General Characteristics		
1	**Abstract of Model Capabilities**	FEM3C is the latest version of a three-dimensional finite element model designed to simulate the atmospheric dispersion of heavier-than-air gas (dense gas) release. The computational approach is based on a solution of the fully three-dimensional, time-dependent conservation equations of mass, momentum, energy, and chemical species. The code may be applied to the release of an inert gas or an atmospheric pollutant in the form of vapor/droplets.
2	**Sponsor and/or Developing Organization**	U.S. Army Chemical Research, Development and Engineering Center (CRDEC) Stevens T. Chan Lawrence Livermore National Laboratory Livermore, CA 94551-9900 (510) 422-1822
3	**Last Custodian/ Point of Contact**	Diana L. West, L-795 Technology Transfer Initiative Program Lawrence Livermore National Laboratory Livermore, CA 94551 (510) 423-8030
4	**Life-Cycle**	FEM3 (1983): Modified Galerkin finite element method for solving the time-dependent conservation equations of mass, momentum, energy, and species of an inert gas. FEM3A (1988): Major improvements include: (1) capability for simulating instantaneous releases involving multiple, overlapping sources, (2) the ability to treat obstructions to flow (e.g., buildings, dikes, and tanks), (3) improvement to the K-theory turbulence submodel, (4) addition of a phase-change submodel for treating vapor-liquid transition of the dispersed material, (5) implementation of an incomplete Cholesky conjugate gradient solver as a cost-effective alternative for solving the pressure field of large-scale problems, and (6) a more user-friendly code with simplified input. FEM3B (1990): Extension of model capabilities to include large density changes in both space and time (previous versions did not necessarily conserve species and mass when vapors involving large density changes were analyzed). FEM3C (1994): Upgrades were implemented to include a more advanced turbulence submodel based on solving the (-(transport equations to model the nonlocal conditions of turbulence. The turbulent mixing in previous versions of the code was parameterized via an algebraic K-theory approach where the turbulence was assumed to be in local equilibrium, i.e., upwind transport or flow history effects were only accounted for in the values of average dispersion variables. Local equilibrium is not valid for non-steady flows or predictions of the vapor concentration field in the near vicinity of the vapor source. FEM3C (1997): The University of Arkansas, under the direction of Prof. Jerry Havens, developed A Sparc workstation version of the code. The Gas Research Institute sponsored the code conversion.
5	**Model Description Summary**	FEM3C is a three-dimensional finite element model for the simulation of the atmospheric dispersion of denser-than-air vapor and liquid releases. The simulation model is based on the solution of the conservation equations of mass, momentum, energy, and species with an anelastic approximation (i.e., the continuity equation is written as íEMBED Equation.3ñ Ñ where the total mass of pollutant is assumed to remain constant with time). Major features of the code include: Solution of two- and three-dimensional dispersion problems. Models both isothermal and non-isothermal dense gas releases as well as neutrally buoyant vapor emissions. Treats multiple simultaneous sources of instantaneous, continuous, and finite-duration releases. Models the effects of obstructions to flow and complex terrain on the vapor concentration field. Turbulence is parameterized via the K-theory approach where the user has the option of using similarity theory for the atmospheric boundary layer or solving the (-(transport equations). A local thermodynamic equilibrium submodel with temperature-dependent physical properties is available for analyzing dispersion scenarios involving phase change between liquid and vapor state. Selection available for direct or iterative solution methods for efficiently determining the pressure field.
6	**Application Limitation**	Treatment of jet release, explosive sources, and chemical reactions between the pollutants and the ambient environment is not available. The turbulent mixing models are not universally applicable to all dispersion situations. Physical processes such as rainout, aerosol drop-size distribution, and chemical reactions are not included in the model. Furthermore, the code tends to overestimate the rate of droplet evaporation in the near field and underestimate the dense gas effects in the far field. The grid nodalization assumes a constant number of mesh points in each direction to enable maximum vectorization of the code for computational speed. The computational penalty in speed may be significant when the flow field (obstructions and terrain) is extremely complex, since the grid mapping scheme precludes the use of unstructured grids, which permits irregularities in the domain to be more efficiently modeled.

7	**Strengths/ Limitations**	**Strengths:** FEM3C has modeling capabilities in the computation of complex turbulent fluid flow in the presence of complex terrain and obstacles to flow. Multiple, simultaneous sources may be accommodated and the meteorological conditions and wind flow field may be tailored to satisfy a variety of boundary conditions that give the code the flexibility to model very site-specific release scenarios. **Limitations**: The code cannot accept typical vapor/aerosol source terms (e.g., pressurized jets, time-varying vapor emissions). Furthermore, although the code can treat complex terrain (ground elevation profile), it is difficult to model the presence of inhomogeneous vegetation coverage (i.e., grassland vs. bushes vs. tall trees in the same computational domain). Finally, the aerosol model is incomplete in the sense it does not model all the relevant physical behavior (e.g., droplet evaporation, rainout).
8	**Model References**	! Chan, S.T., December 1994, FEM3C: An Improved Three-Dimensional Heavy-Gas Dispersion Model: User's Manual, UCRL-MA-116567Rev.1., Lawrence Livermore National Laboratory, Livermore, CA.
9	**Input Data/Parameter Requirements**	Does not have a GUI, input files are ASCII. Chemical Data: reference temperature, temperature of the dispersed material, molecular weight, specific heat, Antoine equation for saturation vapor pressure, Watson relation for heat of vaporization. Ambient Conditions: ground level pressure of ambient air, molecular weight of ambient air, specific heat of ambient air. Computational Grid Nodal Coordinates. Terrain Nodal Grids (located at ground surface to reflect changes in elevation). Boundary Conditions: wind velocity components, temperature, mass fraction of species, turbulence kinetic energy, the dissipation rate of turbulence kinetic energy, pressure, normal/tangential stresses, heat flux, mass flux of species, wall functions. Initial Conditions: wind velocity, temperature, and species concentration. Runtime Options: turbulence model, numerical solution method, output time history variable and spatial node selection, convergence tolerance criteria. Friction velocity of the ambient atmosphere, Monin-Obukhov length, effective physical parameters: energy transfer velocity, lower limit of horizontal/vertical diffusivities, coefficient of the buoyancy term in the ,-equation, parameter for anisotropic turbulence, and superheating coefficient.
10	**Output Summary**	Time history data for wind velocity components, temperature of the mixture, volumetric fraction of vapor material, mass fraction of material in liquid/vapor phase, mixture density, dynamic pressure, dosage, turbulent kinetic energy, dissipation rate of turbulence kinetic energy, and turbulent diffusivity in the vertical direction. Wind vector field plots. Concentration isopleths.
11	**Applications**	! This CFD code has been applied to small-scale atmospheric flow and transport/diffusion of pollutants in which the effects of terrain and obstruction are important and/or the coupling between pollutants and flow field must be considered. ! Chan, S.T., 1992, "Numerical Simulations of LNG Vapor Dispersion from a Fenced Storage Area," Journal of Hazardous Materials, 30, 195-224. ! Havens, J., T. Spicer, H. Walker, and T. Williams, 1995, "Regulatory Application of Wind Tunnel Models and Complex Mathematical Models for Simulating Atmospheric Dispersion of LNG Vapor," International Conference and Workshop on Modeling and Mitigating the Consequences of Accidental Releases of Hazardous Materials, American Institute of Chemical Engineers, New York, 435-469. ! Rodean, H.C., 1987, FEM3C Simulations of Vapor Dispersion from a Random Pattern of Munitions, UCRL-53790, Lawrence Livermore National Laboratory, Livermore, CA.
12	**User-Friendliness**	The user manual provides a thorough explanation of all program input and presents several sample problems (input and output). ASCII files are used for all numerical program input. No evaluation was performed for the post-processing graphical utilities.

13	**Hardware-Software Interface Constraints/ Requirements**	**Computer operating system:** Unix-based workstations or UNICOS on CRAY-2, CRAY, Y-MP, DEC alpha, SGI, or compatible series mainframes. **Computer platform:** **Disk space requirements:** The storage space for the programs, executables, and sample input files requires several megabytes of disk space. The output files can potentially be very large depending upon the grid resolution chosen by the user. **Run execution time** (for a typical problem)**:** Run execution time for typical problem (CPU or Real Time) - The runtimes can vary from several minutes to hours on a CRAY, depending upon the complexity of the problem and the options used for grid structuring and turbulence mixing. **Programming language:** FORTRAN supporting simultaneous processing (code vectorization). **Other computer peripheral information:** The two interactive post-processors PLOTRDM and EZPLOT depend heavily on graphics packages available at LLNL and are not readily exportable to other platforms. **Portability:** The pre-processing utility and the computational core program should be portable to any CRAY-2 or upwardly compatible mainframe. The program has also been implemented on select workstations (with significant modifications required.) The post-processing graphics programs are highly non-portable and would require substitution of the most nearly compatible graphics utilities on the target platform.
14	**Operational Parameters**	**Identify whether the code has any error diagnostic messages to assist the user in troubleshooting operational problems:** The user's manual contains a detailed list of internal error diagnostics in the code including a list of error messages, their meaning, and suggested corrective action. Error diagnostics are recorded in a runtime log file for each program execution. **Set up time for:** Setup time for the first problem of moderate complexity can be several days if the user is not familar with the terminology and modeling approaches used in computational fluid dynamics. A more experienced user should be ble to set up the sample problem a 1 day or less. All input is conducted via ASCII data files, so batch mode capability is available by means of a command batch file which in turn can launch a succession of code executions with different input files.
15	**Surety Considerations**	**All quality assurance documentation:** Thorough internal documentation of the source code by means of "comment cards" permits verification of the program. **Benchmark runs:** Havens, J.A., T.O. Spicer, and P.J. Schreurs, 1987, "Evaluation of 3-Dimensional Numerical Models for Atmospheric Dispersion of LNG Vapor, " Proceedings of International Conference on Vapor Cloud Modeling, American Institute of Chemical Engineers, New York, 495-538. **Validation calculations:** **Verification with field experiments that has been performed with respect to this code:** Chan, S.T., D.L. Ermak, and L.K. Morris, 1987, "FEM3 Model Simulations of Selected Thorney Island Phase I Trials, " Journals of Hazardous Materials, 16, 267-292. Ermak, D.L., S.T. Chan, D.L. Morgan, and L.K. Morris, 1982, "A Comparison of Dense-Gas Dispersion Model Simulations with Burro Series LNG Spill Test Results," Journal of Hazardous Materials, 6 129-160.
16	**Runtime Characteristics**	Setup time for the first problem of moderate complexity can be several days if the user is not familiar with the terminology and modeling approaches used in computational fluid dynamics. A more experienced user should be able to set up the sample problem in 1 day or less.

Specific Characteristics

Part A: Source Term Submodel Type

A1	**Source Term Algorithm?**	_✔_ YES __NO

Part B: Dispersion Submodel Type

B4	**Gradient Transport or K-Theory**	An option exists for modeling turbulent diffusion parameterized using a K-theory local equilibrium model.
B9	**Multiple Capabilities**	K-ε Theory: Option to compute dense gas dispersion based on a 6-, turbulence model.

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		
F1	**For Chemical Consequence Assessment Models**	**Health effects:** __ **fatalities** __ **cancers** __ **latent cancers** __ **symptom onset** **Health criteria** __ **IDLH** __ **STEL** __ **TLV** __ **TWA** __ **ERPG** __ **TEEL** __ **AEGL** __ **WHO** **Zones with flammable limits:** __ **UFL** __ **LFL** **Blast overpressure regions:** **Fire radiant energy zones:** **Risk qualification:** **Concentration:** ✔ **single value** ✔ **time-history** __ **integrated dose** **Probits:**
Part G: Effects and Countermeasures Submodel Type (No Information Provided.)		
Part H: Physical Features of Model		
H2	**Release Elevation**	✔ **ground** _ **roof**
H3	**Aerodynamic Effects from Buildings and Obstacles**	✔ **building wake** _ **cavity** _ **K-factors** ✔ **flow separation** ✔
H5	**Horizontal/Vertical Wind Shear:**	Yes
H10	**Deposition**	__ **gravitational setting** ✔ **dry deposition** ✔ precipitation
H13	**Temporally and Spatially Variant Mesoscale Processes**	Urban heat island: Canopies: Complex terrain (land) effects: ✔ mountain-valley wind reversals _ anabatic winds __ katabatic winds Complex terrain (land-water) effects: _ seabreeze airflow trajectory reversals __ Thermally Induced Boundary Layer definition __ seabreeze fumigation __ landbreeze fumigation Thunderstorm outflow: Temporally variant winds: Terrain effects are modeled by means of imposing appropriate boundary conditions (e.g., zero normal gradients in wind flow and potential temperature at the terrain surface) onto the solution of the conservation equations. High velocity wind phenomena: __ tornado __ hurricane __ supercane __ microburst
Part I: Model Input Requirements		
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** **See above.** **Dew point temperature:** __ **single point** __ **single tower/multiple point** ✔ **multiple towers** **See above. The actual measurement is of humidity from which the dew point can be calculated.** **Precipitation:** ✔ **single point** __ **single tower/multiple point** __ **multiple towers** **See above.** **Turbulence typing parameters:** __ **temperature difference** __ **sigma theta** __ **sigma phi** ✔ **Monin-Obukhov length** __ **roughness length** __ **cloud cover** __ **incoming solar radiation** __ **user-specified** **See above. Currently cloud cover is used; however, a conversion to incoming solar radiation will be made in the near future.** **Four dimensional meteorological fields from prognostic model:**

Part J: Model Output Capabilities		
J1	**Hazard Zone**	**Yes**
J2	**Graphic Contours and Resolution**	**Yes**
J3	**Concentration Versus Time Plots**	**Plotted by the GRIZ post-processing graphics utility.**
J4	**Tabular at Fixed Downwind Locations**	**Yes**
Part K: Model Usage Considerations (See Items 5 -7)		