

A REPORT ON

**Fluidyn PANACHE - PANEPR VALIDATION WITH
DENSE GAS DISPERSION EXPERIMENTS**

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Fluidyn PANACHE - PANEPR VALIDATION

With

DENSE GAS DISPERSION EXPERIMENTS

INTRODUCTION

The U.S. Environmental Protection Agency (EPA) has an ongoing program to evaluate the performance of several categories of air quality simulation models by comparing observed and predicted concentrations using performance measures recommended by the American Meteorological Society (AMS). Rural, Urban, Mobile, Complex Terrain and long-range transport models are categories of models that have already been evaluated. Models for toxic pollutant releases represent a broad class of models for which EPA has previously performed little evaluation work.

Releases of toxic chemicals to the atmosphere can involve complex source dynamics and chemistry. A toxic chemical release can be modeled using the procedures developed for criteria air pollutants, provided that the gas is not dense or highly reactive and it does not rapidly deposit on surfaces. In order to select an appropriate modeling approach for a toxic chemical, the release must first be categorized in terms of physical state, release condition and dispersive characteristics.

An understanding of the process/release condition of a toxic release is required to model the atmospheric dispersion of a toxic chemical. This condition can help determine both the physical state and dispersive characteristics of the released chemical. For example, if the release is from a leak in a pressurized liquefied gas storage tank, additional source modeling is required to determine the state of the material as it enters the atmosphere, since the release may include both liquid and gaseous (aerosol) components, in addition to the source term and initial dispersive characteristics, air toxics models must also provide proper simulation of the cloud characteristics downwind of the release. The cloud characteristics are often complex when dense, highly reactive or rapidly depositing chemicals are released.

Toxic chemicals are often short duration and the concentrations of interest are near instantaneous averages. Typical concerns from a toxic release are the maximum instantaneous concentration and the maximum dosage. Many toxics models are designed to provide concentration predictions or unit averaging times ranging from 0.1 sec. to 1 hour. By contrast, regulatory models for most criteria pollutants have a basic averaging time of one hour for concentration estimates.

DESCRIPTION OF THE STUDY

This report describes briefly the experimental set up, model input data, observed results and comparison of PANEPR and some of the public domain models (like DEGADIS and SLAB) and proprietary models' (viz., AIRTOX, CHARM, FOCUS, SAFEMODE and TRACE) predictions for three dense gases dispersions namely, liquefied ammonia - NH₃, anhydrous hydrofluoric acid - HF and liquefied natural gas - LNG (the experiments are called Desert Tortoise, Goldfish and Burro series respectively).

EXPERIMENTAL SET UP

1. DESERT TORTOISE PRESSURIZED AMMONIA RELEASES

Four large scale (ranging from 15 – 60 m³) pressurized liquid ammonia experiments called “Desert Tortoise Series” were conducted in 1983 at the Liquefied Gaseous Spill Test Facility in Nevada (which later became a permanent test facility for the U.S Department of Energy and later for the U.S EPA. Lawrence Livermore National Laboratory conducted the releases with the sponsorship of the U.S. Coast Guard, the Fertilizer Institute and Department of Environment Canada. The experiments were carried out with a 81-133 Kg/sec horizontal flash boiling jet source and the duration were 1 to 8 minutes. The wind speeds were fairly strong with 5 – 7 m/sec, and the air was dry and hot with 30 – 33° C and just 10 –21 % relative humidity. The site was a normally dried out lakebed, but prior to the experimental campaign it was flooded by unusually heavy rainfall, and during the experimental period the surface changed from moist soil with scattered water pockets to a dry surface.

The experimental design included two lines of 7 and 5 masts distributed across the plume at 100 m and 800 m distance from the source. Each mast was equipped with concentration and temperature sensors at three levels. Pressure, flow and temperature measurements were made on the release system and the soil in front of the release was equipped with heat flux gauges and temperature sensors.

Ammonia tanks were used to feed a six-inch pipeline leading to the spill point. Ammonia was released at elevated (storage) pressure and ambient temperature with a nitrogen system used to provide constant tank pressure. The actual release was made through an orifice plate at the end of the spill pipe at a height of 0.79 m the jet release was directed horizontally down the grid. An analysis of time of arrival of the gas cloud as indicated by the temperature and concentrations time series on both the 100 m and 800 m arcs indicated that the evidence of a momentum jet (i.e., cloud speed in excess of the wind speed) at 100 m in all tests and at 800 m for tests 2 and 4. Release pressures were approximately 150-170 psia at temperatures 20-24°C.

Table 1 Release volumes and rates for Ammonia Release

<i>Test</i>	<i>Volume (m³)</i>	<i>Spill Rate (m³/min.)</i>
1	14.9	7.0
2	43.8	9.8
4	60.3	8.5

Numerous measurements were made in the area of the spill. The temperature of the fluid just prior to its exit from the spill pipe was recorded. Heat flux sensors were placed just below the surface of the soil at different locations. Also, a thermocouple rake assembly was installed in the spill area for the purpose of determining the temperature gradient within the liquid for the confined spills. Thermocouples were installed at the ground level and at different heights. Provision was also made for measuring the depth (pressure head) of the liquid NH₃ during the confined spills.

In addition to the spill area measurements, flow rates, temperatures and pressures near the release point and liquid flow rates and temperature measurements in the soil designed to evaluate pooling, atmospheric boundary layer, wind field, vapor cloud temperature and concentration and surface heat flux measurements were also made using an extensive diagnostic system developed by LLNL.

Several assumptions were made regarding the release configuration for the evaluation. The release configuration resulted in a complex two-phase, horizontal jet with substantial momentum. Documentation indicates that some liquid pooling was observed near the release point, but pool characteristics were not reported. As a result, the release configuration for the data archive assumes a gaseous release of heavy gas, with unspecified initial cloud dimensions. For the archive, emissions were estimated using mass flux estimation techniques using observed concentration data at 800 m downwind of the release point. Only 70% of mass could be accounted for with this technique.

Three tests were conducted for similar meteorological conditions. Tests were performed under D and E stability conditions in moderate winds of 4.5 to 7.4 m/sec. ambient temperatures ranged from 28.8 to 33.7°C. Wind measurements were taken at 2.0 m height and averaged for test duration were included in the data archive.

The site is a desert location on a normally dry lakebed. Surface roughness for the site was reported as 0.003 m, but various portions of the sampling grid were covered with water in three of the four tests, due to unusual rainfall in the area. Humidity on the site could be assumed high due to evaporation of the lake, but humidity and pressure measurements are not available at the site. Model input data is shown below.

Table 2 MODEL INPUT DATA

Sl. No.	Input Data	Desert Tortoise		
		DT1	DT2	DT4
1.	TERRAIN			
	Longitude	-25.57	-25.57	-25.57
	Latitude	36.48	36.48	36.48
	Roughness Length (m)	0.003	0.003	0.003
	Computation Domain (m ³)	1600x1000x50	1600x1000x50	1600x1000x50
2.	Monitor Point Height (m)	1.0	1.0	1.0
	SOURCE			
	Source Type	Point	Point	Point
	Exit Velocity (m/sec)	81.2	85.2	92.5
	Source Height (m)	0.79	0.79	0.79
	Mass Flux (Kg/sec.)	81.0	117.0	108.0
	Release Temperature (°C)	21.50	20.10	24.10
3.	Release Duration (sec.)	126	255	381
	WEATHER			
	Wind Speed (m/sec.)	7.42	5.76	5.50
	Wind Direction (Degrees)	267.30	271.20	274.30
	Anemometer Height (m)	2.0	2.0	2.0
	Relative Humidity (%)	13.2	17.5	21.0
	Ambient Temperature (°C)	29.30	30.50	33.00
	Ambient Pressure (m bars)	909.00	910.00	903.00
	Cloud Cover (10's of %)	1	4	1
	Stability Class	D	D	D
	Wind Profile	Power Law (exp. = 0.007)	Power Law (exp. = 0.007)	Power Law (exp. = 0.00555)
	Temperature Profile	Two Step	Two Step	Two Step
	Lapse Rate (°C/m)	0.057083	0.04094	0.04933
Mixing Height (m)	100	100	100	
Inv Lapse Rate (°C/m)	0.01	0.01	0.01	
4.	SIMULATION			
	Mesh Size Chosen	53, 33, 10	53, 33, 10	53, 33, 10
	Grid Fineness Parameter	7	7	7
	Date	24/08/1983	01/09/1983	06/09/1983
	Time	16:37:47	11:20:56	18:15:07
	Time Zone	- 6.0	- 6.0	- 6.0
	Duration (Sec.)	600	900	1000
	Fluid Type	Compressible	Compressible	Compressible
	Wind Model	Solve	Solve	Solve
	Buoyancy Model	Bouyancy (gz=9.803)	Bouyancy (gz=9.803)	Bouyancy (gz=9.803)
	Wall Type	Log Law2	Log Law2	Log Law2
	Turbulence Model	K Diff	K Diff	K Diff

Ammonia concentrations were sampled on a downwind grid at distances of 100m and 800 m from the spill location. At 100 m downwind, gas samplers were located at heights of 1.0, 3.5 and 6.0 m above ground. A second sampling arc was located at 800 m with five 10 m towers sampling gas at 1.0, 3.5 and 8.5 m with 100 m crosswind separation. Further downwind, eight portable sensors were used to sample concentrations at either 1400 m, 2800 m or 5500 m at a height of 1.0 m. concentrations were averaged to obtain 30 second values for the data archive.

It may be noted that out of the five monitor stations installed at different heights on each arc (with different cross wind separations) the one which was located at 1m level showed a maximum pollutant concentration and the same is taken here for the model prediction comparison purpose.

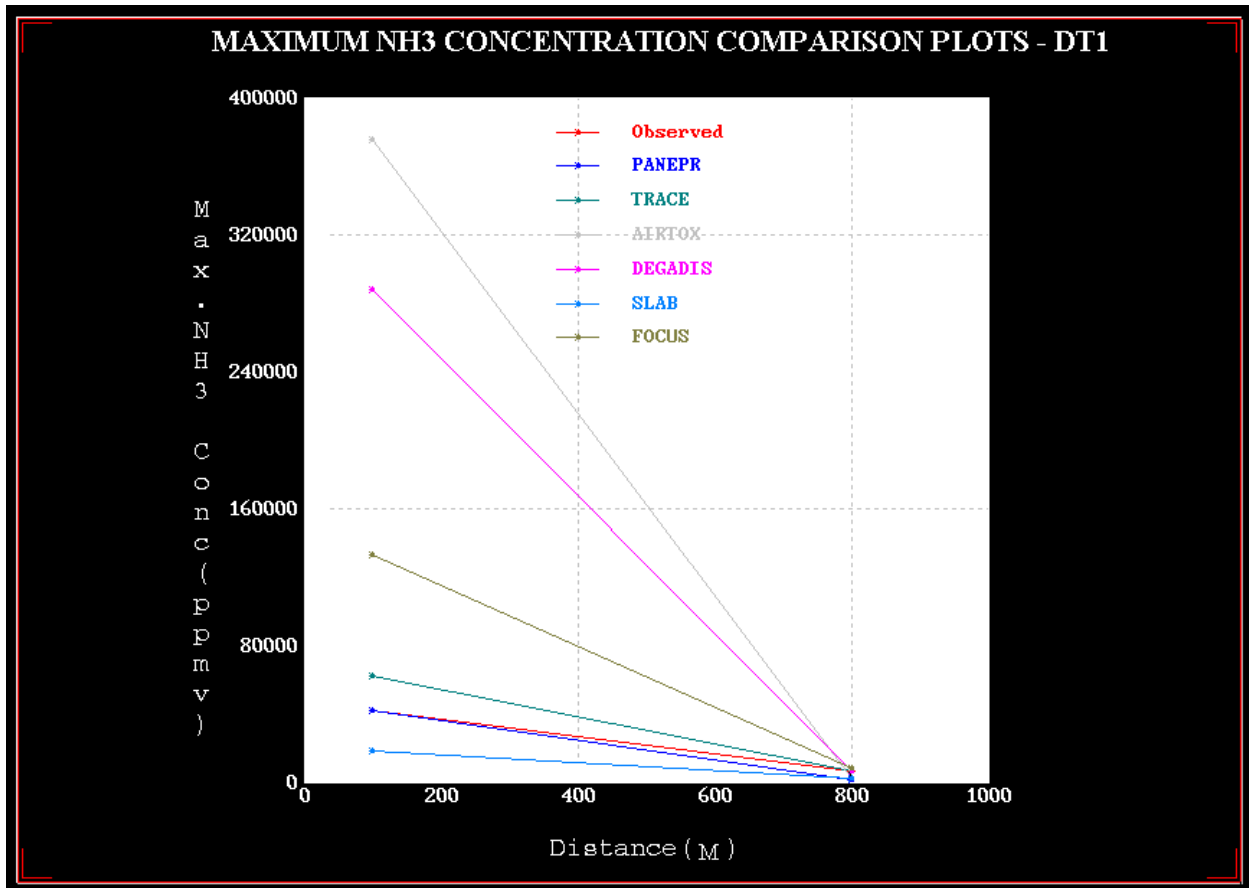
Further, in model input data we have considered different options and the significant features of them are as follows:

- **Power Law** – this option takes in to account the vertical wind velocity profile, which in turn depends on two major factors viz., ground roughness and atmospheric stability.
- **Fluid Type** – here “compressible” option has been used since, this will take in to account the density and temperature variations between ambient air and the pollutant dispersion.
- **Buoyancy Model** – Since, density of heavy gas is the principal driving force for atmospheric dispersion.
- **Log Law2** - this option considers the velocity profile shape both on ground and buildings.
- **K-Diff** – the turbulence model is used for the flat terrain without any obstacles.

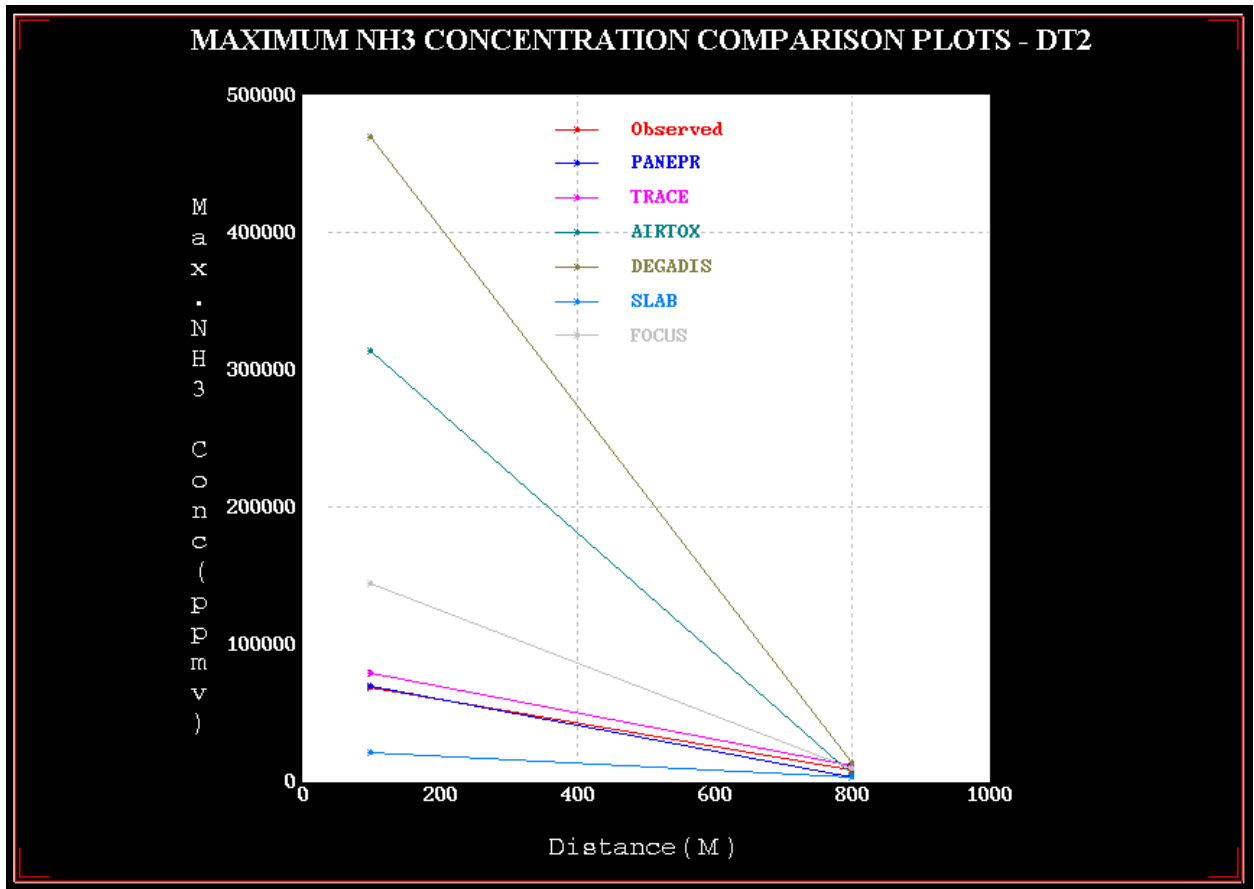
Table 3 Model Predicted and Observed Maximum Centerline Concentrations

Particulars/Model	(Predicted) Max. Centerline NH ₃ Concentration (ppmv)					
	DT1		DT2		DT4	
	100m	800m	100m	800m	100m	800m
Observed	42483	6975	68664	8991	49307	14562
PANEPR	41928	2081	70088	3961	49361	2211
TRACE	62250	6882	79488	11441	72181	12081
CHARM	---	8074	---	2917	---	6321
AIRTOX	375519	3001	313333	5931	226266	35943
DEGADIS	288000	7198	469740	13760	566000	19500
SLAB	18900	2980	21100	3840	21400	4374
FOCUS	133400	8824	144100	10190	138530	15360
SAFEMOD	---	3638	---	5037	---	6249

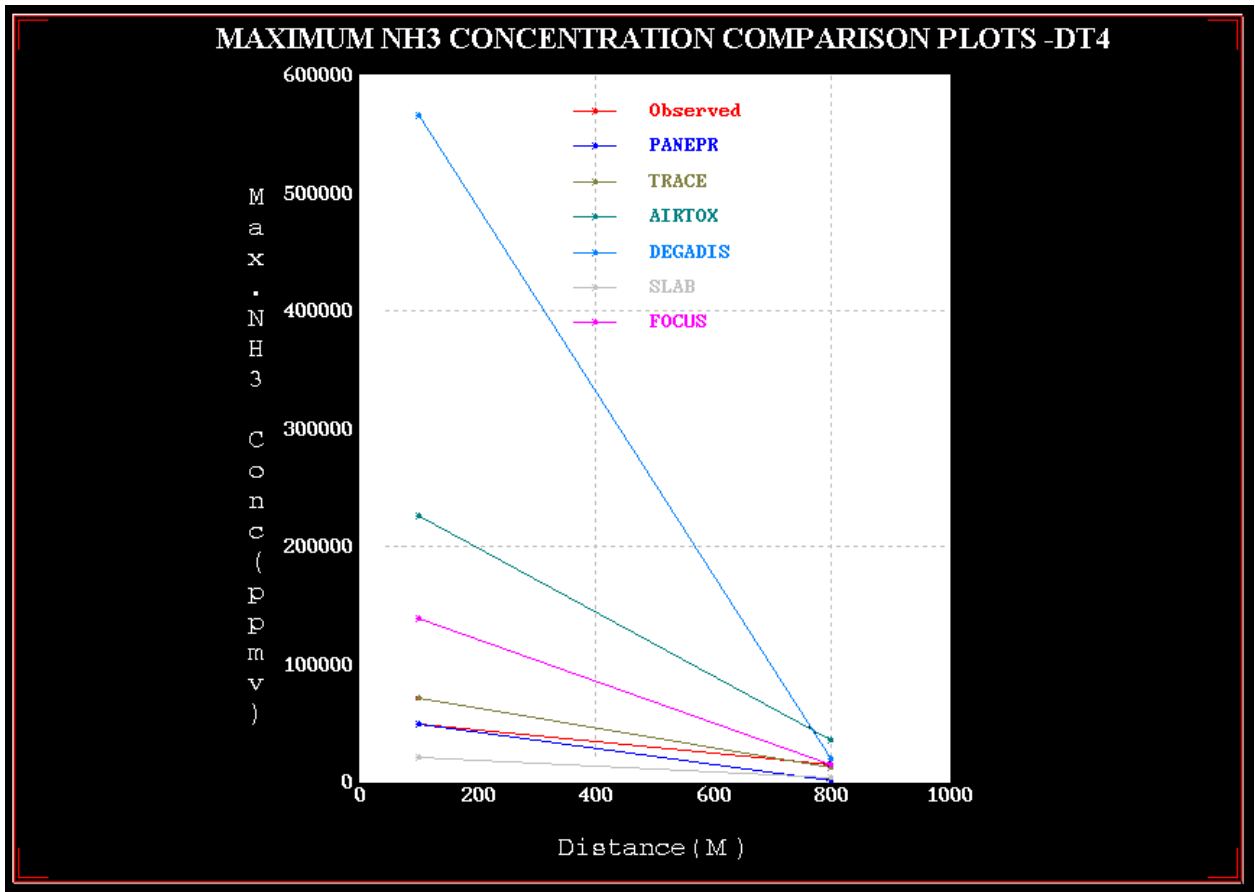
Plot 1



Plot 2



Plot 3



2. GOLDFISH ANHYDROUS HYDROFLUORIC ACID SPILL EXPERIMENTS

In 1986, AMOCO Oil Company and Lawrence Livermore National Laboratory conducted six experiments to study atmospheric releases of anhydrous hydrofluoric acid (HF) from heated, pressurized storage (40°C, 6.8 atm). Three of the six tests (Tests 1-3) were designed primarily to study vaporization and aerosol generation, cloud density and dispersion. The other three were designed to study the effect of water sprays as mitigation measures in the event of a release. Tests 1-3 are included in the EPA's Model Evaluation Support System (MESS) archive.

Releases were made as a horizontal liquid jet from a spill pipe. Concentrations were sampled at vertical levels on three sampling arcs. Sampling distances were sufficient to record concentrations at trace levels. In one of the archived dispersion experiments (Test 3), additional moisture was added to the air upwind of the source using a combination of a pond and stream generators.

Liquid anhydrous hydrofluoric acid was spilled at the Liquefied Gaseous Fuels Spill Test Facility, using a release system similar to the Desert Tortoise Ammonia Tests. The HF releases were made from a tank truck at constant pressure maintained with a nitrogen purging system. From the tank, the HF was carried under pressure by pipe to the spill point. The HF exited the pipe horizontally through an orifice plate, 1.0 m above the surface of an impermeable spill pad. In addition, the pad was designed to collect any pooling HF. In the tests conducted, pooling was not observed. The spill rate data chosen for the archive were obtained by performing a linear regression of the load cell data. The horizontal jet was directed downwind. HF release rates for the three experiments were 1.78 m³/min, 0.65m³/min and 0.66 m³/min with release times of 2 minutes, 6 minutes and 6 minutes respectively.

The release configuration was designed to provide reliable source estimates for dispersion testing. To this, source definition was a major consideration. Three approaches were used to quantify emissions: 1) load cells 2) mass flux and 3) orifice calculations.

Table 4 Release characteristics for the Goldfish Experiments

<i>Test</i>	<i>HF Spill Rate (m³/min)</i>	<i>Duration (sec)</i>	<i>HF Temperature(°C)</i>	<i>HF Pressure (psi)</i>
1	1.78	125	40	111
2	0.65	360	38	115
3	0.66	360	39	117

Liquid volume rate was converted to mass release rate (g/sec) for data archiving. Concentration data collected included measurements on three sampling arcs (300, 1,000 and 3,000 m). For test 1, cloud transport and dispersion was centered on the grid axis resulting in steady state plumes at all three arc distances. In test 2, the peak concentration at 3,000 m was measured at the edge of the sampling array. This makes it impossible to determine the maximum concentration or plume width. In test 3, sensor problems led to inadequate plume coverage at the 3,000 m arc.

Averaging times for concentration measurements were 66.6 seconds, 83.3 seconds or 100 seconds depending on the sample's location and the test conditions.

Wind measurements at a height of 2 m were made at 18 sites ranging from 2 km upwind to 3 km downwind of the release. The archived meteorological data represent test –average values. The atmospheric stability was neutral for the three tests. Wind speeds ranged from 4.2 to 5.6 m/sec. and ambient temperature from 26.5 to 37.0° C.

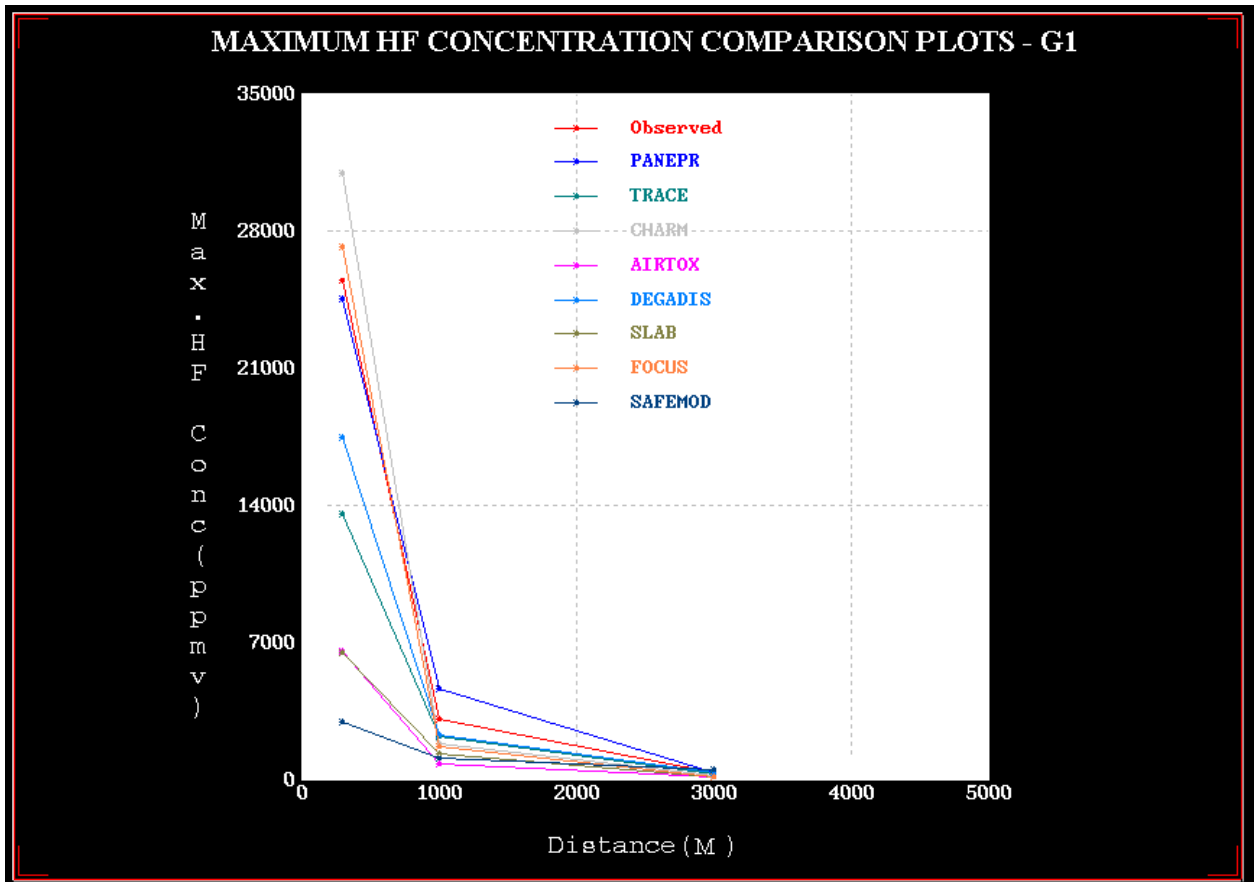
Table 5 MODEL INPUT DATA

Sl. No.	Input Data	Gold Fish		
		G1	G2	G3
1.	TERRAIN			
	Longitude	-25.57	-25.57	-25.57
	Latitude	36.48	36.48	36.48
	Roughness Length (m)	0.003	0.003	0.003
	Computation Domain (m ³)	4000x1200x100	4000x1200x100	4000x1200x100
	Monitor Point Height (m)	1.0	1.0	1.0
2.	SOURCE			
	Source Type	Point	Point	Point
	Exit Velocity (m/sec)	3.89	1.34	1.34
	Source Height (m)	1.0	1.0	1.0
	Mass Flux (Kg/sec.)	30.20	10.40	10.40
	Release Temperature (°C)	40.00	38.00	39.00
	Release Duration (sec.)	125	360	360
3.	WEATHER			
	Wind Speed (m/sec.)	5.60	4.20	5.40
	Wind Direction (Degrees)	270	270	270
	Anemometer Height (m)	2.0	2.0	2.0
	Relative Humidity (%)	4.90	10.50	27.60
	Ambient Temperature (°C)	37.00	36.00	26.5
	Ambient Pressure (m bars)	891.00	900.00	900.00
	Cloud Cover (10's of %)	0	0	0
	Stability Class	D	D	D
	Wind Profile	Power Law (exp. 0.14)	Power Law (exp. 0.19)	Power Law (exp. 0.19)
	Temperature Profile	Two Step	Two Step	Two Step
	Lapse Rate (°C/m)	-0.009766	-0.009766	-0.009766
	Mixing Height (m)	100	100	100
Inverse Lapse Rate (°C/m)	0.01	0.01	0.01	
4.	SIMULATION			
	Mesh Size Chosen	79, 24,10	79, 24,10	79, 24,10
	Grid Fineness Parameter	7	7	7
	Date	16/07/1986	26/07/1986	21/08/1986
	Time (Hours)	11:30:00	12:40:00	15:30:00
	Time Zone	- 6.0	- 6.0	- 6.0
	Duration (Sec.)	1500	1500	1500
	Fluid Type	Compressible	Compressible	Compressible
	Wind Model	Solve	Solve	Solve
	Buoyancy Model	Buoyancy (gz=9.803)	Buoyancy (gz=9.803)	Buoyancy (gz=9.803)
	Wall Type	Log Law	Log Law	Log Law
	Turbulence Model	K Diff	K Diff	K Diff

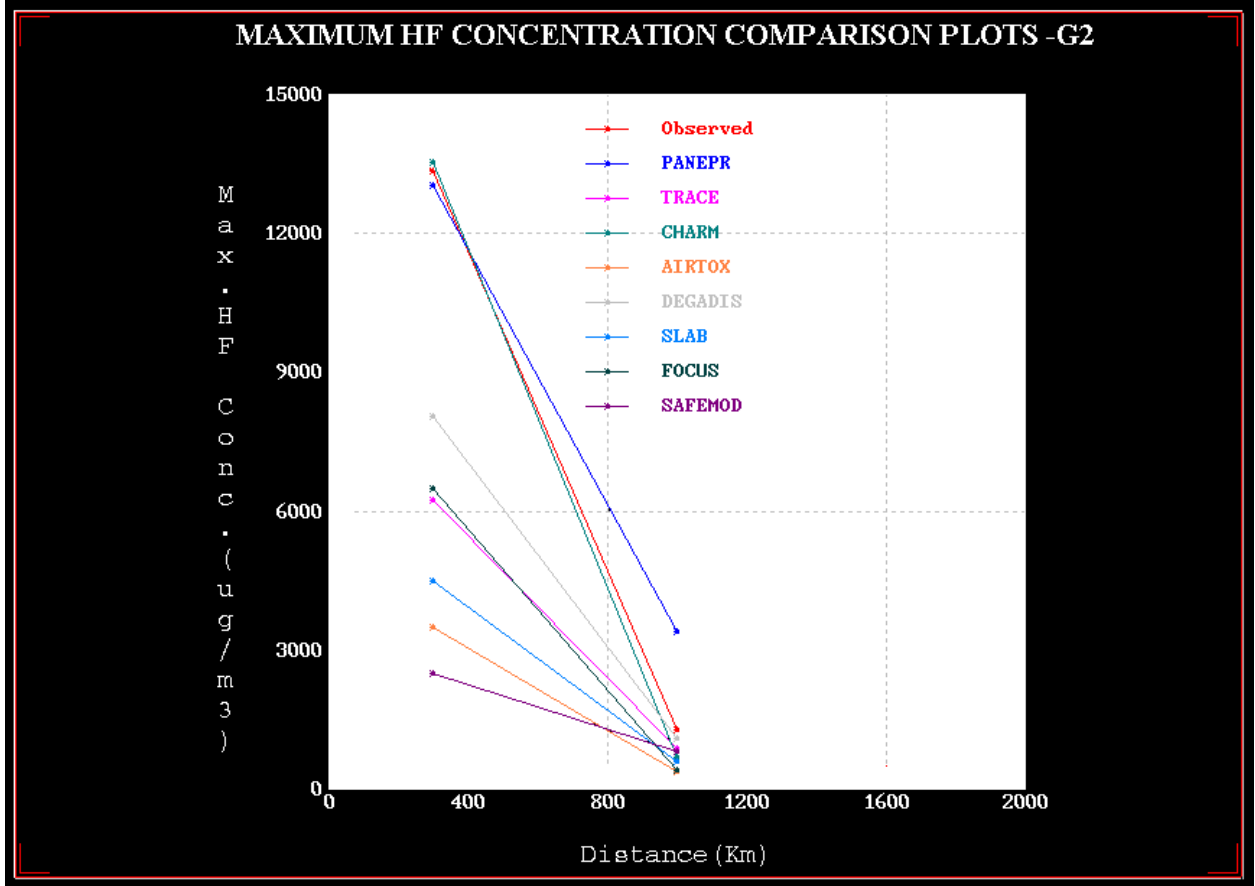
Table 6 Model Predicted and Observed Maximum Centerline Concentrations

Particulars/Model	(Predicted) Max. Centerline HF Concentration (ppmv)						
	G1			G2		G3	
	300m	1000m	3000m	300m	1000m	300m	1000m
Observed	25473	3098	411	13347	1287	12515	2042
PANEPR	24549	4680	389	13011	3418	11428	4190
TRACE	13588	2211	315	6226	894	5359	816
CHARM	30920	1868	258	13520	702	10550	592
AIRTOX	6582	813	138	3501	390	3435	308
DEGADIS	17500	2321	408	8050	1103	7060	881
SLAB	6520	1340	185	4490	600	3590	445
FOCUS	27170	1699	141	6490	425	13240	352
SAFEMOD	2968	1145	520	2499	822	2366	753

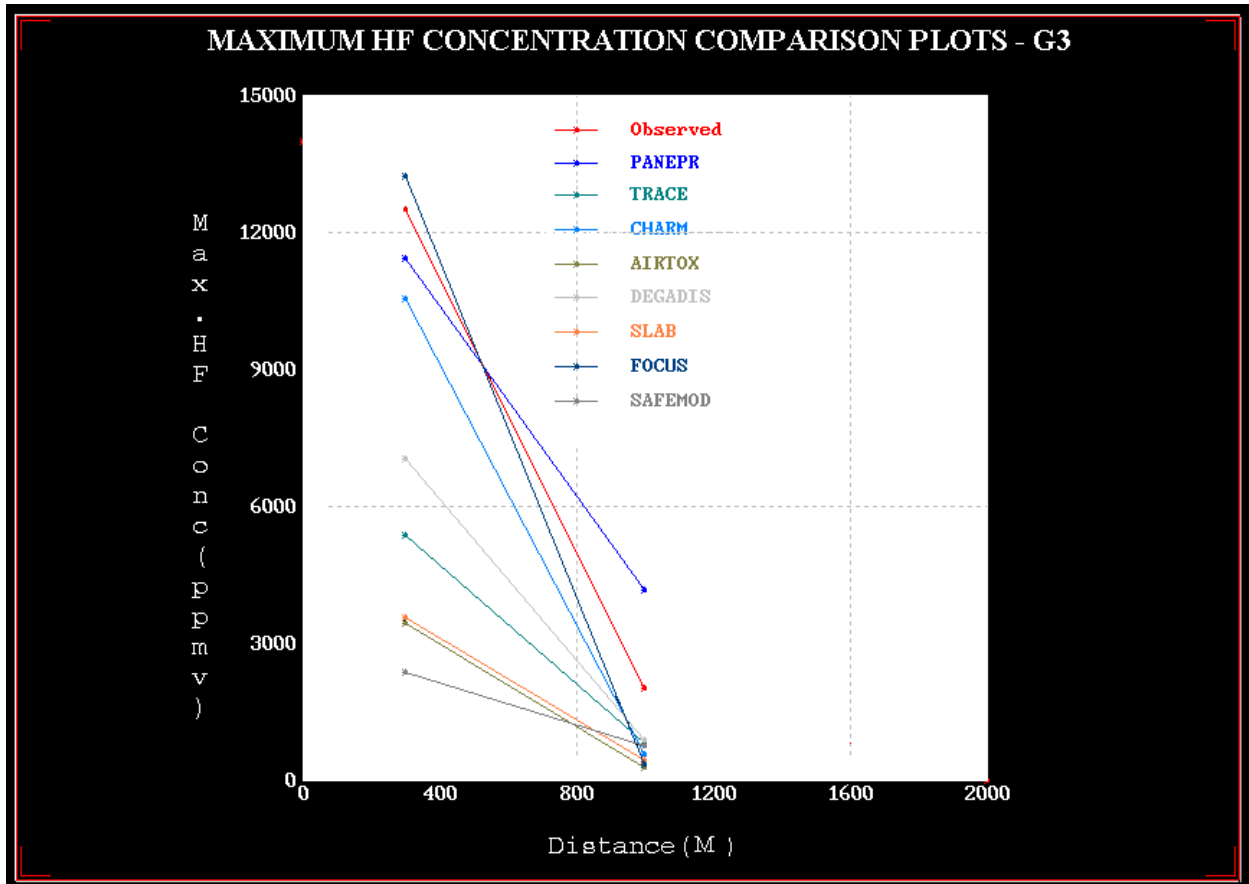
Plot 4



Plot 5



Plot 6



3. BURRO LIQUEFIED NITROGEN GAS SPILL TESTS

The Burro Series of liquefied Natural Gas (LNG- a composition of Methane, Ethane and Propane in the reducing order) spill experiments were performed at the Naval Weapons Center, China Lake, California during the summer and fall of 1981. Personnel from Naval Weapons Center (NWC) and Lawrence Livermore National Laboratory (LLNL) conducted the tests jointly. A total of nine spills of LNG onto water were made between 6th June and 17th September. The first test, Burro1, was a spill of approximately 40 m³ of Liquefied Nitrogen (LN₂) on to water, for the purpose of developing a fog for correction algorithm for the Infra red (IR) gas sensors. The remaining eight tests Burro 2 through Burro 9, were all nominally 40 m³ spills of LNG on to water at spill rates of 11 to 18-m³/min, to measure the dispersion of the LNG vapor cloud in the atmosphere under various conditions. Concentration measuring devices are located at radii of 57, 140, 400 and 800 m from the source. The meteorological data included wind, turbulence and temperature measurements to describe the turbulent atmospheric boundary layer.

All tests were conducted over a desert range with a steep slope rising 7.0 m in elevation from the pond 80.0 m downwind. Beyond 80.0 m the terrain was relatively level with a slight slope (less than 1 degree) north to south, left to right for cloud travel.

The water test basin has an average diameter of 58 m, with an average water level about 1.5 m below the surrounding ground level. The average depth of the water is approximately 1.0 m. The slopes of all but the south bank have been reduced to provide less turbulent wind flow over the water test basin.

Of the eight Burro tests conducted, Nos. 3, 5 and 8 were selected for inclusion in the ESS Archive. Tests 6 and 9 were excluded due to several rapid phase transitions, or small explosions, which occurred during the releases. Burro tests 4 and 7 appeared to have centerline concentrations outside the grid and were not included. Test2 was excluded on the advice of Lawrence Livermore National Laboratory staff, because of data uncertainty.

Test conditions are summarized in Table – 3 below. Wind speeds averaged from 5.4 to 7.4 m/sec. For the unstable and slightly unstable atmospheric conditions in tests 3 and 5. Wind speed averaged only 1.8 m/sec for test 8, with slightly stable conditions.

Table 7 Burro Series Test Summary (1980)

Test Name	Date	Spill Volume (m ³)	Spill Rate (m ³ /min)	Averaged Wind Speed (m/sec)	Atmospheric Stability
Burro 3	2 July	34.0	12.2	5.4	Unstable
Burro 5	16 July	35.8	11.3	7.4	Slightly Unstable
Burro 8	3 Sept.	28.4	16.0	1.8	Slightly Stable

The LNG was released from a cryogenic liquid storage tank. A 25 cm diameter stainless steel spill line ran from the tank to the center of a 58 m diameter spill pond filled with water to a depth of approximately 1 m. the water level was 1.5 m below the surrounding ground level. The spill pipe was directed straight down toward the water with a splash plate installed below the spill pipe outlet at a shallow depth beneath the water surface to limit penetration of the LNG into the water, it was directed radially outward along the surface of the water. Little information is available to accurately define the liquid pool area, although, for modeling total pool flux is assumed to be equal to release rate as pool spreading and vaporization reach equilibrium with the release rate. Spill rates were close to 12 m³/min for Burro tests 3 and 5, and then increased to 16.0 m³/min for test 8.

Gas concentration data were measured at heights of 1, 3 and 8 m above the ground at distances of 57, 140,400 and 800 m from the source. A total of 30 stations recorded gas concentrations. Gas concentration data were originally recorded at rates of 1 to 5 Hertz. All concentration data were averaged to 10 seconds for the MESS archive.

Meteorological data were collected using standard cup and vane anemometers 2.0 m above the ground, located at 20 stations upwind and downwind of the spill source. Wind data from the 20 cup and vane anemometers were averaged to obtain single values of wind speed and direction for the MESS archive. An average value for the test duration for temperature, humidity, stability and Monin-Obukhov length were taken from the Burro data report.

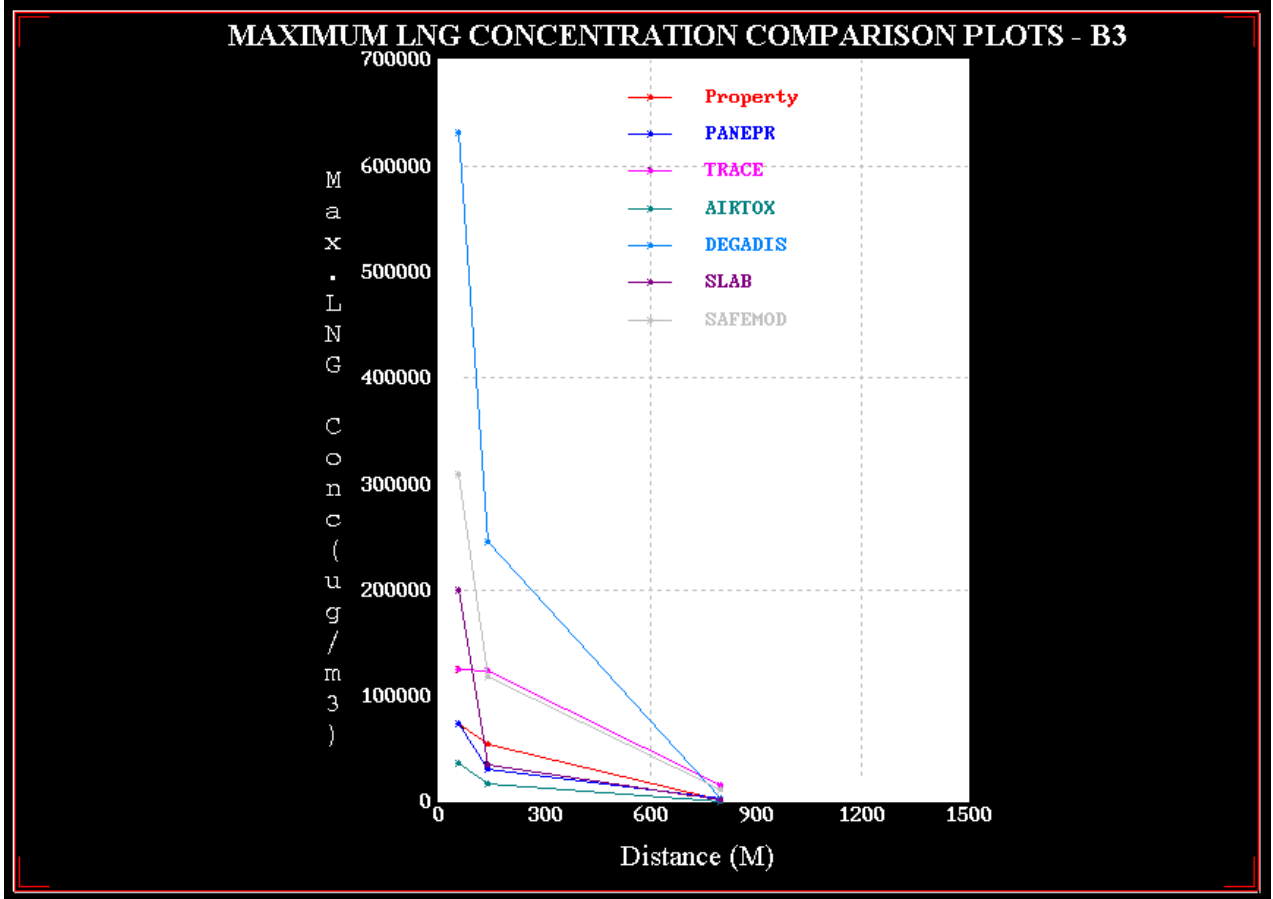
Table 8 MODEL INPUT DATA

Sl. No.	Input Data	Burro		
		B3	B5	B8
1.	TERRAIN			
	Longitude	-27.683	-27.683	-27.683
	Latitude	36.683	36.683	36.683
	Roughness Length (m)	0.002	0.002	0.002
	Computation Domain (m ³)	1400 x 500 x 50	1400 x 500 x 50	1400 x 500 x 50
2.	Monitor Point Height (m)	1.0	1.0	1.0
	SOURCE			
	Source Type	Area	Area	Area
	Pool Diameter (m)	58.0	58.0	58.0
	Source Height (m)	0.0	0.0	0.0
	Mass Flux (Kg/sec.)	88.00	81.80	116.90
	Release Temperature (°C)	-164.00	-164.00	-164.00
3.	Release Duration (sec.)	167	190	107
	WEATHER			
	Wind Speed (m/sec.)	5.40	7.40	1.80
	Wind Direction (Deg)	269.00	263.00	279.80
	Anemometer Height (m)	2.0	2.0	2.0
	Relative Humidity (%)	5.20	5.60	4.50
	Ambient Temp (°C)	33.80	40.5	33.10
	Ambient Press (m bars)	948.00	941.00	941.00
	Cloud Cover (10's of %)	0	0	0
	Stability Class	B	C	E
	Wind Profile	Log Law	Log Law	Log Law
	Temperature Profile	Two Step	Two Step	Two Step
	Lapse Rate (°C/m)	-0.107692	-0.073846	-0.010769
	Mixing Height (m)	100.0	100.0	100.0
Inverse Lapse Rate (°C/m)	0.01	0.01	0.01	
4.	SIMULATION			
	Mesh Size Chosen	79, 28, 10	79, 28, 10	79, 28, 10
	Grid Fineness Parameter	7	7	7
	Date	02/07/1980	16/07/1980	03/09/1980
	Time (Hrs)	15:08:06	16:19:36	19:09:22
	Time Zone	- 6.0	- 6.0	- 6.0
	Duration (Sec.)	700	900	900
	Fluid Type	Compressible	Compressible	Compressible
	Wind Model	Solve	Solve	Solve
	Buoyancy Model	Bouyancy (gz=9.803)	Bouyancy (gz=9.803)	Bouyancy (gz=9.803)
	Wall Type	Log Law2	Log Law2	Log Law2
	Turbulence Model	K- Diff	K- Diff	K- Diff

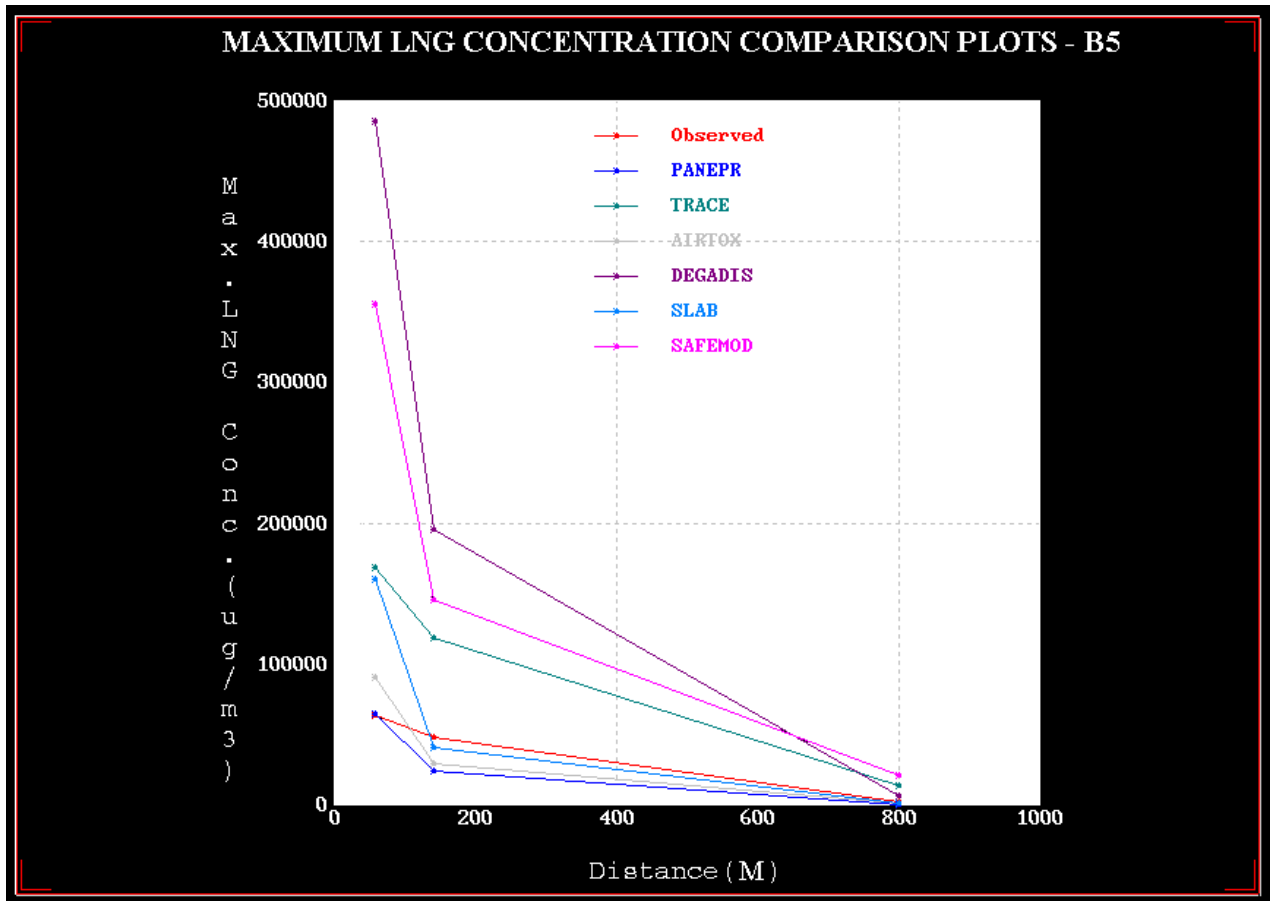
Table 9 Model Predicted and Observed Maximum Centerline Concentrations

Particulars/Model	(Predicted) Max. Centerline LNG Concentration (ppmv)								
	B3			B5			B8		
	57m	140m	800m	57m	140m	800m	57m	140m	800m
Observed	74000	54640	1167	63478	47535	2236	283390	34507	20810
PANEPR	74318	30483	3786	64948	24530	596	283112	23917	7300
TRACE	125401	123472	16043	168815	118118	14226	211543	90562	40144
CHARM	---	---	8180	---	---	4425	---	37310	8532
AIRTOX	36465	17507	698	90184	29103	1133	616281	385947	164520
DEGADIS	631000	246000	3760	485000	195000	6723	853000	65870	21500
SLAB	199000	34400	1180	160000	40400	1820	328000	46900	17500
FOCUS	---	890260	191000	---	843000	50630	---	76700	18220
SAFEMOD	308703	118471	11485	355297	146070	20929	622197	312103	187380

Plot 7



Plot 8



Plot 9

