	General Characteristics	
1	**Abstract of Model Capabilities**	HGSYSTEM is a collection of computer programs designed to predict the source-term and subsequent dispersion of accidental chemical releases with an emphasis on denser-than-air (dense gas) behavior. Multi-component releases may be modeled as well as chemicals that exhibit non-ideal behavior. Chemical reactivity may be modeled for hydrogen fluoride (HF) and uranium hexafluoride (UF6) in HGSYSTEM-UF6. This version of HGSYSTEM includes all of the features and capabilities contained in HGSYSTEM 3.0 plus several code enhancements, including the addition of chemistry and thermodynamic modules simulating UF6 hydrolysis reaction influence on plume characteristics and dispersion. HGSYSTEM offers a broad spectrum of accidental release modeling capabilities.
2	**Sponsor and/or Developing Organization**	**Sponsors:** 1.Shell Research, Industry Co-operative HF Mitigation/Assessment Program, Ambient Impact Technical Subcommittee [HGSYSTEM Version 1.0] 2. American Petroleum Institute (API) [HGSYSTEM Version 3.0] 3.U.S. DOE [HGSYSTEM-UF6] **Developers:** Shell Research Limited [HGSYSTEM] Shell Research and Technology Centre Thornton, P.O. Box 1, Chester, CH1 3SH Earth Tech., Inc/ORNL- Lockheed Martin Energy Research Corp. [HGSYSTEM-UF6] Steven Hanna and Joseph Chang/Sanford Bloom
3	**Last Custodian/ Point of Contact**	Contacts: Shell Research and Technology Centre ORNL, Doug Lombardi Thornton, P.O. Box 1 Bethel Valley Rd., Chester, CH1 3SH Oak Ridge, TN 37831-6200 Phone: 44 151 373 5851 [HGSYSTEM] (423) 576-9231 [HGSYSTEM-UF6] Fax: 44 151 373 5845 (423) 574-5788 E-mail: hgsystem@msmail.trctho.simis.com
4	**Life-Cycle**	The first public domain release of HGSYSTEM version 1.0 was released in November of 1990 followed by version 1.1 in 1991. Several later versions of the code were developed but not made publicly available. Version 3.0, released August 1995, is the second public domain version of HGSYSTEM.
5	**Model Description Summary**	Computer-based model to calculate the release properties of an accidental release of hydrogen fluoride (HF) including simulation of plume and jet behavior. Three areas where a great deal of uncertainty existed in previous models, which the code explicitly addresses, are: (1) the modeling of the complex thermodynamics of HF/H2O/air mixtures (including aerosol effects on cloud density), (2) the treatment of a wide range of surface roughness conditions, and (3) jet flow and air entrainment for pressurized release of HF, followed by transition to ground-based dense gas dispersion.
6	**Application Limitation**	Some of the source-term models cannot be extended to highly stable meteorological conditions (e.g., no pool evaporation results can be obtained for a 1 m/s, F stability wind field). Furthermore, low momentum plumes, in general, are difficult to model when the initial plume velocity is small in magnitude. Overall, many of the computational models in HGSYSTEM are coupled to empirical correlations providing values for turbulence and dispersion parameters which are not robust for all meteorological conditions that may need consideration in a SAR analysis (i.e., low likelihood/worst-case meteorological conditions).

7	**Strengths/ Limitations**	**Strengths**: HGSYSTEM offers the most rigorous treatments of HF source-term and dispersion analysis available for a public domain code. The code also offers modeling capabilities to other chemical species with complex thermodynamic behavior. Some special features in HGSYSTEM include Aerosols and multi-component mixtures: Ability to model spillage of a liquid non-reactive compound from a pressurized vessel. Time-dependent dispersion: Ability to carry out more efficient simulations of time-dependent dispersion problems by automating the selection of output times and output steps in the HEGADAS-T model. Improve dosage calculations and time averaging (HEGADAS-T/HTPOST). Ability to model dispersion on terrain with varying surface roughness. Evaporating pools: Ability to include effects of dike containment (LPOOL). General upgrade of evaporating pool model. User friendliness of HGSYSTEM: Upgrading of post-processors HSPOST and HTPOST. Shared input parameter file. Sensitivity analyses performed for LPOOL, SPILL, AEROPLUME, HEGADAS-S and HEGADAS-T to ensure robustness and correctness of code and to evaluate effect of model parameters on dispersion analysis. Concentration predictions: Inclusion of a concentration profile in AEROPLUME that provides smooth transitions with the concentration profiles adopted in PGPLUME for airborne plumes. Re-examination of crosswind concentrations formulation in HEGADAS. Improved aerosol model.
7	**Strengths/ Limitations** (Cont.)	**Limitations:** It is difficult to extend the physical/chemical data base utility DATAPROP to include additional chemical species. Such modifications would require an extremely good knowledge of the HGSYSTEM program structure and some consultation with the code developers. Releases from pipes cannot be calculated by HGSYSTEM. Liquid aerosol rainout is not modeled C all aerosol component is assumed to remain airborne until complete evaporation.
8	**Model References**	! McFarlane, K., A. Prothero, J.S. Puttock, P.T. Roberts, H.W.M. Witlox, November 1990, "Development and Evaluation of Atmospheric Dispersion Models for Ideal Gases and Hydrogen Fluoride — Part 1: Technical Reference Manual," Report No. TNER.90.015, Shell Research Ltd., Thornton Research Centre, Thornton, Chester, CH1 3SH, England. ! L. Post (editor), 1994, HGSYSTEM 3.0 Technical Reference Manual, Report No. TNER.94.059, Shell Research Limited, Thornton Research Centre, P.O. Box 1, Chester, England, Shell Internationale Research Maatschappij B.V. ! L. Post, "HGSYSTEM 3.0 User Guide," Report No. TNER.94.058, Shell Research Ltd., Thornton Research Centre, Thornton, Chester, CH1 3SH, England.

9	**Input Data/Parameter Requirements**	Input is provided by means of the NAMELIST feature where a descriptive variable name is equivalent to a numeric value. Input file comment statements are also permitted to aid the description of input entries. In addition to the source-term model input requirements, detailed in the APAC Spills Model Review, the following AEROPLUME, LPOOL, PGPLUME, HFPLUME, HEGABOX, and HEGADAS inputs are used for subsequent dispersion analysis. AEROPLUME (Near Field Dispersion of High Momentum Jets) RESERVOIR Block — parameters describing the reservoir fluid thermodynamic state RELEASE Block — temperature of a stack release GASDATA Block — initial composition of the reservoir mixture and the relevant thermodynamic data including mole fraction of water, vapor specific heat at constant pressure, molecular weight natural convection heat transfer group, and species complete thermodynamic data PIPE Block — release pipe/orifice-plane conditions AMBIENT Block — conditions of the ambient environment DISP Block — parameters describing the dispersion characteristics (surface roughness and wind stability) MMESOPT Block — “switches” that indicate the use of the options for the modeling of wet/dry deposition, canyon effects, center-line concentration fluctuations, and plume lift-off) TERMINAT Block — sets reservoir release termination criteria MATCH Block — transition criteria for interface between AEROPLUME and on the far-field dispersion models LPOOL - single or multi-component (simulates boiling and time-dependent evaporation of a single or multi-component liquid pool on land or water) GROUND Block — parameters used to describe the ground composition, temperature, and the dike composition and size (where applicable) SPILL Block — Spill type (user defined rate, Bernoulli, or choked flow), user-defined spills may consist of a sequence of up to 5 distinct spill rate and duration pairs. RESERVOIR Block — includes radius of a cylindrical tank, initial fluid level, equivalent diameter of reservoir orifice, and elevation of the orifice. LPOOL - multi-component (simulates the time-dependent evaporation of a multi-component liquid pool on land or water). CONTROL Block — parameters for determining maximum simulation time, minimum film thickness of pool, and time step for pool data used to link to dispersion model GROUND Block AMBIENT Block — describes atmospheric conditions; includes relative air humidity, fraction of sky covered by clouds, spill starting time, and times for sunrise and sunset FLASH Block — user-specified flash and aerosol fractions; options of using HGSYSTEM to calculate the flashing fraction and aerosol generation or define the fractions of both. GASDATA Block MMESOPT Block — only contains 1 Y/N switch for the option associated with plume lift-off HEGABOX (Initial Spreading Phase of a Stagnant, Dense Cloud) CONTROL Block — specifies run control parameters (maximum simulated dispersion time, maximum time step, output printing control, and final termination Richardson number) SPILL Block — describes the spill of pollutant (spill size and initial cloud radius) AMBIENT Block — same as in AEROPLUME DISP Block — includes the option of specifying the Monin-Obukhov length rather than permit the code to compute the value GASDATA Block — same as in AEROPLUME with the natural convection heat transfer group replaced with: type of thermodynamic model, mole fraction of water adsorbed from earth’s surface, dilution by initial entrainment, thermal diffusivity of the dry pollutant, and kinematic viscosity

9	**Input Data/Parameter Requirements (Cont.)**	MMESOPT Block — same as in AEROPLUME except no plume lift-off option available HEGADAS (Area Source Dense Gas Dispersion Model: Transient and Steady-State) CONTROL Block — specifies run control parameters (surface heat effects, concentration output, transient vs. steady-state simulation, cloud shape correction, convergence tolerance) AMBIENT Block — same as in AEROPLUME DISP Block — parameters describing the dispersion characteristics (surface roughness, wind stability, concentration, Monin-Obukhov length (optional), crosswind dispersion parameters, gravity spreading law constants, downwind dispersion coefficient formula) GASDATA Block — same as in AEROPLUME with the addition of the following parameters: type of thermodynamics model, dry pollutant source emission rate, mole fraction of water adsorbed by pollutant, pollutant temperature, pollutant enthalpy, and liquid mass fraction in initial HF release CLOUD Block — controls the output of gas cloud information CALC Block — specifies output time for which cloud concentration is calculated and printed AUTOTIM Block — specification of an “optimal” set of output times POOL Block — pool dimensions TIMEDATA Block — specifies the time-dependent source data either following release initiation or at a spatial breakpoint following post-jet/plume transition TRANSIT Block — specification of break point conditions MMESOPT Block — same as in AEROPLUME with the addition of an option for calculation of variation of concentration with averaging time
10	**Output Summary**	Each source-term module creates a number of different ASCII text output files including intermediate data values, time-dependent source-term results, and data files used by the dispersion analysis modules. A summary of the dispersion model output quantities follows: Dependent Variable (output) Independent Variable Centerline volume percent gas fraction Vertical dispersion coefficient Crosswind dispersion coefficient Half-width of middle part of crosswind concentration profile Temperature Effective cloud half-width Effective cloud height Cloud half-width (normal definition) Vapor concentration (x, y, z) Vapor dose (x, y, z) x = downwind location, y = crosswind from plume centerline, z = vertical distance above grade
11	**Applications**	HGSYSTEM has been used in select cases to support Risk Management Plans (RMPs) for local emergency planning committees (LEPs) and analyses at the Gaseous Diffusion Plant Safety Analysis Report Upgrade Program.
12	**User-Friendliness**	Program is run in batch mode using a combination of customized batch files and input data files. Some manual manipulation of the data may be necessary when using utility programs such as DATAPROP results as input into a successive source-term model.
13	**Hardware-Software Interface Constraints/ Requirements**	a. Operating system: IBM PC compatible with a 80386 processor or greater, 4 Mbytes of RAM, and math coprocessor chip is optional but highly recommended b. Disk space required: 22 Mbytes hard disk space c. Run execution time for typical problem (CPU or Real Time): Several minutes (real time) maximum. d. Programming language: Microsoft FORTRAN Power station e. Interface with other codes: None f. Portability: Intended for compilation under Microsoft FORTRAN Power station and execution on a PC, but adaptable to any platform possessing a standard FORTRAN 77 compiler. DOS batch files are used to pipe input and output.
14	**Operational Parameters**	**Error Diagnostics** Variety of diagnostic messages including input data file validation, runtime error messages, numeric convergence information, warning messages, as well as run information detailing the progress of the calculations. **Batch Mode Capability (several cases at once)** The individual program segments are executed at the DOS prompt by means of the desired program name followed by a list of input file(s) and an optional output file name. Although batch mode capability is not explicitly provided with the program, it would be a simple task to construct a DOS batch file that would execute the desired individual DOS command statements.

15	**Surety Considerations**	**Quality Assurance** It is unknown to what extent the source code has been verified. In some instances, modeling features documented in the user's manual have been deactivated with no accompanying explanation in the source code or an accompanying "README" file. The source code has been made available since 1990 to permit verification of the way in which the models have been implemented. **Benchmark Runs (comparison with other codes)** HGSYSTEM has been benchmarked in comparison to 9 independent dense gas models: DEGADIS, SLAB, AIRTOX, CHARM, FOCUS, GASTAR, PHAST, TRACE, and the Britter & McQuaid model. Details are provided in Hanna, S.R., D.G. Strimaitis, and J.C. Chung, 1993, "Hazardous Gas Model Evaluation with Field Observations," Atmospheric Environment, Vol. 27A, No. 15, pp. 2265-2285. **Comparison with Field Experiments** Comparison of code results to large scale field data has been performed with the Burro, Coyote, Desert Tortoise, Goldfish, Hanford Kr85, Maplin Sands, Prairie Grass, and Thorney Island data sets. Details are provided in Hanna, S.R., D.G. Strimaitis, and J.C. Chung, 1993, "Hazardous Gas Model Evaluation with Field Observations," Atmospheric Environment, Vol. 27A, No. 15, pp. 2265-2285.
16	**Runtime Characteristics**	**Setup Time (first run, subsequent run)** A first-time user may need between 2 and 1 day to completely set up a release analysis and complete the source-term, dispersion, and post-processing analyses, assuming that all the necessary input data is readily available. Approximately 2 hours should represent the setup and processing time for an experienced user. In the event that the analysis requires modeling of a chemical that is not included in the chemical database, several hours may be required to obtain all the necessary physical/chemical property data, depending upon the availability of data and estimation methods and property correlations.

Specific Characteristics

Part A: Source Term Submodel Type		
A1	**Source Term Algorithm?**	_✔_YES __NO
A2	**For Chemical Consequence Assessment Models**	**Liquid spill: _✔_ pool evaporation __ particulate resuspension** **Pressurized releases:_✔_ two-phase jets_✔_ flashing_✔_ entrainment__ aerosol formation** **Solid spills: __ resuspension __ sublimation**
Part B: Dispersion Submodel Type		
B1	**Gaussian**	**_✔_Straight-line plume __Segmented plume __ Statistical plume _✔_ Statistical puff**
Part C: Transport Submodel Type		
C2	**Deterministic**	Yes
C4	**Frame of Reference**	**_✔_ Eulerian __ Lagrangian __ Hybrid __ Eulerian-Lagrangian**
Part D: Fire Submodel Type (Not Applicable)		
Part E: Energetic Events Submodel Type (Not Applicable)		
Part F: Health Consequence Submodel Type (No Information Provided.)		
Part G: Effects and Countermeasures Submodel Type (No Information Provided.)		
Part H: Physical Features of Model		
H2	**Release Elevation**	**_✔_ ground __ roof**
H7	**Cloud Buoyancy**	**_✔_ neutral [passive] _✔_ dense [negative] __ plume rise [positive]**

Part I: Model Input Requirements		
I1	**Radio(chemical) and Weapon Release Parameters**	**Release rate: _✔_ Continuous _✔_ Time dependent _✔_ Instantaneous** **Release container characteristics: _✔_ vapor temperature _✔_ tank diameter _✔_ tank height _✔_ tank temperature _✔_ tank pressure _✔_ nozzle diameter _✔_ pipe length** **Jet release: _✔_ initial size _✔_ shape __ concentration profile at end of jet affected zone** **Release dimensions: _✔_ point __ line _✔_ area** **Release elevation: _✔_ ground __ roof __ stack**
I2	**Meteorological Parameters**	**Wind speed and wind direction: _✔_single point __ single tower/multiple point __ multiple towers** **Temperature: _✔_ single point __ single tower/multiple point __ multiple towers** **Dew point temperature: __ single point __ single tower/multiple point** **__ multiple towers** **Precipitation: __ single point __ single tower/multiple point __ multiple towers** **Turbulence typing parameters: __ temperature difference __ sigma theta __ sigma phi _✔_ Monin-Obukhov length __ roughness length __ cloud cover __ incoming solar radiation __ user-specified** **Four dimensional meteorological fields from prognostic model:**
Part J: Model Output Capabilities		
J1	**Hazard Zone**	HEGADIS model has a post-processor that provides the calculation of the hazard zone.
J3	**Concentration Versus Time Plots**	Concentration values at select time intervals can be requested for output
J4	**Tabular at Fixed Downwind Locations**	Virtually all output variables are presented in a tabular format
Part K: Model Usage Considerations (See Items 5 - 7.)		