PACKAGE ID - 001242IBMPC00 HGSYSTEMUF6

KWIC TITLE - Model for Simulating Dispersion due to Atmospheric Release of UF6

AUTHORS - Hanna, G
George Mason University, (United States)

Chang, J.C.
Earthtech, Inc., (United States)

Zhang, J.X.
BlazeTech Corporation, (United States)

Bloom, S.G.
Lockheed Martin Energy Systems, Oak Ridge, TN (United States)

Goode, W.D. Jr
Bechtel Jacobs Company, Oak Ridge, TN (United States)

Lombardi, D.A.
JBF Associates, (United States)

Yambert, M.W.
LMERC, Oak Ridge, TN (United States)

LIMITATION CODE -UNL **AUDIENCE CODE -** UNL

COMPLETION DATE - 08/01/1998 **PUBLICATION DATE -** 08/01/1998

DESCRIPTION - HGSYSTEMUF6 is a suite of models designed for use in estimating consequences associated with accidental, atmospheric release of Uranium Hexafluoride (UF6) and its reaction products, namely Hydrogen Fluoride (HF), and other non-reactive contaminants which are either negatively, neutrally, or positively buoyant. It is based on HGSYSTEM Version 3.0 of Shell Research LTD., and contains specific algorithms for the treatment of UF6 chemistry and thermodynamics. HGSYSTEMUF6 contains algorithms for the treatment of dense gases, dry and wet deposition, effects due to the presence of buildings (canyon and wake), plume lift-off, and the effects of complex terrain. The models components of the suite include (1) AEROPLUME/RK, used to model near-field dispersion from pressurized two-phase jet releases of UF6 and its reaction products, (2) HEGADAS/UF6 for simulating dense, ground based release of UF6, (3) PGPLUME for simulation of passive, neutrally buoyant plumes (4) UF6Mixer for modeling warm, potentially reactive, ground-level releases of UF6 from buildings, and (5) WAKE, used to model elevated and ground-level releases into building wake cavities of non-reactive plumes that are either neutrally or positively buoyant.

SOURCE CODE INCLUDED? - Yes

PACKAGE ID - 001242IBMPC00 HGSYSTEMUF6

MEDIA QUANTITY - Media Directory; Software Abstract; Media Includes Source Code, Executable Modules, Sample Problem Data, Batch and PIF Files, User Guides;/ 1 CD Rom

METHOD OF SOLUTION - The atmospheric release and transport of UF6 is a complicated process involving the interaction between dispersion , chemical, and thermodynamic processes. This process is characterized by four separate stages (flash, sublimation, chemical reaction entrainment, and passive dispersion) in which one or more of these processes dominate. The various models contained in the suite are applicable to one or more of these stage. For Example, for modeling reactive, multiphase releases of UF6, the AEROPLUME/RK component employs a process-splitting scheme which numerically integrates the differential equations governing dispersion, UF6 chemistry, and thermodynamics. This algorithm is based on the assumption that, for a given time step, the equations governing the processes of dispersion, chemical reaction, and thermodynamics can be solved sequentially and independently. Here, a Runge-Kutta solver is employed to solve the equations governing dispersion, a simple, first-order forward finite difference scheme is used to solve the rate equations for the consumption and production of reactants, while the proprietary nonlinear algebraic equation solver NAESOL, developed by Shell Research LTD. is used to solve equations governing thermodynamic balances of molar fraction, enthalpy and molar flow rate of HF. Conversely, for simulating downwind dispersion of a passive, ideal gas, the WAKE component employs equations based on advanced empirical formulations of wind tunnel data in conjunction with the standard gaussian plume model formation.

COMPUTER - IBM PC

OPERATING SYSTEMS - Windows 95, Windows Nt and Windows 3.1, OS/2

PROGRAMMING LANGUAGES - FORTRAN

SOFTWARE LIMITATIONS - HGSYSTEMUF6 is designed for a single user on a single personal computer. Array dimensions have been initially set to reflect realistic, limiting values. By modification of these limits the user may create executable versions of model files that are limited only by the hardware configuration of their machine. HGSYSTEMUF6 is designed specifically for the simulation of atmospheric releases of Uranium Hexafluoride and its reaction products. For other sinmultions which involve the dispersion of vapour from gas, liquid or two-phase releases including multi-component mixtures, HGSYSTEM, is available at no charge from the official Shell Research LTD HGSYSTEM Web site: http:;//www.users.virtual-chester.com/hgsystem or email HGSystem@OPC.shell.com&quot.

SOURCE CODE AVAILABLE (Y/N) - Y

PACKAGE ID - 001242IBMPC00 HGSYSTEMUF6

UNIQUE FEATURES - HGSYSTEMUF6 is designed for simulation of atmospheric releases of UF6. It contains a detailed formulation of the dispersion, chemical and thermodynamic processes associated with atmospheric transport of UF6. Furthermore, HGSYSTEMUF6 can also be used to simulate transport of generic, non-reactve heavy gases, and neutral or positively buoyant passive gases in the presence of building wakes.

RELATED SOFTWARE - Offical utility software included with HGSYSTEMUF6 distribution: FFMAIN, official utility used to verify the content and format of model input files; POSTHEG, official post-processing utility for HEGADAS; POSTMIX, official post-processing utility fo UF6MIXER; AMBIEN, meteorological pre-processor; APINST, an initial mixing model which assumes the reaction rate of UF6 is not limited by atmospheric turbulence. The model is used to determine the initial characteristic of the plume; PKZIP/PKKUNZIP, shareware software for compacting/uncompacting files; POETAP, post-processing utility for use with the AEROPLUME/RK model; PPOSTMIX, additional post-processing utility used in combination with UF6MIXER results for simulation of transient releases.

OTHER PROG/OPER SYS INFO - Input/Output naming conventions: AEROPLUME/RK filename.api, filename.apr; HEGADAS/UF6 (transient mode) filename.hti, filename.htr; HEGADAS/UF6 (steady-state model) filename.hsi, filename.hsr; PGPLLUME filename.pgi, filename.pgr; UF6MIXER filename.mxi, filename.out; WAKE filename.wki, filename.out

HARDWARE REQS - Minimum: 486 microprocessor, 8MB memory, and approximately 16 MB free disk space for installation of program files. Recommended: 100 MHZ PENTIUM processor, 16 MB memory, 50 MB free disk space.

TIME REQUIREMENTS - Typical execution times vary from 1-10 minutes depending on the HGSYSTEMUF6 model component selected.

REFERENCES - S.R. Hanna, J.C. Chang, and J.X. Chang, Technical Documentation of HGSYSTEM/UF6 Model, K/SUB/93-XJ947/1, January 1996; Steven R. Hanna and Joseph C. Chang, HGSYSTEM/UF6 Model Enhancements for Plume Rise and Dispersion Around Buildings, Lift-off of Buoyant Plumes, and Robustness of Numerical Solver, K/SUB/93-XJ947/2R1, January 1997; M.W. Yambert, D.A. Lombardi, W.D. goode, Jr and S.G. Bloom, A Summary of Recent Refinements to the WAKE Dispersion Model, a Component of the HGSYSTEM/UF6 Model Suite, ORNL/TM-13666, August 1998.

ABSTRACT STATUS - Released AS-IS August 27, 1998.

SUBJECT CLASS CODE - GR

KEYWORDS -
COMPUTER PROGRAM DOCUMENTATION

PACKAGE ID - 001242IBMPC00 HGSYSTEMUF6

H CODES
DISPERSION RELATIONS
GASES
MIGRATION
ENVIRONMENTAL TRANSPORT
THERMODYNAMIC PROPERTIES
HYDROFLUORIC ACID

EDB SUBJECT CATEGORIES -
990200

SPONSOR - DOE/ER

PACKAGE TYPE - AS - IS