               1687.7 s
 vapor mass rate=        3.7524 kg/s
 height=                   0.00 m
```

These trials have a smaller source diameter, causing VLSTRACK to use a smaller number of munitions. So, the same procedure used in the Burro trials did not give an accurate simulation of the release. Many more puffs were needed for smoother and more accurate model output. To achieve this, a target size 10 times greater was input to get a larger number of munitions. The VLSTRACK parameters for the initial run of this field trial were:

- chem/bio agent = Propane (LPG)
- date = September 28, 1980
- local attack time = 1817 (0118Z) day
- downrange target size = 0.8×14.30×10 = 114.40 m
- crossrange target size = 0.8×14.03 ×10= 114.40 m
- wind measurement height = 10.000 m
- averaging time = 3.000 and 60.000 s (two simulations)
- contour levels = 183000.00 18300.00 1830.000 183.0000 mg-min/m^3
- dosage output height = 0.90 m
- number of munitions = 1027
- rate of fire = 60×1027/1688 = 36.5 rds/min
- height of release = 0.00 m
- fill weight (19.2 kg/s)×(330 s)/1027 = 6.169 kg
- lateral sigma= 0.1×14.3 = 1.430 m
- vertical sigma = 1.000 m
- Pasquill stability category = C (slightly unstable)
- wind speed = 5.8 m/s
- air temperature = 17.0 C
- relative humidity = 70%
- cloud cover = partly cloudy (from MDA value of 50%)

This created a large number of randomly positioned munitions, but over an area 100 times too large. The release coordinates in the .POS file were divided by 10 to cause all of the munitions to be released within the 14.3-m source diameter. VLSTRACK was then run again using detonation coordinates from the .POS file by selecting “read from file.” Everything else was kept the same as the initial run. For the growing area vapor source, FILEGEN was run after the .POS file was adjusted. Refer to Section 3.1 if necessary. Note that the MDA only has a peak averaging time of 3 s, but a long averaging time of 60 s was run for future comparison with

RAILCAR-QUIC and RAILCAR-ALOHA simulation results. The conversion factor for propane is 1.83 mg/ppm-m^3.

3.6 Thorney Island Instantaneous Trials

The nine Thorney Island Instantaneous trials consisted of Freon-12 and nitrogen mixtures released at ground level forming vapor clouds. Thorney Island 12 will be the test case. The field trial summary table in the MDA document states that the cylindrical tent volume was 1950 m^3 and that the relative density of the Freon-12 mixture was 2.37. The entrainment ratio was adjusted to create a cloud that was 2.37 times as dense as air. The 5736 kilograms (kg) in the MDA table represents the combined mass of both Freon-12 and nitrogen; the mass entered into RAILCAR represents only the mass of Freon-12. The initial mass parameter was adjusted to 4350 kg to result in a cloud mass of 5736. RAILCAR does not compute the cloud slumping that occurred during the Thorney Island instantaneous field trials. RAILCAR was executed for the both the initial height of 12.7 m and a slumped height of 4.0 m. RAILCAR was also modified to allow this release to be all vapor at ambient temperature rather than the two-phase, cooled cloud that is normally computed. This switch cannot be set in the GUI; it must be adjusted in the .DAT file (terrain elevation type = 2). The RAILCAR input parameters mapped to the MDA records were:

- initial tank mass = 4350 kg
- tank temperature = 283.29 K – 273.15 = 10.14 C
- inert gas head pressure = 0.00 atm
- roughness length = 0.0180 m
- air temperature = 283.29 K – 273.15 = 10.14 C
- ground temperature = 285.15 K – 273.15 = 12.0 C
- relative humidity = 66.2 %
- wind speed at 10-m height = 2.5 m/s
- friction velocity = 0.1262 m/s (from METPROPS)
- surface height or pressure = 1.000 atm
- equivalent hole/pipe diameter = 12.00 in
- entrainment ratio = 1.33

For both cloud heights, RAILCAR predicted that the release would form a stationary vapor cloud. Without slumping, the cloud duration was computed to be 754 s with a vapor flux at the top of 5.75 kg/s and the cloud diameter equal to the 14-m tent diameter. For the 4-m cloud height, RAILCAR characterized the slumped stationary vapor cloud as:

```
Constant Area Vapor Source Properties:
diameter=                24.86 m
duration=                239.2 s
vapor mass rate=       18.1077 kg/s
height=                   4.00 m
```

The 4-m slumped cloud was used for each of the trials as more realistically portraying the observed cloud shape. The unit conversion for Freon-12 is 5.03 mg/ppm-m^3. The VLSTRACK parameters for this field trial were:

- chem/bio agent = Freon-12
- date = October 15, 1982
- local attack time = 1721 (0121Z) nightfall
- downrange target size = 0.8×24.86 = 19.90 m
- crossrange target size = 0.8×24.86 = 19.90 m
- wind measurement height = 10.000 m
- averaging time = 1.000 s and 60.000 s (two simulations; MDA only has 0.6 s)
- contour levels = 503000.00 50300.00 5030.000 503.0000 mg-min/m^3
- dosage output height = 0.4 m
- number of munitions = 31 (determined from munition density and target size)
- rate of fire = 60×31/239 = 7.8 rds/min
- height of release = 4.00 m
- fill weight = 4350/31 = 140.320 kg
- lateral sigma = 0.1×24.86 = 2.488 m
- vertical sigma = 2.000 m
- Pasquill stability category = E (Slightly Stable)
- wind speed = 2.5 m/s
- air temperature = 10.0 C
- relative humidity = 70%
- cloud cover = overcast (from the MDA value of 88%)

Note: the surface roughness length differed for each trial, so it was necessary to change the OVERWRTE.PAR file for each trial. The MDA only has a peak averaging time of 0.6 s, but a long averaging time of 60 s was run for future comparison with RAILCAR-QUIC and RAILCAR-ALOHA simulation results.

3.7 Thorney Island Continuous Trials

The two Thorney Island continuous trials consisted of 7- to 8-min releases of Freon-12 (dichlorodifluoromethane) in nitrogen (32% by volume) released from a ground area source forming a vapor plume. RAILCAR characterized the trials as horizontal plume vapor sources. Thorney Island 45 will be the test case. As with the instantaneous trials, entrainment ratio and initial mass were adjusted to match relative density and cloud mass, respectively. The hole diameter was adjusted to match the liquid empty time. The RAILCAR input parameters mapped to the MDA records were:

- initial tank mass = 3200.0 kg
- tank temperature = 286.25 K – 273.15 = 13.1 C
- inert gas head pressure = 0
- surface roughness length = 0.01 m
- air temperature = 286.25 K – 273.15 = 13.1 C

- ground temperature = 285.95 K – 273.15 = 12.8 C
- relative humidity = 100 %
- wind speed at 10-m height = 2.3 m/s
- surface height or pressure = 0.897 atm
- friction velocity = 0.1042 m/s (from METPROPS)
- surface pressure = 1.00 atm
- equivalent hole/pipe diameter = 0.9 in
- entrainment ratio = 2.19

RAILCAR characterized this release as a plume:

```
Horizontal Plume Vapor Source Properties:
diameter=                 0.61 m
duration=                 540.1 s
vapor mass rate=        5.8987 kg/s
height=                    2.00 m
```

The diameter was reset to match the MDA value of 2.0 m for the VLSTRACK run. RAILCAR also assigns a default 2.0-m height for any plume source type, whereas the MDA source is on the ground. Since there was a large mass released, 100 stationary sprayers were used to release the Freon-12. The VLSTRACK parameters for this field trial were:

- chem/bio agent = Freon-12
- date = June, 09 1984
- local attack time = 1959 (0359Z) day
- wind measurement height = 10.000 m
- averaging time = 30.000 s (only one simulation)
- contour levels = 503000.00 50300.00 5030.000 503.0000 mg-min/m^3
- dosage output height = 0.4 m
- sprayer duration = 455.000 s
- height of release = 0 m
- fill weight = (10.67 kg/s)×(455 s)/100 = 48.55 kg
- lateral sigma = 2.0/4 = 0.5 m
- Pasquill stability category = E (Slightly Stable)
- wind speed = 2.3 m/s
- air temperature = 13.0 C
- relative humidity = 90%
- cloud cover = clear (from MDA value of 13%)

The unit conversion for Freon-12 is 5.03 mg/ppm-m^3.

3.8 Hanford Instantaneous Trials

The Hanford Instantaneous field trials generated single, neutrally buoyant puffs containing Krypton-85 particles. RAILCAR was not used for neutrally buoyant releases, and the

source parameters were entered directly into VLSTRACK. The test case will be Hanford 8. The VLSTRACK parameters for the initial run of this field trial were:

- chem/bio agent = Krypton-85
- date = November 8, 1967
- local attack time = 0602 (1402Z) night
- wind measurement height = 1.500 m
- averaging time = 5.000 s and 60.000 s (two simulations, MDA only has 4.8 s)
- contour levels = 11.200 1.120 0.112 0.0112 mg-min/m^3
- dosage output height = 1.50 m
- number of munitions = 1
- height of release = 0.00 m
- fill weight = 0.100 kg (scaled from the 10.0 Ci MDA value)
- lateral sigma = 2.000 m
- vertical sigma = 2.000 m
- Pasquill stability category = E (Slightly Stable)
- wind speed = 1.6 m/s
- air temperature = 5.0 C
- relative humidity = 50% (assumed)
- cloud cover = clear (assumed)

Note that the contour levels were set to low values for these tracer releases. Also, the detector threshold was set to 1.0×10^{-4} mg/m^3. Since the fill weight was scaled down from the MDA, the concentration values in the MDA were also scaled down. The unit conversion for hydrogen cyanide representing Krypton-85 is 1.12 mg/ppm-m^3; however, the MDA concentration values are based on a scaled release mass of 10.0 Ci, so the VLSTRACK unit conversion can be assumed to equal 1.

3.9 Hanford Continuous Trials

The five Hanford Continuous trials consisted of 15- to 20-min Krypton-85 tracer releases from a horizontal pipe oriented in the downwind direction forming a particle plume. These trials involved a small release weight, so only one sprayer was used. The same scaling used in the instantaneous trials was used for these trials. The test case will be Hanford 3. The VLSTRACK parameters for the initial run of this field trial were:

- chem/bio agent = Krypton-85
- date = October, 23 1967
- local attack time = 1101 (1901Z) day
- wind measurement height = 1.5 m
- averaging time = 38.000 s and 269.000 s (two simulations)
- contour levels = 11.200 1.120 0.112 0.0112 mg-min/m^3
- dosage output height = 1.50 m
- sprayer duration = 855 s

- number of munitions = 1
- height of release = 1.0 m
- fill weight = (0.0278 kg/s)×(855 s)/100 = .238 kg (scaled from the MDA value)
- lateral sigma = 2.000 m
- Pasquill stability category = C (Slightly Unstable)
- wind speed = 7.1 m/s
- air temperature = 16.0 C
- relative humidity = 50% (assumed)
- cloud cover = clear (assumed)

Again, the unit conversion for hydrogen cyanide representing Krypton-85 is 1.12 mg/ppm-m^3; however, the MDA concentration values are based on a scaled release mass of 10.0 Ci, so the VLSTRACK unit conversion can be assumed to equal 1.

4.0 COMPARISON TO MDA

The detector output files for the short and long averaging time simulations were used to determine the maximum concentration and average concentration, respectively, at the center-line of the output grid in the downwind direction. These values were determined for each downwind distance noted in the MDA records for each test case. The lateral sigma at each downwind distance was determined from the grid output file for the long averaging time simulation for each test case for the dense gas field trials; the lateral sigma in the MDA for each neutrally buoyant field trial is for the peak concentration, so the grid output file for the short averaging time was used for that test type. Maximum concentration is simply the highest concentration recorded by the detector at each downwind distance for the short averaging time simulation. Average concentration is determined by first finding the highest concentration recorded by the detector at each downwind distance for the long averaging time simulation. A time period equal to the averaging time is then roughly centered at the flat part of the concentration profile to also include the highest concentration. The dosage at the start of the time period is subtracted from the dosage at the end of the time period, and the result is divided by the time period duration. The maximum and average concentrations are then converted from mg/m^3 to ppm using conversion factor A (specified for each trial).

VLSTRACK uses Gaussian puffs to represent all source types. The lateral sigma is then one normal distribution away from the highest concentration at a given time and distance. Since dosage is the integral of concentration over time, the lateral sigma can also be determined from the crosswind dosage profile. Dosage at one sigma is 0.61 times the center maximum dosage. At two sigmas, the ratio is 0.14, which is easier to determine. Lateral sigma was thus determined by plotting the crosswind dosage profile at each downwind distance, along with a horizontal line representing 0.14 times the maximum dosage in the profile. The distance between the two intersecting points was then divided by four to get lateral sigma. Figure 4 shows an example of the graph of crosswind dosage profiles that was used to calculate the lateral sigma for each trial. The crosswind grid spacing is the same 4.944 m for each grid output file, so the curves are positioned starting at 0 m.

The three parameters determined from the test case simulations are compared to the MDA values for each set of trials. Not every set of trials has all three parameters in the MDA; thus, in those cases no comparison was made. Tables 1 through 10 provide the measured MDA values for each field trial (e.g., BU2 for Burro 2) at each measurement distance (d) for peak concentration (cp_obs), average concentration (ca_obs), and lateral sigma (sig_obs) and the corresponding RAILCAR-VLSTRACK predicted values (cp_pred, ca_pred, sig_pred). Concentrations are in units of ppm, and lateral sigmas are in units of meters.

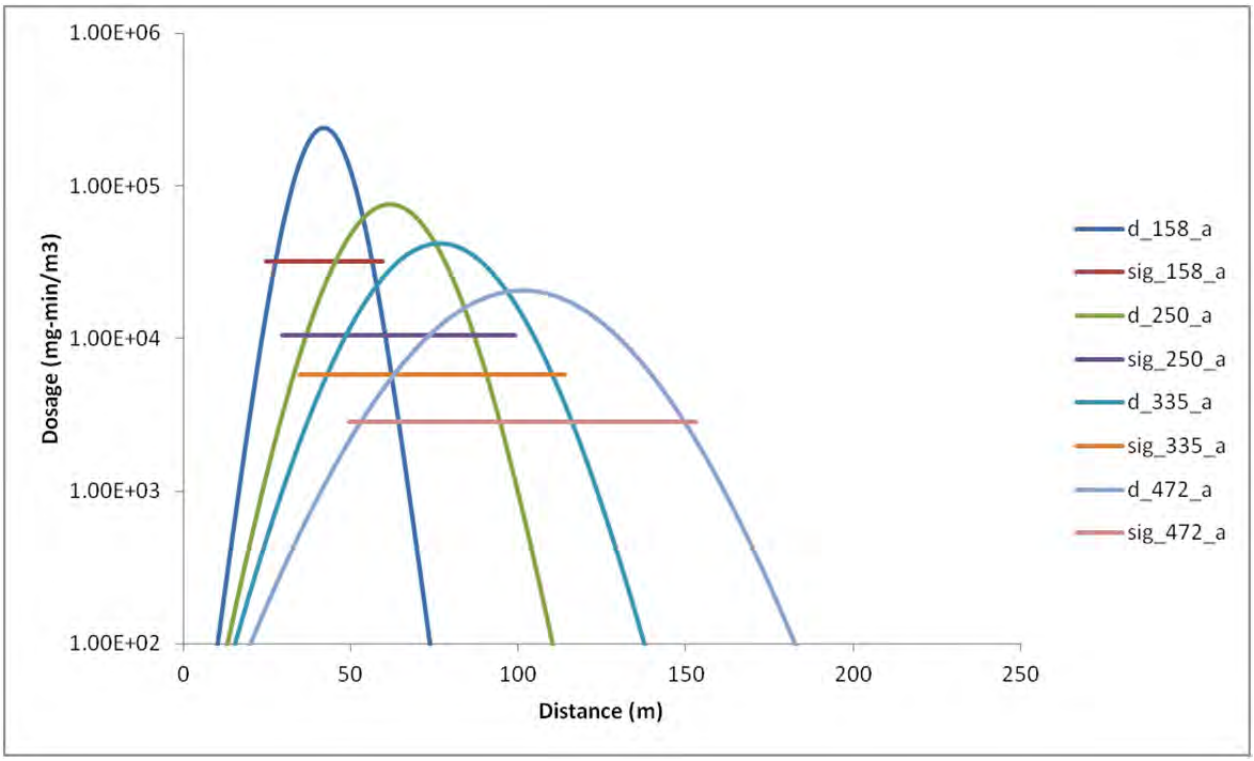


Figure 4. Thorney Island 45 Lateral Sigma

4.1 Burro Trials Comparison

Table 1. Concentrations and Lateral Sigmas for Burro Trials

Trial	d (m)	cp_obs	cp_pred	Trial	d (m)	ca_obs	ca_pred	Trial	d (m)	sig_obs	sig_pred
BU2	57	1.53E+05	1.64E+06	BU2	57	8.70E+04	1.45E+05	BU2	57	N/A	7.42
BU2	140	5.50E+04	5.80E+05	BU2	140	3.00E+04	8.94E+04	BU2	140	N/A	9.89
BU3	57	2.24E+05	1.46E+06	BU3	57	7.91E+04	2.84E+05	BU3	57	20.02	8.65
BU3	140	8.99E+04	5.69E+05	BU3	140	6.37E+04	6.79E+04	BU3	140	N/A	11.12
BU4	57	1.77E+05	1.81E+06	BU4	57	8.55E+04	1.43E+05	BU4	57	14.91	7.42
BU4	140	7.16E+04	8.21E+05	BU4	140	4.03E+04	7.79E+04	BU4	140	N/A	8.65
BU5	57	1.90E+05	2.17E+06	BU5	57	6.89E+04	1.35E+05	BU5	57	13.21	7.42
BU5	140	9.60E+04	8.94E+05	BU5	140	4.99E+04	7.34E+04	BU5	140	10.11	8.65
BU6	57	1.79E+05	1.44E+06	BU6	57	1.27E+05	1.24E+05	BU6	57	N/A	8.65
BU6	140	6.10E+04	6.02E+05	BU6	140	3.67E+04	8.39E+04	BU6	140	20.33	9.89
BU7	57	1.79E+05	1.55E+06	BU7	57	1.44E+05	1.74E+04	BU7	57	N/A	7.42
BU7	140	7.13E+04	7.04E+05	BU7	140	4.42E+04	1.10E+04	BU7	140	20.90	9.89
BU7	400	3.86E+04	4.16E+04	BU7	400	2.35E+04	1.87E+03	BU7	400	N/A	13.60
BU8	57	5.59E+05	6.89E+05	BU8	57	2.95E+05	2.01E+05	BU8	57	27.14	9.89
BU8	140	1.64E+05	1.66E+05	BU8	140	1.62E+05	7.02E+04	BU8	140	N/A	11.12
BU8	400	3.58E+04	1.72E+04	BU8	400	2.92E+04	1.11E+04	BU8	400	84.19	22.25
BU8	800	2.12E+04	4.57E+03	BU8	800	2.09E+04	1.98E+03	BU8	800	N/A	48.20
BU9	140	1.06E+05	3.17E+05	BU9	140	6.52E+04	9.80E+04	BU9	140	26.72	11.12
BU9	400	3.96E+04	2.85E+04	BU9	400	2.29E+04	1.71E+04	BU9	400	44.63	16.07
BU9	800	1.40E+04	4.69E+03	BU9	800	1.10E+04	2.45E+03	BU9	800	57.06	32.14

4.2 Coyote Trials Comparison

Table 2. Concentrations and Lateral Sigmas for Coyote Trials

Trial	d (m)	cp_obs	cp_pred	Trial	d (m)	ca_obs	ca_pred	Trial	d (m)	sig_obs	sig_pred
CO 3	140	1.07E+05	3.31E+05	CO 3	140	5.42E+04	7.92E+04	CO 3	140	23.52	9.888
CO 3	200	4.86E+04	1.40E+05	CO 3	200	2.33E+04	4.83E+04	CO 3	200	N/A	11.124
CO 3	300	1.91E+04	4.38E+04	CO 3	300	6.96E+03	2.10E+04	CO 3	300	N/A	14.832
CO 5	140	1.15E+05	4.20E+05	CO 5	140	3.28E+04	1.10E+05	CO 5	140	N/A	9.888
CO 5	200	8.09E+04	2.10E+05	CO 5	200	2.47E+04	5.98E+04	CO 5	200	N/A	12.36
CO 5	300	3.17E+04	7.55E+04	CO 5	300	7.20E+03	2.98E+04	CO 5	300	N/A	17.304
CO 5	400	2.30E+04	3.23E+04	CO 5	400	6.34E+03	1.60E+04	CO 5	400	N/A	21.012
CO 6	140	1.27E+05	2.57E+05	CO 6	140	8.25E+04	7.35E+04	CO 6	140	15.41	11.124
CO 6	200	8.50E+04	1.31E+05	CO 6	200	4.53E+04	4.56E+04	CO 6	200	17.13	12.36
CO 6	300	4.18E+04	5.07E+04	CO 6	300	2.19E+04	2.28E+04	CO 6	300	N/A	13.596
CO 6	400	3.29E+04	2.44E+04	CO 6	400	1.73E+04	1.25E+04	CO 6	400	N/A	14.832

4.3 Desert Tortoise Trials Comparison

Table 3. Concentrations and Lateral Sigmas for Desert Tortoise Trials

Trial	d (m)	cp_obs	cp_pred	Trial	d (m)	ca_obs	ca_pred	Trial	d (m)	sig_obs	sig_pred
DT 1	100	6.33E+04	5.59E+05	DT 1	100	4.99E+04	4.66E+05	DT 1	100	11.83	2.47
DT 1	800	1.10E+04	7.56E+03	DT 1	800	8.84E+03	3.86E+03	DT 1	800	61.79	39.55
DT 2	100	1.10E+05	8.20E+05	DT 2	100	8.32E+04	6.64E+05	DT 2	100	14.72	3.71
DT 2	800	1.86E+04	1.16E+04	DT 2	800	1.08E+04	4.99E+03	DT 2	800	88.19	28.38
DT 3	100	9.73E+04	6.12E+05	DT 3	100	7.69E+04	5.98E+05	DT 3	100	15.24	4.94
DT 3	800	1.56E+04	1.13E+04	DT 3	800	7.09E+03	1.06E+04	DT 3	800	73.4	30.90
DT 4	100	8.43E+04	8.73E+05	DT 4	100	5.73E+04	6.71E+05	DT 4	100	15.67	4.94
DT 4	800	2.09E+04	1.19E+04	DT 4	800	1.67E+04	4.28E+03	DT 4	800	85.99	59.33

4.4 Goldfish Trials Comparison

Table 4. Concentrations and Lateral Sigmas for Goldfish Trials

Trial	d (m)	cp_obs	cp_pred	Trial	d (m)	ca_obs	ca_pred	Trial	d (m)	sig_obs	sig_pred
GF 1	300	2.55E+04	8.64E+03	GF 1	300	2.55E+04	8.35E+03	GF 1	300	25.13	9.888
GF 1	1000	3.10E+03	4.07E+02	GF 1	1000	3.10E+03	3.91E+02	GF 1	1000	63	44.496
GF 1	3000	4.11E+02	3.15E+01	GF 1	3000	4.11E+02	2.94E+01	GF 1	3000	113.89	155.736
GF 2	300	1.94E+04	3.49E+03	GF 2	300	1.94E+04	3.39E+03	GF 2	300	29.93	11.124
GF 2	1000	2.39E+03	1.66E+02	GF 2	1000	2.39E+03	1.61E+02	GF 2	1000	54.65	48.204
GF 3	300	1.86E+04	3.21E+03	GF 3	300	1.86E+04	3.12E+03	GF 3	300	25.06	9.888
GF 3	1000	2.49E+03	1.45E+02	GF 3	1000	2.49E+03	1.42E+02	GF 3	1000	49.83	43.26
GF 3	3000	2.24E+02	1.23E+01	GF 3	3000	2.24E+02	1.20E+01	GF 3	3000	75.19	155.736

4.5 Maplin Sands Trials Comparison

Table 5. Concentrations and Lateral Sigmas for Maplin Sands LNG Trials

Maplin Sands (LNG)			
Trial	d (m)	cp_obs	cp_pred
MS 27	89	1.23E+05	7.90E+04
MS 27	131	9.49E+04	4.60E+04
MS 27	324	3.56E+04	6.45E+03
MS 27	400	2.91E+04	3.73E+03
MS 27	650	5.70E+03	9.31E+02
MS 29	58	1.42E+05	1.28E+05
MS 29	90	1.14E+05	9.94E+04
MS 29	130	6.19E+04	6.42E+04
MS 29	182	5.43E+04	3.82E+04
MS 29	252	2.04E+04	1.76E+04
MS 29	324	1.65E+04	1.01E+04
MS 29	403	1.35E+04	5.50E+03
MS 34	87	1.18E+05	7.01E+04
MS 34	179	4.55E+04	3.09E+04
MS 35	129	7.74E+04	5.88E+04
MS 35	250	3.07E+04	1.88E+04
MS 35	406	2.28E+04	5.72E+03

Table 6. Concentrations and Lateral Sigmas for Maplin Sands LPG Trials

Maplin Sands (LPG)			
Trial	d (m)	cp_obs	cp_pred
MS 42	28	1.13E+05	9.29E+04
MS 42	53	1.11E+05	7.48E+04
MS 42	83	6.67E+04	4.19E+04
MS 42	123	4.15E+04	1.83E+04
MS 42	179	2.17E+04	8.09E+03
MS 42	247	2.18E+04	3.39E+03
MS 42	398	1.05E+04	1.05E+03
MS 43	88	5.65E+04	3.27E+04
MS 43	129	3.51E+04	1.64E+04
MS 43	249	1.89E+04	3.09E+03
MS 43	400	7.50E+03	8.96E+02
MS 46	34	9.76E+04	5.90E+05
MS 46	91	5.72E+04	5.05E+05
MS 46	130	3.76E+04	2.94E+05
MS 46	182	2.61E+04	1.48E+05
MS 46	250	1.85E+04	6.07E+04
MS 46	322	1.67E+04	3.29E+04
MS 46	401	7.20E+03	1.89E+04
MS 47	90	8.09E+04	4.34E+04
MS 47	128	4.02E+04	2.51E+04
MS 47	182	3.13E+04	1.40E+04
MS 47	250	1.55E+04	6.12E+03

Maplin Sands (LPG)			
Trial	d (m)	cp_obs	cp_pred
MS 47	321	1.44E+04	3.43E+03
MS 47	400	9.50E+03	2.00E+03
MS 49	90	7.21E+04	2.63E+04
MS 49	129	4.67E+04	1.39E+04
MS 49	180	4.35E+04	7.40E+03
MS 49	250	2.50E+04	3.23E+03
MS 49	322	1.48E+04	1.87E+03
MS 49	400	7.60E+03	1.13E+03
MS 50	59	1.03E+05	5.72E+04
MS 50	93	5.71E+04	4.19E+04
MS 50	182	3.08E+04	1.77E+04
MS 50	400	1.19E+04	2.75E+03
MS 52	61	5.63E+04	5.41E+04
MS 52	95	3.38E+04	4.54E+04
MS 52	178	2.60E+04	1.93E+04
MS 52	249	1.12E+04	9.51E+03
MS 52	398	1.18E+04	3.20E+03
MS 52	650	7.50E+03	7.96E+02
MS 54	56	2.27E+05	7.43E+04
MS 54	85	1.20E+05	3.31E+04
MS 54	178	5.34E+04	6.78E+03
MS 54	247	4.95E+04	2.80E+03

4.6 Thorney Island Trials Comparison

Table 7. Concentrations and Lateral Sigmas for Thorney Island Instantaneous Trials

Thorney Island Instantaneous							
Trial	d (m)	cp_obs	cp_pred	Trial	d (m)	cp_obs	cp_pred
TI 6	71	9.04E+04	4.19E+04	TI 13	71	7.33E+04	1.07E+05
TI 6	141	3.67E+04	1.08E+04	TI 13	100	6.46E+04	5.84E+04
TI 6	180	2.62E+04	6.02E+03	TI 13	224	2.54E+04	1.12E+04
TI 6	283	9.76E+03	1.66E+03	TI 13	316	1.25E+04	4.41E+03
TI 6	424	5.29E+03	4.47E+02	TI 13	361	9.26E+03	3.12E+03
TI 7	71	1.32E+05	3.54E+04	TI 13	412	7.29E+03	1.93E+03
TI 7	100	5.92E+04	1.58E+04	TI 17	40	1.27E+05	4.70E+05
TI 7	150	3.38E+04	5.67E+03	TI 17	50	8.51E+04	3.55E+05
TI 7	180	2.54E+04	4.16E+03	TI 17	71	4.76E+04	2.28E+05
TI 7	224	1.98E+04	2.41E+03	TI 17	100	3.19E+04	1.07E+05
TI 7	361	1.19E+04	7.20E+02	TI 17	141	1.49E+04	4.59E+04
TI 7	500	6.02E+03	2.99E+02	TI 17	224	6.52E+03	1.34E+04
TI 8	71	9.25E+04	4.10E+04	TI 17	500	3.33E+03	1.33E+03
TI 8	100	6.11E+04	1.82E+04	TI 18	40	2.42E+05	7.66E+04
TI 8	150	4.03E+04	5.74E+03	TI 18	60	8.61E+04	6.15E+04
TI 8	200	2.81E+04	3.18E+03	TI 18	70	6.27E+04	5.27E+04
TI 8	364	1.08E+04	6.56E+02	TI 18	80	5.25E+04	5.40E+04
TI 8	412	6.92E+03	4.50E+02	TI 18	100	4.08E+04	5.18E+04
TI 8	510	4.26E+03	2.57E+02	TI 18	200	1.61E+04	1.62E+04
TI 9	71	1.23E+05	1.78E+04	TI 18	224	1.10E+04	1.24E+04
TI 9	100	7.06E+04	9.18E+03	TI 18	300	8.06E+03	6.53E+03
TI 9	141	3.58E+04	4.84E+03	TI 18	400	4.87E+03	3.10E+03
TI 9	180	2.65E+04	3.09E+03	TI 18	510	3.49E+03	1.41E+03
TI 9	224	2.07E+04	2.10E+03	TI 19	40	1.84E+05	1.86E+05
TI 9	316	1.14E+04	1.13E+03	TI 19	60	8.24E+04	1.30E+05
TI 9	503	5.45E+03	5.39E+02	TI 19	71	7.22E+04	1.02E+05
TI 12	71	1.16E+05	5.26E+04	TI 19	100	5.39E+04	5.37E+04
TI 12	150	3.17E+04	7.93E+03	TI 19	224	1.36E+04	9.71E+03
TI 12	200	1.85E+04	4.32E+03	TI 19	361	6.77E+03	2.56E+03
TI 12	361	9.99E+03	1.11E+03	TI 19	583	2.99E+03	6.10E+02
TI 12	500	3.68E+03	5.05E+02				

Table 8. Concentrations and Lateral Sigmas for Thorney Island Continuous Trials

Thorney Island Continuous			
Trial	d (m)	cp_obs	cp_pred
TI 45	40	2.00E+05	1.33E+05
TI 45	53	1.29E+05	7.68E+04
TI 45	72	8.90E+04	4.07E+04
TI 45	90	6.20E+04	2.19E+04
TI 45	112	3.79E+04	1.34E+04
TI 45	158	2.62E+04	6.16E+03
TI 45	250	7.60E+03	2.24E+03
TI 45	335	5.00E+03	1.24E+03
TI 45	472	3.60E+03	6.19E+02
TI 47	50	1.59E+05	6.38E+04
TI 47	90	7.40E+04	4.35E+04
TI 47	212	1.47E+04	1.57E+04
TI 47	250	6.70E+03	1.22E+04
TI 47	335	4.80E+03	7.88E+03
TI 47	472	2.40E+03	4.59E+03

4.7 Hanford Trials Comparison

Table 9. Concentrations and Lateral Sigmas for Hanford Instantaneous Trials

Hanford Instantaneous							
Trial	d (m)	cp_obs	cp_pred	Trial	d (m)	sig_obs	sig_pred
HI 2	200	3.63E+00	7.29E+00	HI 2	200	5.05	7.416
HI 2	800	3.84E-01	3.00E-01	HI 2	800	N/A	27.192
HI 3	200	9.05E-01	9.59E+00	HI 3	200	11.62	7.416
HI 3	800	7.39E-02	1.29E-01	HI 3	800	22.14	33.372
HI 5	200	1.72E+00	1.06E+01	HI 5	200	8.68	7.416
HI 5	800	6.81E-02	1.14E-01	HI 5	800	N/A	38.316
HI 6	200	1.89E+00	1.04E+01	HI 6	200	7.86	8.652
HI 6	800	5.54E-02	1.11E-01	HI 6	800	39.09	46.968
HI 7	200	1.73E+00	8.12E+00	HI 7	200	9.13	11.12
HI 7	800	2.00E-02	7.62E-02	HI 7	800	49.07	46.97
HI 8	200	1.53E+00	6.12E+00	HI 8	200	9.32	8.65
HI 8	800	9.47E-02	1.49E-01	HI 8	800	27.51	29.66

Table 10. Concentrations and Lateral Sigmas for Hanford Continuous Trials

Hanford Continuous											
Trial	d (m)	cp_obs	cp_pred	Trial	d (m)	ca_obs	ca_pred	Trial	d (m)	sig_obs	sig_pred
HC 1	200	4.97E-01	1.50E-01	HC 1	200	3.30E-01	1.18E-01	HC 1	200	15.61	11.124
HC 1	800	3.39E-02	1.13E-02	HC 1	800	2.63E-02	8.83E-03	HC 1	800	70.69	43.26
HC 2	200	4.90E-02	8.01E-02	HC 2	200	2.33E-02	5.91E-02	HC 2	200	15.06	18.54
HC 2	800	4.20E-03	2.28E-03	HC 2	800	1.90E-03	1.67E-03	HC 2	800	36.20	100.116
HC 3	200	7.24E-02	1.61E-01	HC 3	200	4.54E-02	1.33E-01	HC 3	200	13.74	11.124
HC 3	800	4.40E-03	4.44E-03	HC 3	800	2.60E-03	3.66E-03	HC 3	800	38.65	72.924
HC 4	200	1.40E-01	2.58E-01	HC 4	200	6.68E-02	2.13E-01	HC 4	200	19.65	16.068
HC 4	800	1.17E-02	7.34E-03	HC 4	800	4.30E-03	6.04E-03	HC 4	800	55.24	87.756
HC 5	200	1.38E-01	1.41E-01	HC 5	200	6.33E-02	1.09E-01	HC 5	200	15.47	11.12
HC 5	800	1.95E-02	6.15E-03	HC 5	800	9.70E-03	4.72E-03	HC 5	800	37.81	49.44

5.0 STATISTICAL ANALYSIS

To quantitatively compare the predicted concentrations and lateral sigmas to those in the MDA, geometric mean and geometric variances were calculated for each set of trials. Geometric mean represents bias; a value of 1 indicates no bias. A value greater than one indicates an underprediction, a value less than one indicates an overprediction. Geometric variance represents accuracy; a value of 1 indicates perfect accuracy. The MDA developers evaluated model performance by plotting geometric mean versus geometric variance. A parabolic curve represents the lower bound for the paired statistics. The bottom of the curve at (1,1) represents no bias and perfect accuracy. As geometric mean increases or decreases, geometric variance must increase. The plots also include lines representing a factor of two in bias, which has been determined to be the typical prediction accuracy based on the variability of the atmospheric transport and dispersion processes. It is generally accepted that models within a factor of 2 are sufficiently accurate. This corresponds to a geometric mean between 0.5 and 2. A factor of 2 in accuracy is represented by a geometric variance of 1.6, while a factor of 10 in accuracy has a geometric variance of 201.

Geometric mean, MG, and geometric variance, VG, are computed from the ratios of observed, C_obs, over predicted, C_pred, concentrations and lateral sigmas:

$$MG = \exp[\left(\frac{1}{N}\right) \sum Ln(C_{obs}/C_{pred})]$$

$$VG = \exp[\left(\frac{1}{N}\right) \sum Ln^2(C_{obs}/C_{pred})]$$

N represents the number of observations.

5.1 Individual Trial Analysis

Geometric mean and variance for each set of trials, along with overall values, are shown in Table 11. Figure 5 shows these values plotted on geometric mean versus geometric variance.

Table 11. Geometric Mean and Variance for Each Set of Trials

Trial	MG	VG
Overall	1.43	5.83
Burro	0.82	7.19
Coyote	0.61	1.85
Desert Tortoise	0.82	8.24
Goldfish	4.84	38.88
Hanford	0.77	1.97
Hanford (cont)	1.01	1.64
Hanford (Inst)	0.54	2.52
Maplin Sands	2.04	5.33
Maplin Sands (LNG)	2.01	2.42
Maplin Sands (LPG)	2.05	7.24
Thorney Island	2.54	8.23
Thorney Island (cont)	1.85	2.54
Thorney Island (Inst)	2.75	10.99

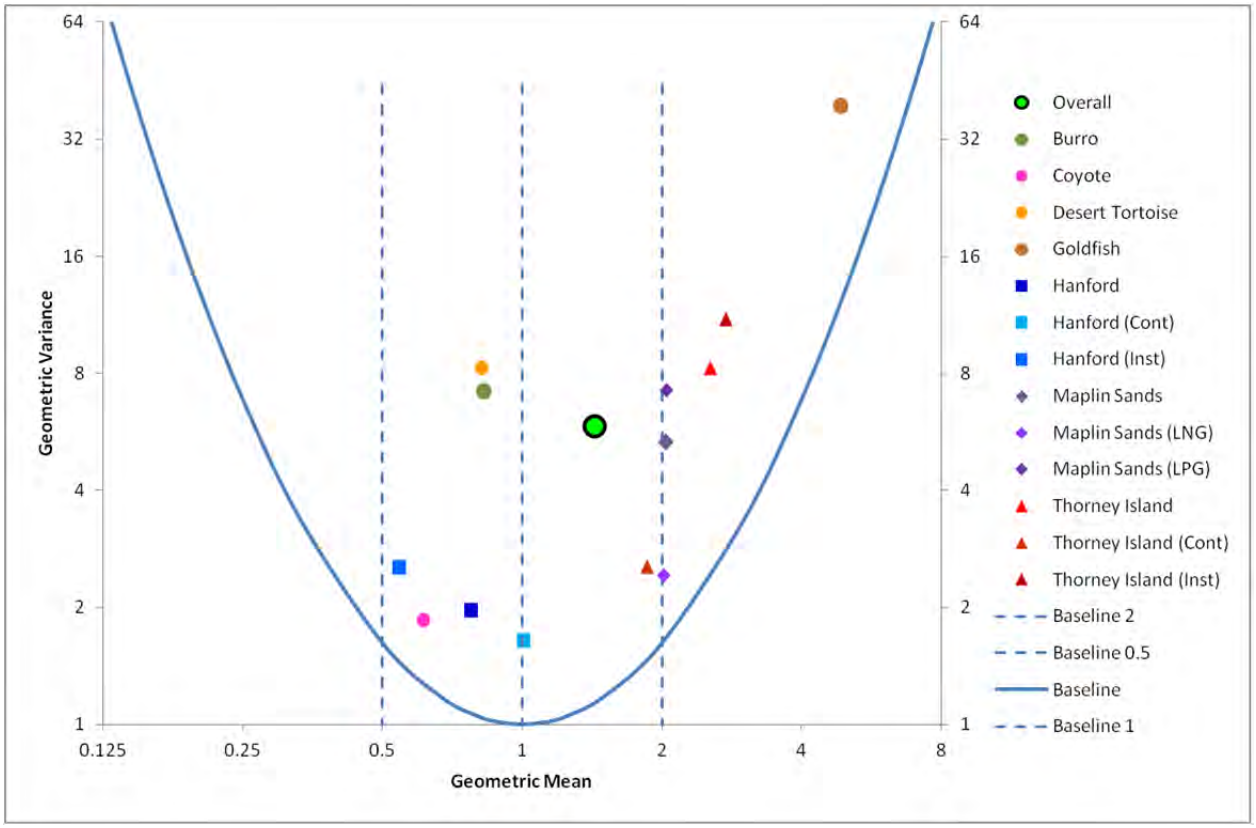


Figure 5. Plot of Geometric Mean Versus Variance for Each Set of Trials

The majority of the trials have a geometric mean between 0.5 and 2; however, results are inconsistent. The geometric variances are all above a factor of 2 accuracy and also indicating inconsistency. There is not much of a pattern to indicate whether trial results were over- or underpredicted.

The trials that overpredicted (Desert Tortoise, Burro, Coyote, and Hanford Instantaneous) tended to be overpredicting by a large margin at detectors close to the source. As the distance from the source increased, this overprediction decreased to the point, typically around 300 to 400 m, where the predicted values were less than observed values.

The trials that underpredicted (Maplin Sands LPG and LNG, Goldfish, Thorney Island continuous and instantaneous) tended to have predicted values closer to observed values at shorter distances. As the distance increased, the underprediction continued to get worse.

Overall, with all of the trials combined together, the geometric mean is safely within the region that indicates that this coupled model is relatively accurate but has a higher geometric variance than desired; average accuracy is within a factor of 3.8.

5.2 Comparison of RAILCAR-VLSTRACK to Other ATD Models

The MDA developers grouped trials based on similarities to reveal release types for which a model is accurate or inaccurate. They created five groups and compared other ATD models on the same parabolic curve described above. These five groups are:

- Group 1: All continuous-release dense gas dataset, for short averaging times (Burro, Coyote, Desert Tortoise, Goldfish, Maplin Sands, Thorney Island Continuous)
- Group 2: Same as Group 1, but for longer averaging times
- Group 3: All continuous-release, neutrally buoyant passive gas datasets (Prairie Grass and Hanford Continuous)
- Group 4: All instantaneous-release dense gas datasets (Thorney Island Instantaneous)
- Group 5: All instantaneous-release neutrally buoyant passive gas datasets (Hanford Instantaneous)

Figure 6 shows the comparison of the concentrations of continuous dense gas with short averaging times (Group 1).

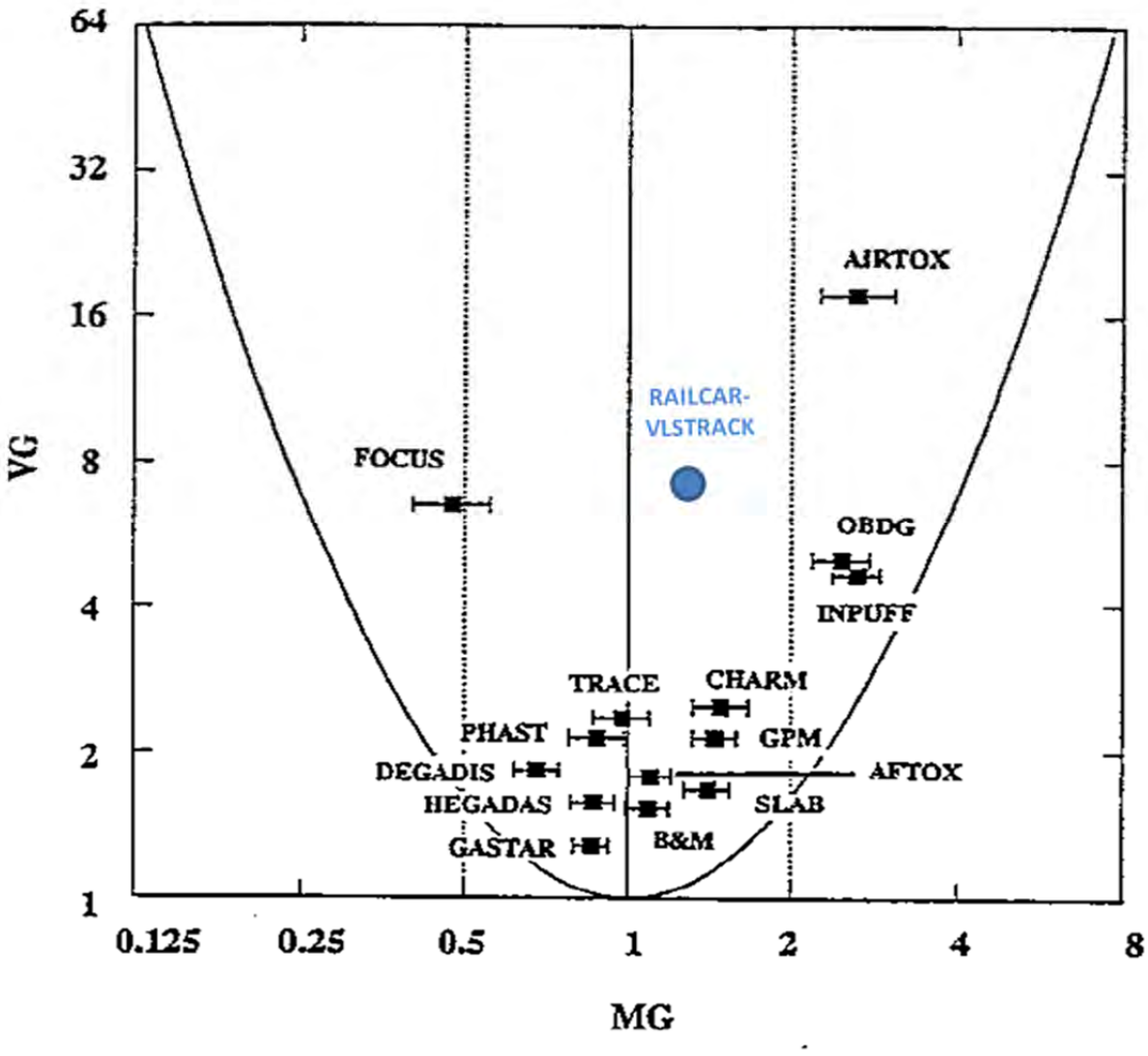


Figure 6. Comparison of ATD Models in Group 1

This comparison is similar to the comparison of all trials, with the RAILCAR-VLSTRACK geometric mean and variance being 1.29 and 7.56, respectively. Figure 7 shows the comparison of Group 2.

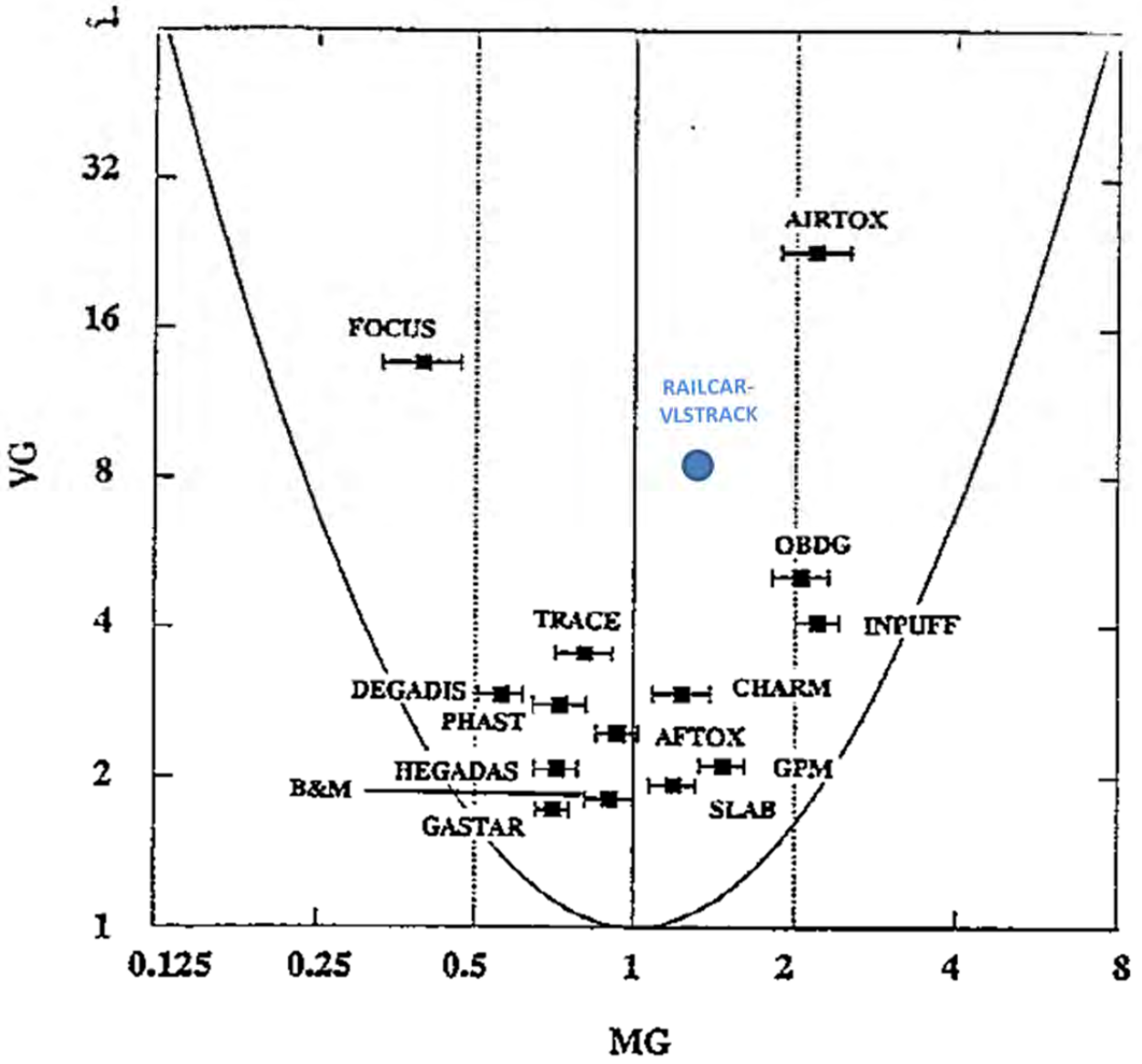


Figure 7. Comparison of ATD Models in Group 2

Again, the trend continues for the longer averaging times. The RAILCAR-VLSTRACK geometric mean and variance are 1.27 and 8.49, respectively. Figure 8 shows the comparison of the concentrations of instantaneous dense gas releases (Group 4).

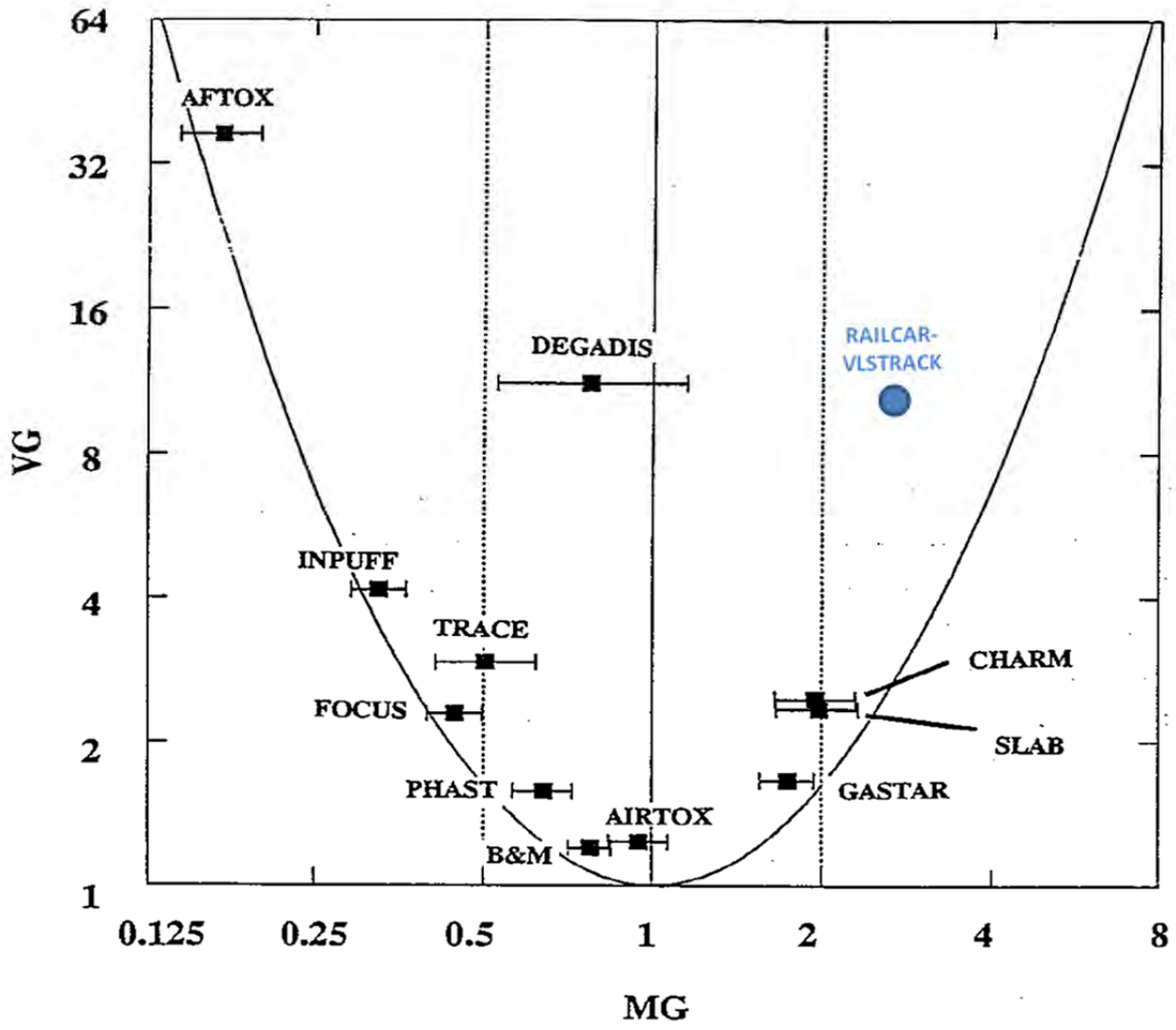


Figure 8. Comparison of ATD Models in Group 4

This comparison, which is just for the Thorney Island Instantaneous trials, shows RAILCAR-VLSTRACK severely underpredicting trial results, whereas most other ATD models overpredicted concentrations. Figure 9 shows the comparison of Group 1 trials at distances equal to or over 200 m.

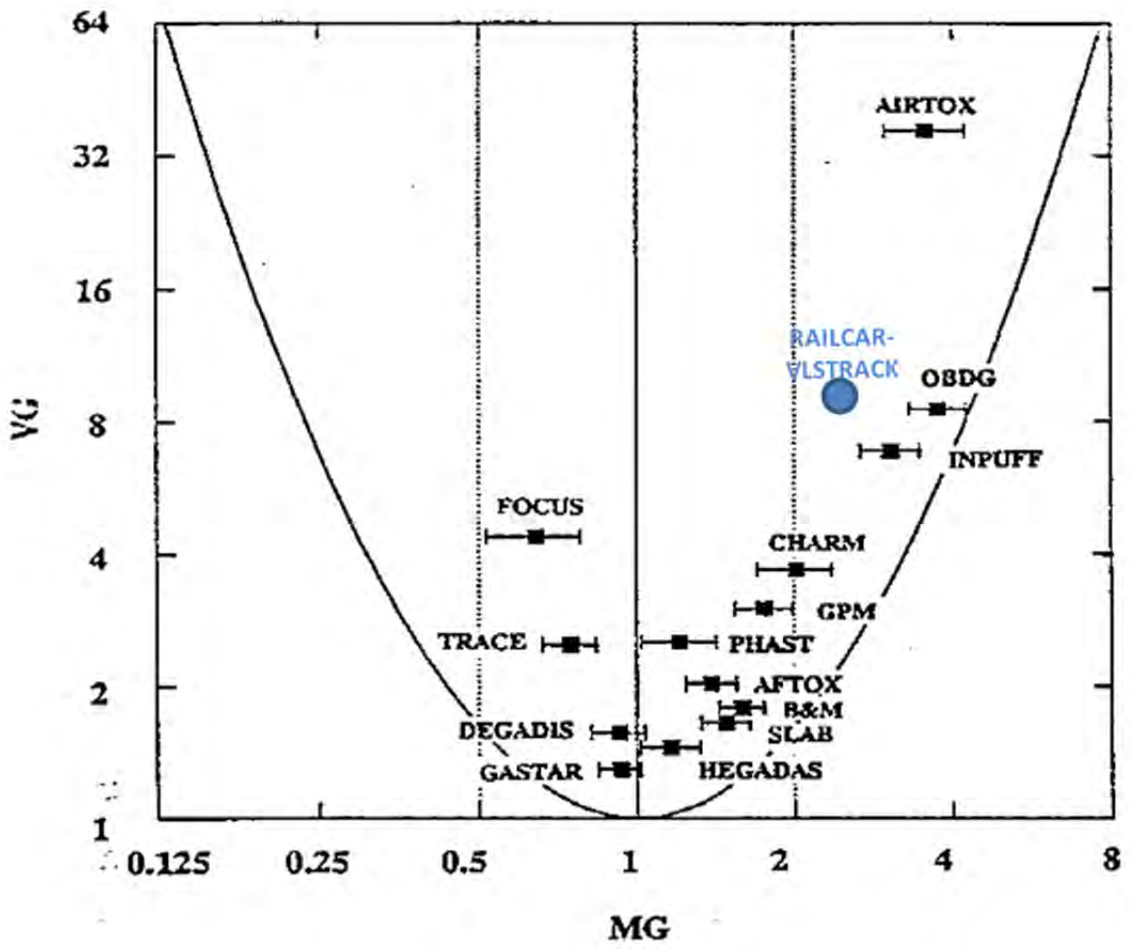


Figure 9. Group 1 Concentrations at Distances Equal to or Greater than 200 Meters

It is evident that most ATD models underpredict on distances greater than 200 m. RAILCAR-VLSTRACK is no different with a geometric mean and variance of 2.51 and 8.72, respectively. Similarly, Figure 10 shows comparisons of the concentrations of Group 4 at distances equal to or greater than 200 m.

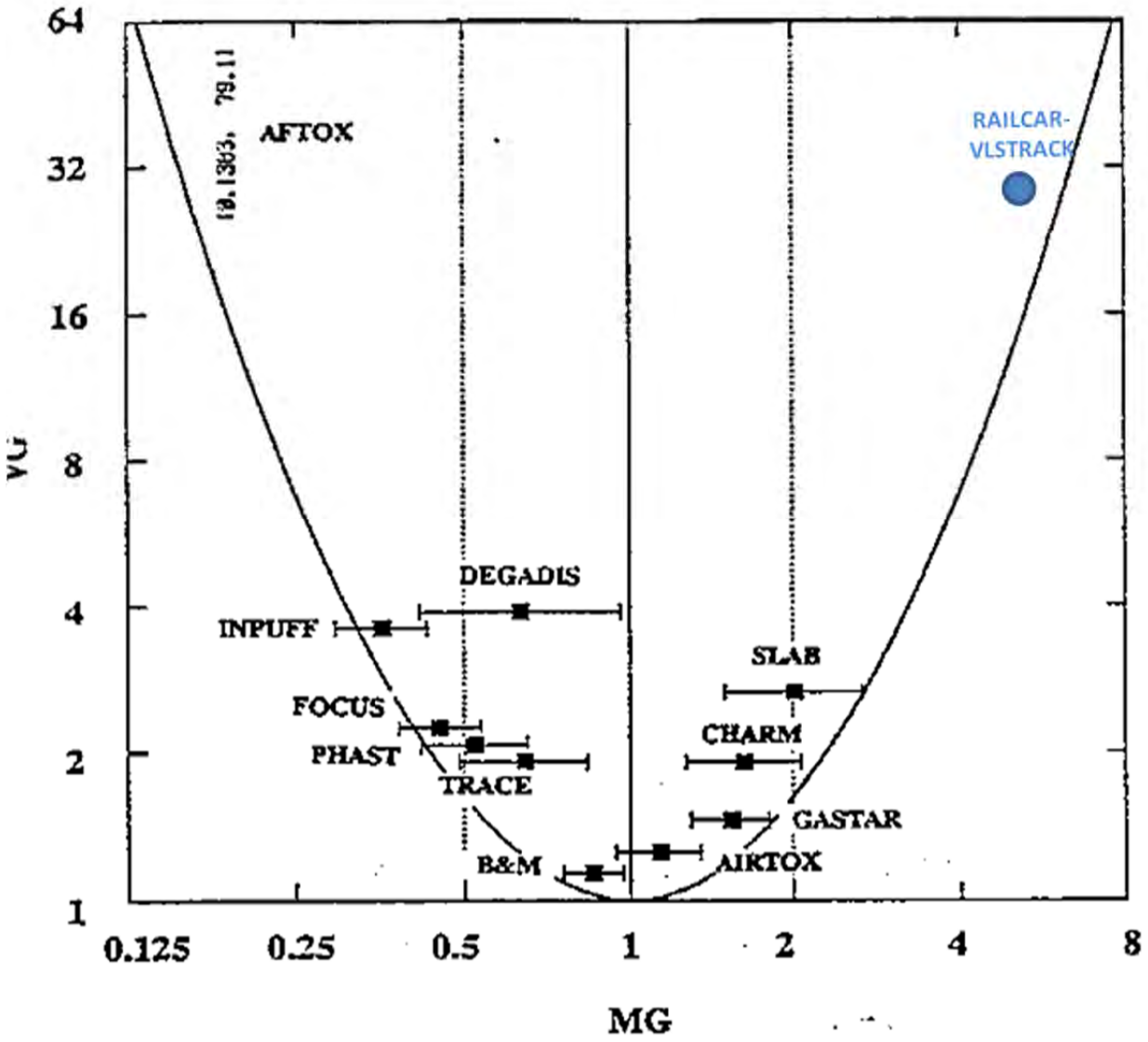


Figure 10. Group 4 Concentrations at Distances Equal to or Greater than 200 Meters

The RAILCAR-VLSTRACK model vastly underpredicts concentration in this comparison. The geometric mean and variance were 4.57 and 27.48, respectively. Figure 11 shows the comparison of concentrations from Group 1 at distances under 200 m.

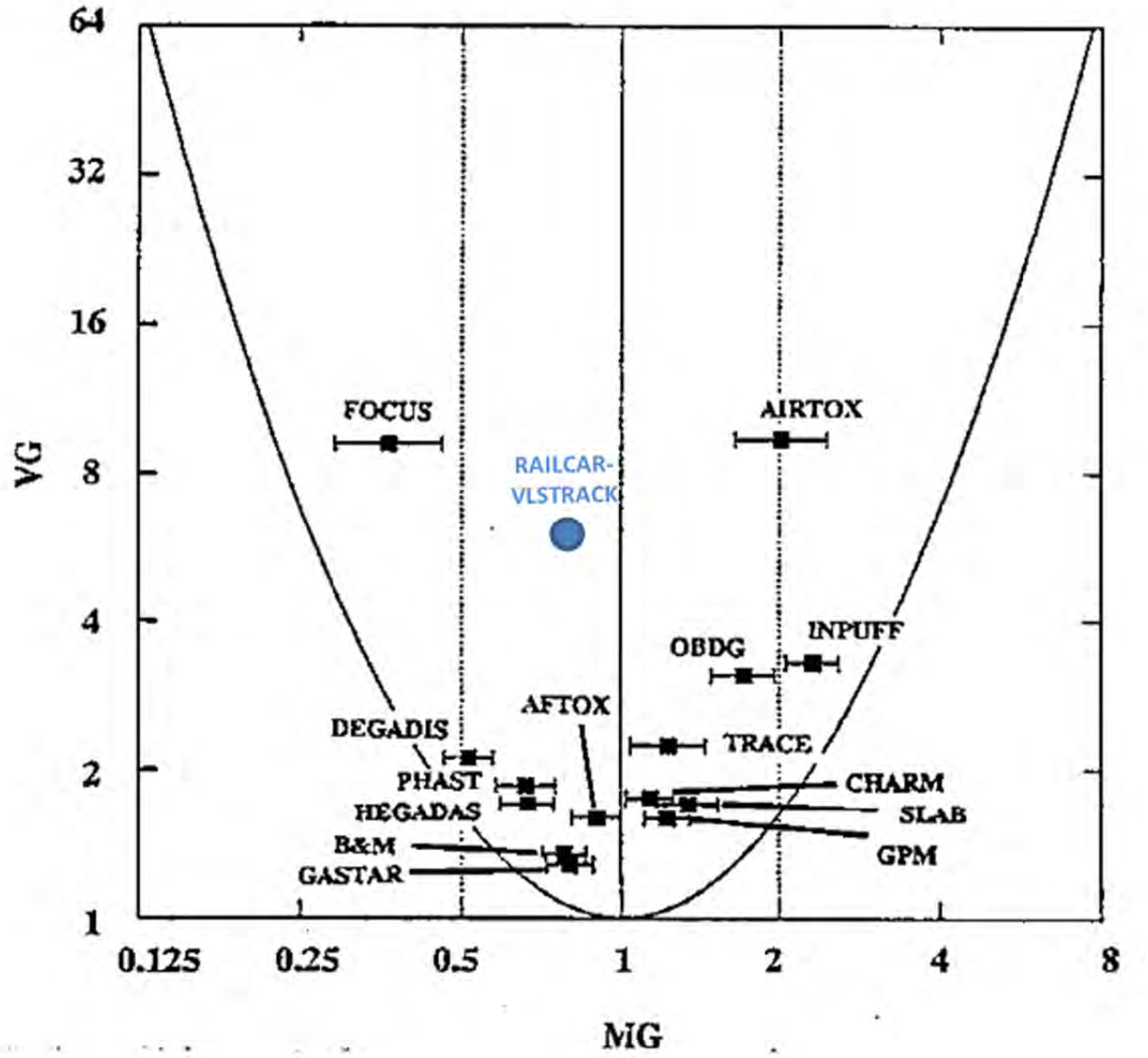


Figure 11. Group 1 Concentrations at Distances Less than 200 Meters

As observed in Section 5.1, at closer distances, this coupled model overpredicts concentrations, resulting in a geometric mean and variance of 0.79 and 6.14, respectively. Figure 12 displays the comparison of concentrations of Group 4 at distances under 200 m.

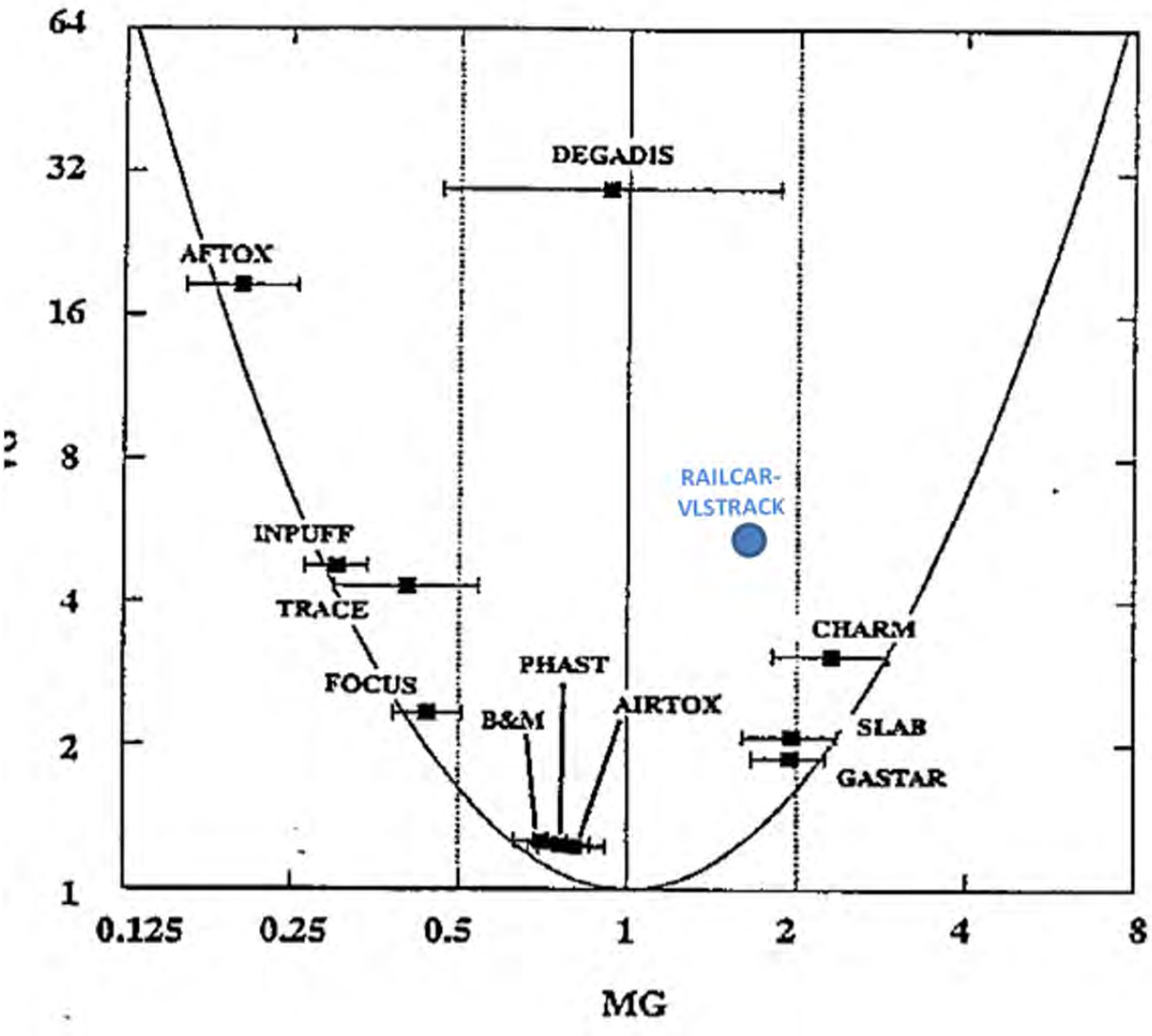


Figure 12. Group 4 Concentrations at Distances Less than 200 Meters

This plot reflects considerable inaccuracy for most models predicting the Thorney Island Instantaneous trials, as most other models overpredict at a close range but RAILCAR-VLSTRACK underpredicts: MG = 1.73 and VG = 4.79. Figure 13 shows the comparisons of concentrations from continuous passive, neutrally buoyant gas trials (Group 3).

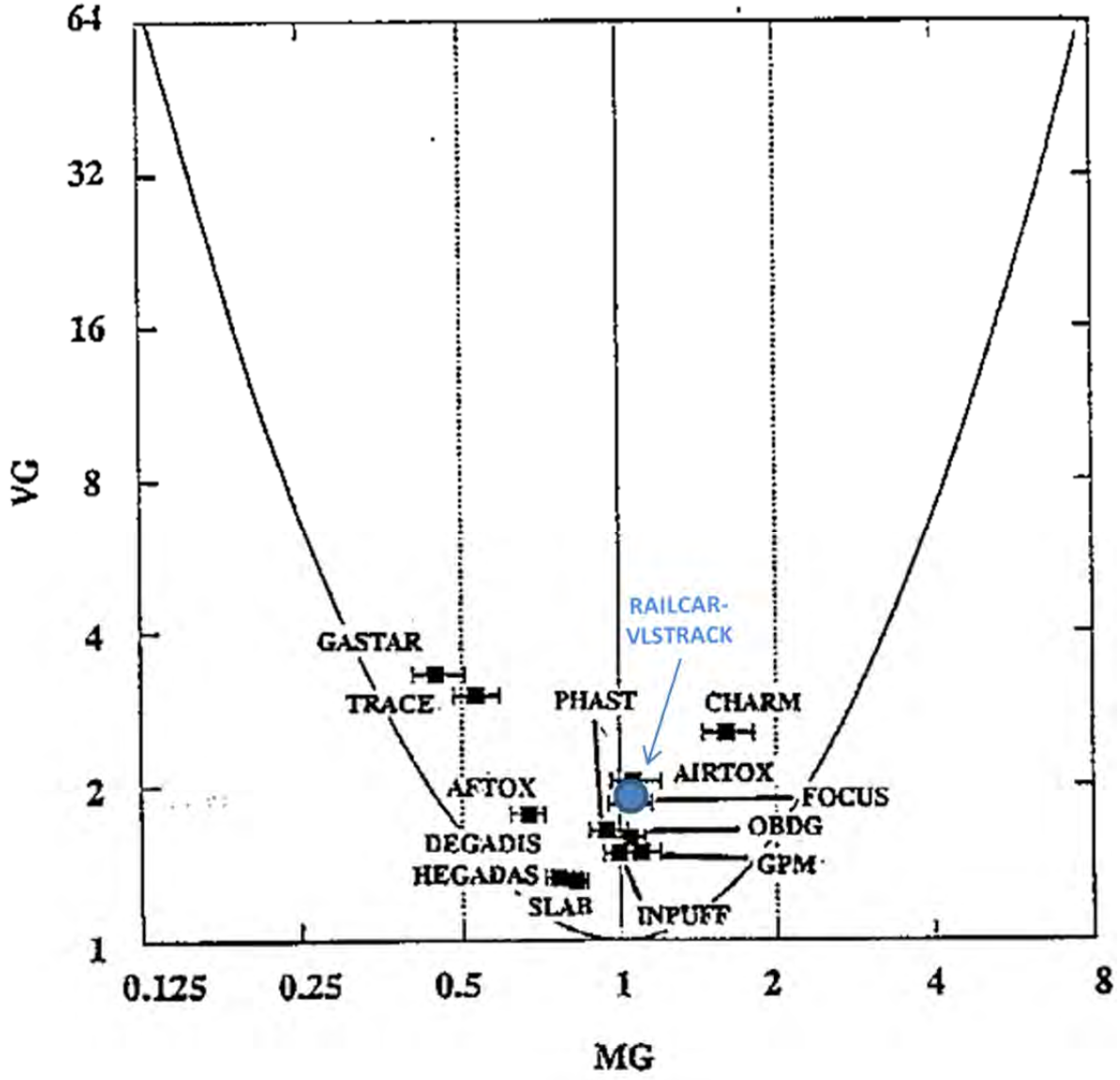


Figure 13. Comparison of Concentrations of ATD Models in Group 3

The RAILCAR-VLSTRACK model simulates this dataset very accurately, with geometric mean and variance of 1.06 and 1.87, respectively. Note Prairie Grass trials have not yet been simulated, so this data point was calculated with only Hanford Continuous trials. Figure 14 displays comparisons of ATD models from Group 5.

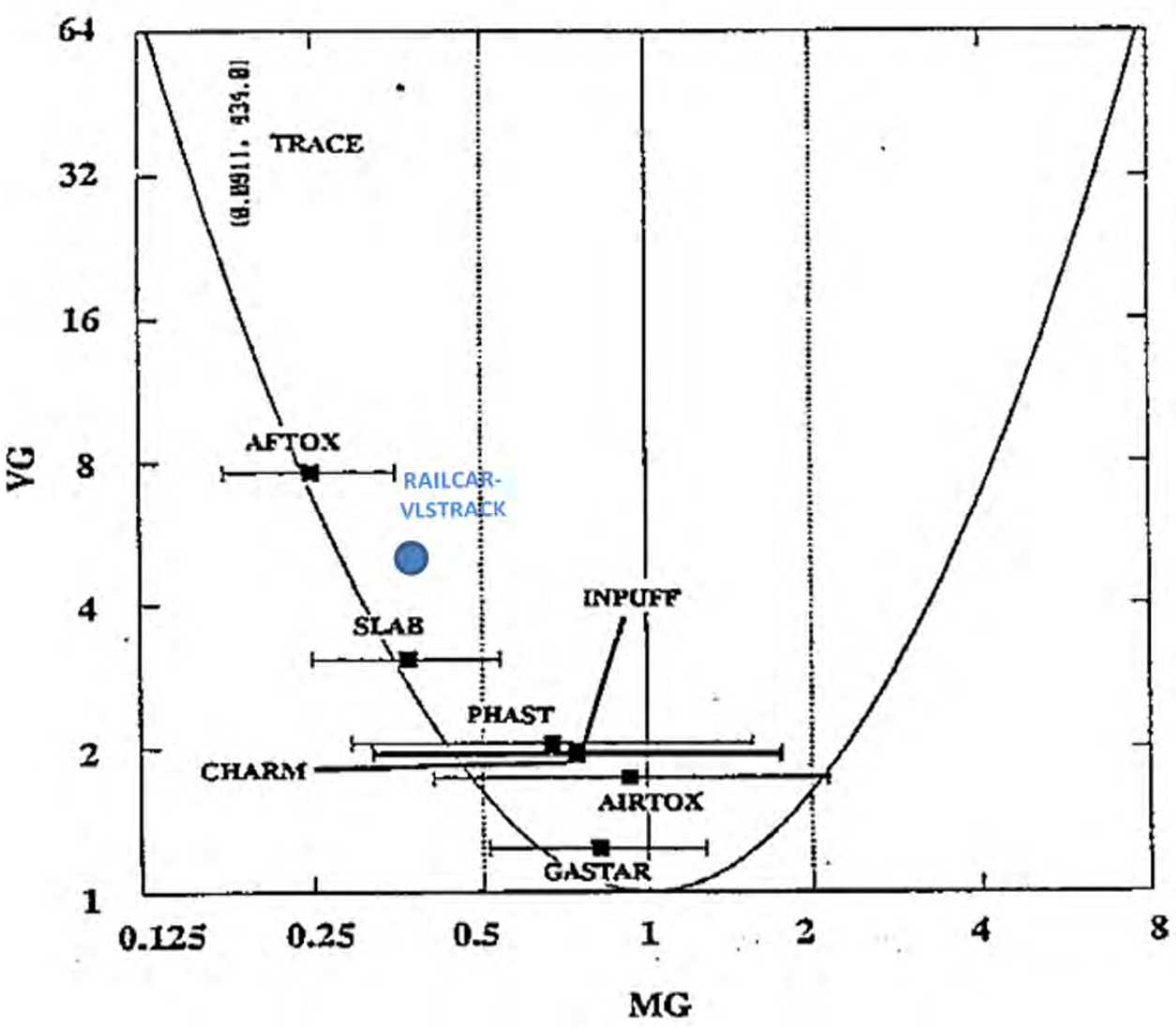


Figure 14. Comparison of Concentrations of ATD Models in Group 5

The large overprediction here (MG = 0.35 and VG = 5.17) is consistent with other ATD models which also overpredict. Figure 15 compares the concentration of continuous dense gas trials for distances equal to or greater than 200 m with stable ambient conditions (Pasquill stability category of E or F).

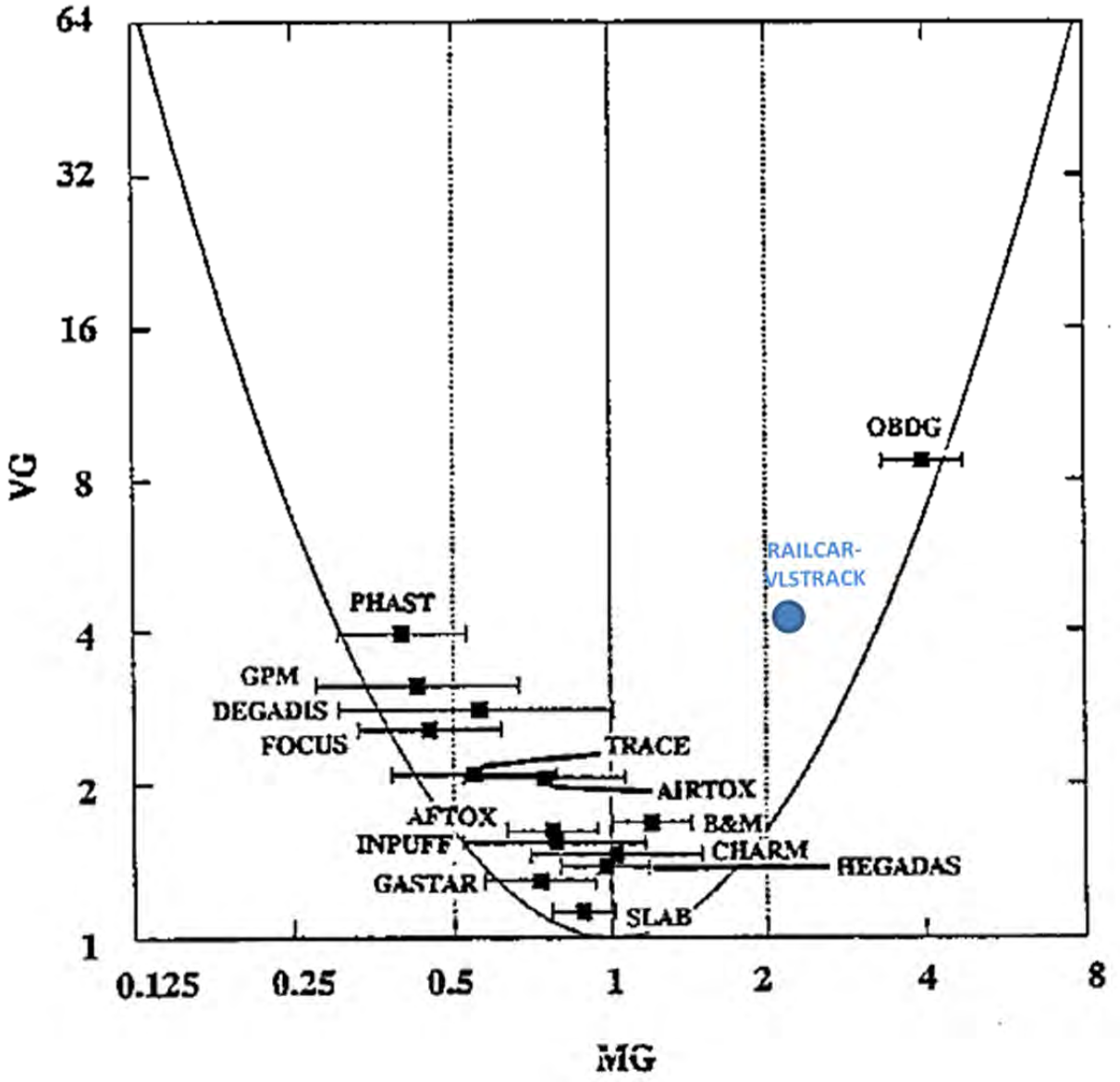


Figure 15. Group 1 Concentrations at Distances ≥ 200 m with Stable Ambient Conditions

RAILCAR-VLSTRACK severely underpredicts the concentrations at longer distances with stable conditions. Other ATD models tend to overpredict in this situation. Figure 16 shows the same comparison as Figure 15, except with Group 4 rather than Group 1.

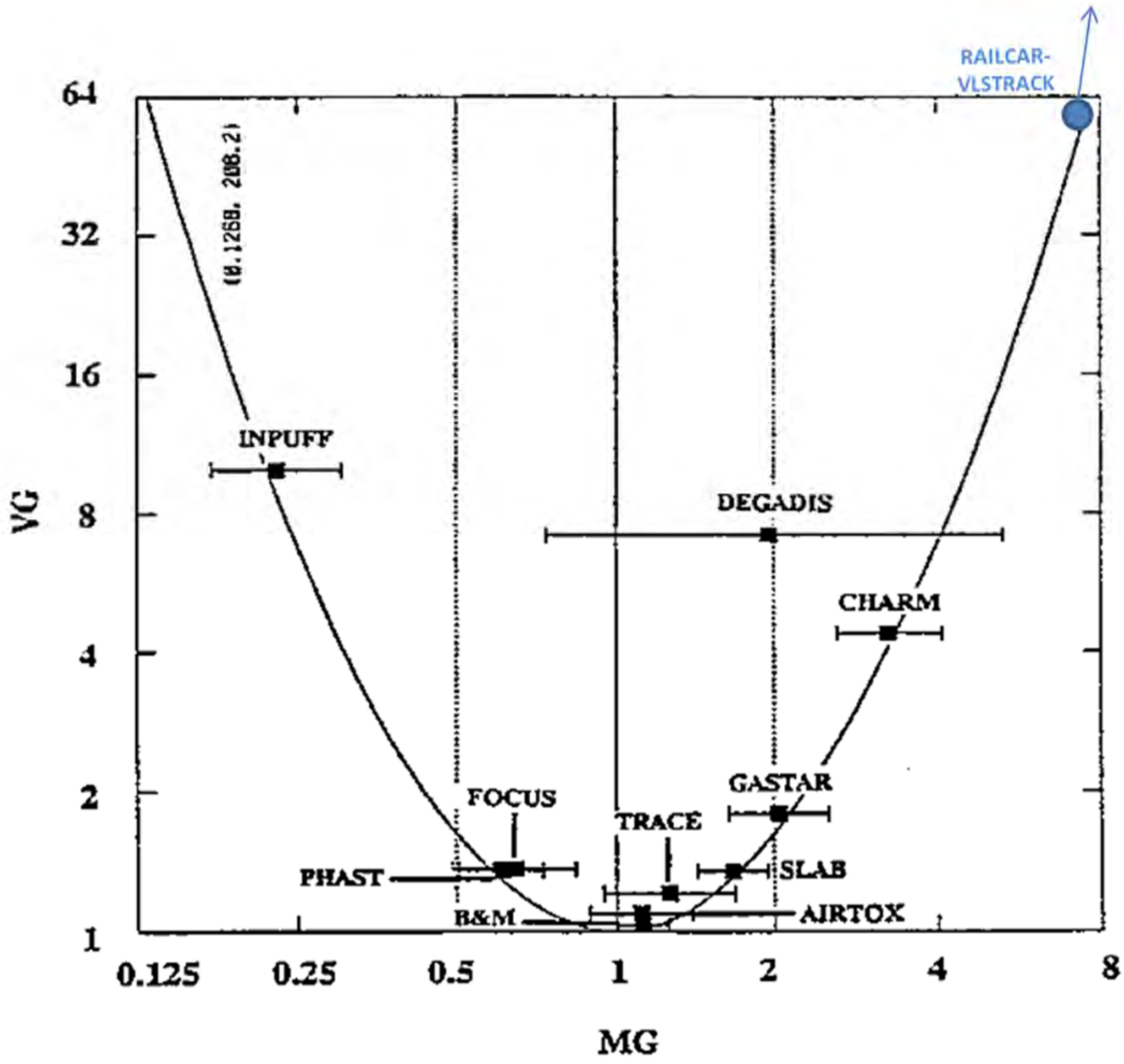


Figure 16. Group 4 Concentrations at Distances ≥ 200 m with Stable Ambient Conditions

Sadly, this data point is not even on the plot with a very severe underprediction resulting in a geometric mean and variance of 10.47 and 295.68, respectively. This result is not surprising as this comparison is a small subset of the Thorney Island Instantaneous trials and it was already noted that this set of trials as a whole was not accurate. Figure 17 compares the plume widths from Group 2 trials.

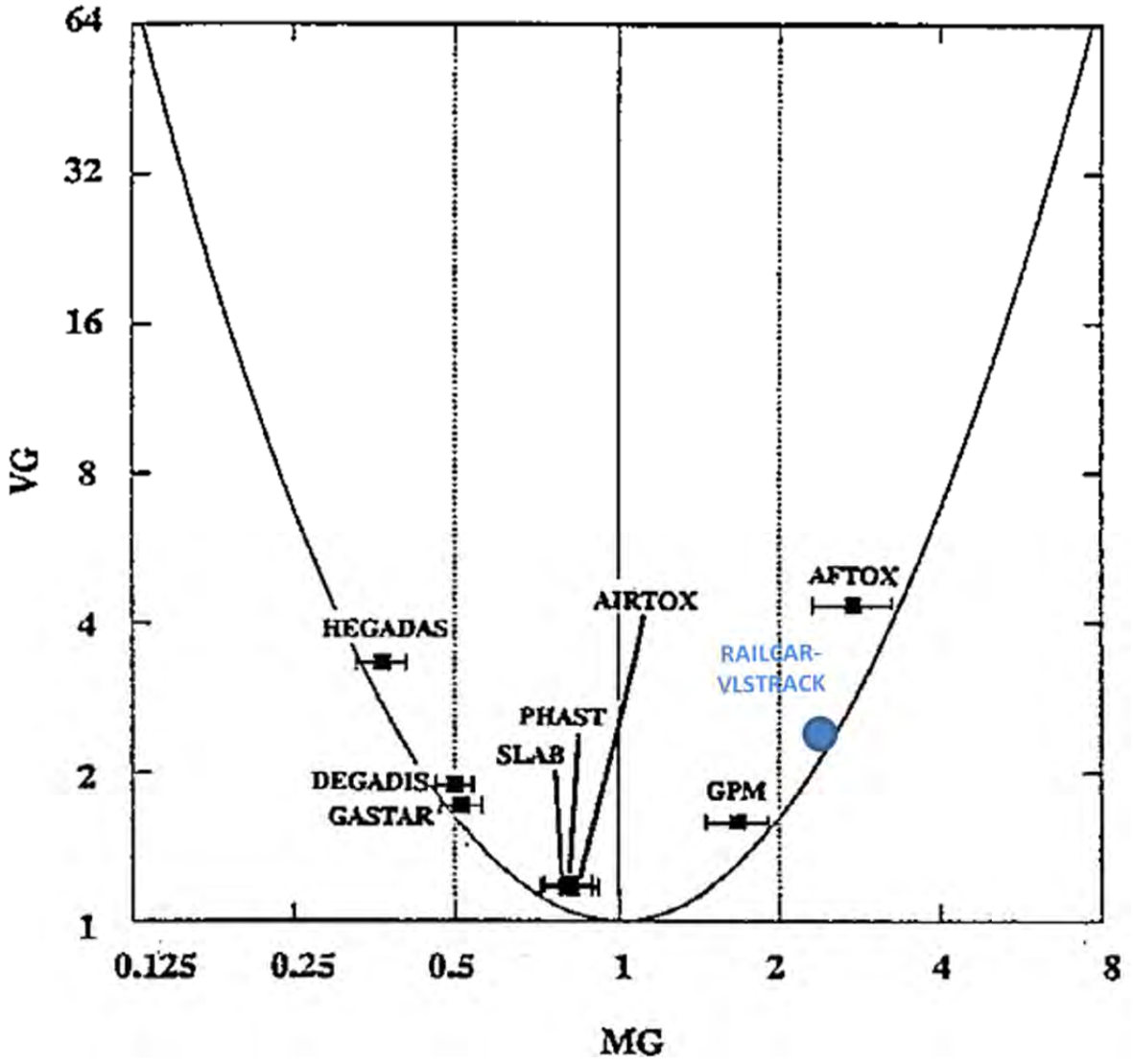


Figure 17. Comparison of Plume Widths from Group 2 Trials

This plot shows the RAILCAR-VLSTRACK model tends to underpredict the plume width, but it does so without much variation, resulting in a geometric mean and variance of 2.35 and 2.33, respectively. Figure 18 compares the plume widths from Group 4 trials.

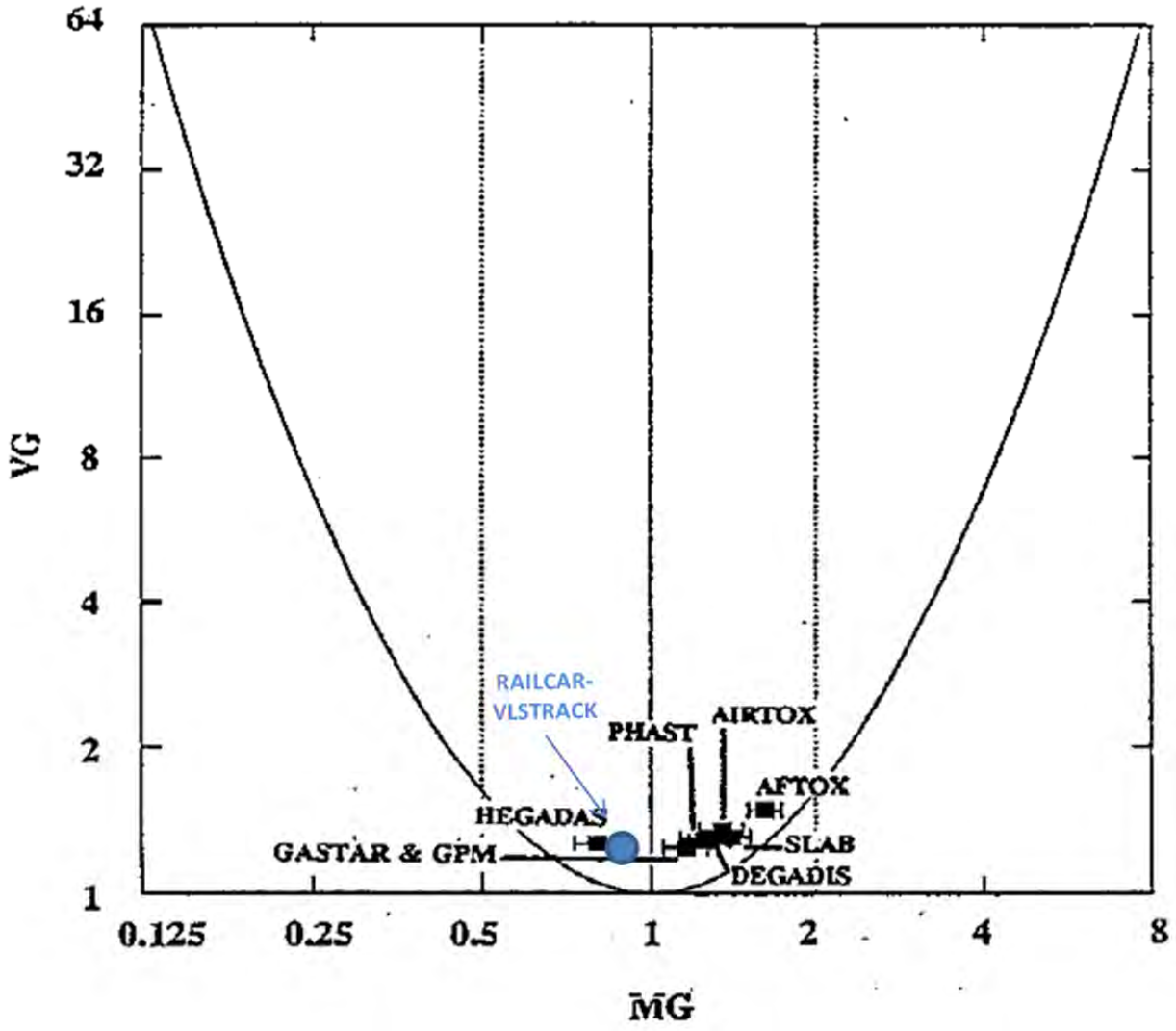


Figure 18. Comparison of Plume Widths from Group 4 Trials

While the concentrations predicted by RAILCAR-VLSTRACK may not have been accurate for the Thorney Island Instantaneous trials, the plume width was accurate, resulting in a geometric mean and variance of 0.90 and 1.26, respectively.

6.0 CONCLUSION

As evidenced in the analyses in Sections 5.1 and 5.2, the RAILCAR-VLSTRACK model proves to be a viable model for the release of TICs into the environment. Although, it has a large variation of whether it under- or overpredicts the concentrations of TIC downwind, it suffices as a feasible model that will give relatively accurate predictions. Overall, the geometric mean is acceptable (1.43), but the geometric variance (5.83) was higher than most other ATD models. In general, as the distance downwind increased, the RAILCAR-VLSTRACK model simulated more of an underprediction of concentration. However, this trend was similar in other ATD models that have also been validated using the MDA.

It is entirely possible that, in an uncontrolled event, this coupled model would be more accurate. VLSTRACK was designed to simulate an attack, whereas the field trials in the MDA were conducted in a highly controlled manner. Although RAILCAR and VLSTRACK were executed separately, it is not possible at this time to separate the relative accuracy of each model. The greatest source of error is likely due to the inability of VLSTRACK to simulate an area vapor source. Representing a large area source as many small Gaussian puffs leads to large concentration fluctuations near the source location; however, the relative diffusion of a small puff will also be different than that of an area source. The majority of the modeling error is tentatively attributed to VLSTRACK and not RAILCAR.

This validation process is not completed. Although the emphasis was on the dense gas field trials in the MDA, the remaining neutrally buoyant gas trials can also be used to validate VLSTRACK. The project time period ended before the Prairie Gas field trials could be simulated. VLSTRACK readily simulates the Prairie Grass sulfur dioxide plumes. Also, Jack Rabbit II field trials are set to be completed during FY16. Once these data are available, they will also be used to validate the combined models. This validation may prove to be more useful, as the Jack Rabbit II will release chlorine into the environment from a large transportation tank, which is the type of release that RAILCAR was created to simulate. Resulting chlorine clouds, though, will still have to be represented as many small puffs for VLSTRACK simulations.

RAILCAR integration into the ALOHA and QUIC ATD models is near completion. The above process will be repeated to validate these two coupled models using the MDA. Both of these ATD models simulate area vapor sources without having to approximate them as done for VLSTRACK. Significantly improved statistical results compared to these RAILCAR-VLSTRACK results will first verify the benefit of the RAILCAR source characterization and second support the assumption that the VLSTRACK puff approximation is the primary cause of the validation inaccuracy.

7.0 REFERENCES

1. Bauer, T. J., *Software User's Manual for the RAILCAR4 Toxic Industrial Chemical Source Characterization Program*, NSWCDD/TR-12/68, Naval Surface Warfare Center, Dahlgren Division, Dahlgren, VA, August 2011.

2. Bauer, T. J., and Wolski, M. G., *Software User's Manual for the Chemical/Biological Agent Vapor, Liquid, and Solid Tracking (VLSTRACK) Computer Model, Version 3.1*, NSWCDD/TR-01/83, Naval Surface Warfare Center, Dahlgren Division, Dahlgren, VA, April 2001.

3. Hanna, S. R.; Strimaitis, D. G.; and Chang, J. C., *Hazard Response Modeling Uncertainty (A Quantitative Method), Volume II, Evaluation of Commonly Used Hazardous Gas Dispersion Models*, Sigma Research Corporation, Westford, MA, September 1991.

DISTRIBUTION

	Copies
DOD ACTIVITIES (CONUS)	
DEFENSE TECH INFORMATION CTR 8725 JOHN J KINGMAN RD SUITE 0944 FORT BELVOIR VA 22060-6218	2
NON-DOD ACTIVITIES (CONUS)	
ATTN DOCUMENT CENTER THE CNA CORPORATION 4825 MARK CENTER DRIVE ALEXANDRIA VA 22311-1850	1
ATTN GOVERNMENT DOCUMENTS SECTION LIBRARY OF CONGRESS 101 INDEPENDENCE AVENUE SE WASHINGTON DC 20540-4172	4

	Copies
INTERNAL	
1033 (TECHNICAL LIBRARY)	2
Z24 (DAVË)	1
Z24 (BAUER)	1

DAHLGREN