DEGADIS (Dated 12260) Readme File

The source code and procedures for running and recompiling this model have been updated. While changes have been made to the source code, the source code algorithms have remained the same. The updated code now conforms to current Fortran standards. This update was performed with the collaboration of Dr. Tom Spicer, original developer of DEGADIS, who played a major role in updating this source code, recompile instructions, and test case procedures.

This file includes updated information on the following topics:

      1. Background
      2. Installation
      3. Model input information and format
      4. Diagnostic (TRAP) messages
      5. Miscellaneous fixes

   1. Background

The DEGADIS model was originally developed for the U.S. Coast Guard and the Gas Research Institute primarily for simulation of the dispersion of cryogenic flammable gases. Subsequent work sponsored by the U.S. Environmental Protection Agency extended DEGADIS for simulation of the dispersion of vertical jets. Implementation of DEGADIS on a personal computer was sponsored by the Gas Research Institute and the American Petroleum Institute.

Basic information concerning the theoretical development of DEGADIS v2.1, its applicability, and its general implementation may be obtained from "User's Guide for the DEGADIS 2.1 Dense Gas Dispersion Model," Tom Spicer and Jerry Havens, EPA-450/4-89-019, November 1989. This document and an evaluation of toxic gas dispersion models is available from the EPA SCRAM web site at: http://www.epa.gov/ttn/scram/dispersion_alt.htm#DEGADIS

A Degadis software package for a PC is also available from the Gas Research Institute for a fee at: http://sales.gastechnology.org/Products-Software.html The Gas Research Institute report provides specific guidance on liquefied natural gas (LNG) vapor dispersion. Their freeware PDF reader, "Foxit Reader", would not open the above page for one of our colleagues.

In the United States, Title 49, Code of Federal Regulations (C.F.R.), Part 193 prescribes the federal safety standards for liquefied natural gas (LNG) facilities. The siting requirements in Subpart B specify that each LNG container and LNG transfer system must have vapor-gas dispersion exclusion zones calculated in accordance with §193.2059. The regulation specifically approves the use of two models for performing these calculations, DEGADIS and FEM3A, but also allows the use of alternative models approved by the U.S. Department of Transportation. http://www.ferc.gov/industries/gas/indus-act/lng/safety/DEGADIS-report.pdf

2. **Installation**

This section summarizes the suggested methods for installing and using DEGADIS v2.1 under DOS for a Windows Operating System.

Previous references to installing and operating DEGADIS under a VMS system have been deleted. However, the source code has been standardized and recompiling under other operating systems should be doable.

2.1 Directory Organization

The target directory of the installation is where the executable files are stored which make up DEGADIS. Make the installation target directory a first level directory off the root directory (e.g., \DEG). The discussion which follows assumes the target directory is \DEG under DOS.

Subdirectories can be created in \DEG to organize the simulations made with DEGADIS. Examples of subdirectories might include \DEG\LNG, \DEG\NH3, or \DEG\BURRO.

2.2   Download and Installing DEGADIS

These instructions apply to a PC with the Windows operating system installed. These instructions can be paralleled for other operating systems such as MAC OSX, and Linux.

1) Download the software and documentation from the EPA SCRAM web site at: http://www.epa.gov/ttn/scram/dispersion_alt.htm#DEGADIS
2) Save the packages to the subdirectory, C:\DEG on your hard drive.
3) Unzip the files into that subdirectory, C:\DEG.
   Note: Some of our users have experienced decompression problems using third party decompression programs. We advise our users to use either WinZip or PKUNZIP.

2.3   Notes about the test cases

Five test cases were selected for DEGADIS, B9, B9T, EX1, EX2 and EX3. As denoted below, each test case tests various aspects of DEGADIS. The test cases can be used as templates but the primary goal here is to make sure that DEGADIS has been downloaded and installed properly.

Here is a brief synopsis of each test case:

    B9 - steady state, ground-level plume,
    B9T - transient, ground-level plume,
    EX1 - steady state, vertically oriented jet that does not return to
          ground level before diluting below the target concentration,

    EX2 - steady-state, vertically oriented jet that returns to ground

level with subsequent ground-level plume, and
        EX3 – steady-state, vertically oriented jet that returns to ground
                    level with subsequent ground-level plume using a simplified
                    relationship between contaminant concentration and air mixture
                    density

    2.4   Preparing for a Simulation

All simulations are run through the Windows' Command Prompt. The Command
Prompt is executed by clicking on Start | All Programs | Accessories |
Command Prompt.

Clicking on the Command Prompt item starts the Command Prompt window
(CMD). The CMD will open up in a default subdirectory such as:
C:\Documents and Settings\UserName>. The ">" symbol is the prompt and the
user types various DOS commands and names after this prompt followed by
pressing the "Enter" key. DOS commands are used to move around and to
create/delete files and subdirectories.

Here is a list of common DOS commands used in the DEGADIS batch
files(*.bat):

Note: Any double quotes are not entered but are there to offset the actual
command sequence from the rest of the sentence text.

FC – file compare. Compares lines of text in one file with lines of text
in another file. The lines that are different are noted. The execution
line is: "FC *file1 file2"*. If the files are in different directories,
then the paths have to be added. Some text editors such as UltraEdit have
built in FC comparable functions where two files can be brought into the
editor and a Compare function is executed.

REM – remark. Comments can be added after each rem.

Rem, as with this line, starts in column 1.

CD – change directory. Allows the user to switch to a different directory.
If a "\" (root) is present before any directory name, the change begins at
the top main (root) directory and not from the present subdirectory
location. Examples and details can be found on the Internet by searching
under "MS-DOS CD"

N: - where "N" is a drive letter. This moves the user from their current
location to the root directory of the "N" drive. For example, "I:" may
take you to a USB thumb drive that has been mapped as drive I:

SET – Displays, sets or removes DOS environmental variables. Just
entering "SET" will produce a list of already set environmental variables.

For instance, entering: "set DEGADIS=C:\DEG" will set DEGADIS as an environmental variable so that when you enter:

"copy %DEGADIS%\example.er1 b9.er1" no matter where you are in the drive – subdirectory structure, the file, example.er1 will be copied from: C:\deg\example.er1 to your current location and named b9.er1. This works for executable files also so you can run DEGADIS from any subdirectory as long as you have your environmental variable set correctly. With the Windows Operating System, commands are **not** case sensitive as with other operating systems such as Unix.

DEL – delete file. This command will delete the file appearing after this command. For example: "Del NoLongerNeededFile.Old" will delete this file: "NoLongerNeededFile.Old".

There are a number of other DOS commands that can be found that maybe useful. Either an old DOS reference manual or a search on line for DOS commands will uncover a lot more useful information. Some of the older DOS commands may not work because they have been deleted.

Before running the DEGADIS test case batch files, the "DEGADIS" environmental variable needs to be set for the location where the DEGADIS exe files are located. If you took our suggestion and placed them in the C:\DEG subdirectory, the set command is:

Set DEGADIS=C:\DEG

If this variable is **not** set, you will not be able to run the test cases.

   2.5 Setting Up to Run the Test Cases via Batch Files

The DEGADIS packages on SCRAM come with 5 test cases. They can be run manually or by using their respective batch files. The batch files follow the nomenclature of the 5 types of runs mentioned above. The files are B9.BAT, B9T.BAT, EX1.BAT, EX2.BAT, and EX3.BAT. Their input data files all bear the same respective test case filename but have various extensions such as .IN, .ER1, .ER2, .LIS, etc. (e.g. B9.er1, EX3.LIS) Some temporary files are created during execution and then deleted after the run is done. If the data needs to be examined, the "del" of these temporary files can be "rem"'ed out and later reinstituted.

One word of caution, the degbridge.for program will output a "Ignore any file-not-found messages to follow." It will likely output a number of "File-not-found" messages. **This is "not" an actual error** but something left over from the original code that will be addressed in a later update.

To start:

1) Create subdirectories for each test case from your equivalent of C:\DEG (e.g. mkdir B9 or MD EX3) MKDIR and MD are the same "make (or create) subdirectory" command. This will create the new subdirectories: C:\DEG\B9 or C:\DEG\EX3.

2) Copy test run input data and batch file into each respective subdirectory (e.g. copy b9.* b9*.*).

3) Set your environmental command for the executable and support data files (e.g., SET DEGADIS=C:\DEG). **Note that the SET DEGADIS command needs to be done every time a CMD window is opened.**

4) Change directory and run each test case (e.g. cd B9 then enter B9) Note: to change from subdirectory B9 to EX3 under directory DEG, the following command structure can be used: cd ..\ex3) ".." moves up one directory level toward root (main directory from which all subdirectories are created.) So this moves the subdirectory location or focus from B9 up to DEG, the parent directory, and then down to EX3.

5) File compare (FC) command lines have been added to each batch file. The output has a "LIS.DIF" suffix to the general filename. The three characters to the left of the dot denote the extension of the output file while the "DIF" indicates that it contains the output of any differences between the original file and the file you just ran. For instance, the original B9 test case output file is B9OLD.LIS and the batch file is set up to recreate this file as B9.LIS. The file compare will output the differences as the file B9LIS.DIF.

6) The next paragraph will explain what to look for when examining the DIF files for major differences. However, a pre-explanation is needed. When the latest executables were used, the downwind distances calculated were different from the original downwind distances calculated in 1992 for some of the previous DEGADIS test cases such as EX3. The previous downwind **unit** values were mostly "2"'s while the current downwind unit values are mostly "5"'s (e.g. 162 versus 195). Calculating concentrations for these different downwind distances produces different concentrations. However, when the concentration values are graphed by their respective downwind distances, the two resultant lines coincide. Therefore, the results are "the same".

7) After running each test case, the results are compared to the 2012 results that have an "Lis" extension (e.g. *.Lis) as opposed to the original 1992 results that have an "L92" extension (e.g. *.L92). These L92 files now have the word "old" in the filename with the "Lis" extension instead of "L92". There should be no significant differences between the old and new results. The results will produce: 1) date and time differences, 2) the same values printed differently such as 0.005 versus .005, and/or 3) very minor differences in values such as 12.3456789 versus 12.3456791 where

differences are in the 10,000ths to millionths positions to the right of the decimal point. Any significant differences should be reported via the SCRAM "Contact Us" page http://www.epa.gov/ttn/scram/comments.htm.

The next two major topics have been copied from the previous Readme file:

3. <u>Model input information and format</u>

DEGINP, JETINT, and JETPLUIN are the programs used to enter simulation information; DEGINP and JETINT are interactive programs. In DEGINP and JETINT, the questions asked depend on previous responses. On-line help is available for all questions. Default responses are shown for each question along with a list of possible responses. The following conventions are used:

* A line terminator (carriage return) must end every line entered by the user.

* The file name specification RUN_NAME must satisfy operating system restrictions.

* When the user is asked to choose an option, responses are a single character (capital or lower case). The default responses are denoted by a capital letter inside angle brackets (e.g. <N>). When applicable, a menu of responses is included inside square brackets.

* When a file is used as input (i.e. for the density or transient source input), DEGINP and JETINT read the same information from the file which would be entered at the terminal in the same order and in the same format.

DEGINP and JETINT use a simple text file format for storing contaminant properties; an example file EXAMPLE.GAS is included with the code. The first line of the file contains column headings with the following meanings:

Gas   The three letter designation used to identify the contaminant with a text description in the next column.

GASMW   is the contaminant molecular weight (kg/kmole). When blank, GASMW is the molecular weight of air.

GASTEM   is the contaminant temperature as it is released to the atmosphere (after any depressurization) (K). When blank, GASTEM is the ambient temperature.

GASRHO   is the contaminant density as it is released
             to the atmosphere (after any depressurization)
             (kg/m**3). When blank, GASRHO is calculated
             using the ideal gas law.

CPK   is q1 in the equation used to describe the
             contaminant heat capacity.

CPP   is p1 in the equation used to describe the
             contaminant heat capacity.

GASULC   is the upper level of concern.

GASLLC   is the lower level of concern.

GASZZC   is the elevation for contour calculations.

Any text editor can be used to add other contaminants by
following the example format. Also, different file names can
be used for the property file.

3.1 Jet releases

     JETINT is the interactive input module which defines a
jet or elevated release simulation. (As discussed earlier,
JETINT creates IN files for use by JETPLUIN.) The following
summarizes the structure of the input file RUN_NAME.IN
required by JETPLUIN to simulate jet releases:

     TITLE1
     TITLE2
     TITLE3
     TITLE4
     U0   Z0
     ZR
     INDVEL   ISTAB   RML
     TAMB   PAMB   RELHUM
     TSURF
     GASNAM
     GASMW
     AVTIME
     TEMJET
     GASULC   GASLLC   GASZZC
     INDHT   CPK   CPP
     NDEN
     ERATE
     ELEJET   DIAJET
     TEND
     DISTMX

A description of each variable follows. After each line of
input, an explanation is included. All units are SI (meter,
kilogram, second) except as noted.

```
TITLE1
TITLE2
TITLE3
TITLE4
        TITLE1, TITLE2, TITLE3, and TITLE4 are four lines of
        up to 80 characters each of a title for this
        simulation.

U0  Z0
        U0 (m/s) is the ambient wind velocity at Z0 (m).

ZR
        ZR is the surface roughness (m).

INDVEL  ISTAB  RML
        INDVEL is an indicator which determines the method of
        calculation for the ambient velocity profile in the
        jet/plume model as follows:

        For INDVEL=1, the Pasquill-Gifford stability category
        (in ISTAB using 1 for A, 2 for B, etc.) is used along
        with ZR to determine the Monin-Obukhov length RML;
        the log velocity profile is then determined using
        RML.

        For INDVEL=2, the Monin-Obukhov length RML is
        supplied by the user; the log velocity profile is
        then determined using RML.  Note that ISTAB must
        still be specified.

TAMB  PAMB  RELHUM
        TAMB, PAMB, and RELHUM are the ambient temperature
        (K), the ambient pressure (atm or N/m**2), and the
        relative humidity (%), respectively.

TSURF
        TSURF is the surface temperature (K); if TSURF < 250
        K, TSURF is set to TAMB.

GASNAM
        GASNAM is a three-letter designation for the
        contaminant name.  Any character string of three
        letters or less is valid; this is for user run
        identification and does not access property data.

GASMW
        GASMW is the contaminant molecular weight (kg/kmole).

AVTIME
        AVTIME is the averaging time (s) used to estimate
        DELTAY.

TEMJET
```

TEMJET is the temperature of the contaminant as it is released to the atmosphere (K).

GASULC GASLLC GASZZC

GASULC and GASLLC are the concentrations to be used for estimating contours for an upper and lower concentration level in DEGADIS. The calculations are made for the elevation GASZZC. Note that the DEGADIS computations will be carried out to GASLLC for steady-state simulations and to GASLLC/4 for transient simulations.

INDHT CPK CPP

INDHT is used to include heat transfer in the DEGADIS computations. Heat transfer is not included for INDHT=0. For INDHT=1, heat transfer is included, and the heat transfer coefficient is calculated by DEGADIS. CPP and CPK are used to calculate the heat capacity as a function of temperature. If a constant heat capacity is desired, set CPP to 0. and CPK to the desired heat capacity (J/kg K); JETPLUIN calculates the appropriate value for q1.

NDEN

NDEN is used to specify the contaminant density profile. There are three cases for NDEN:

NDEN = -1; "isothermal" mode. The simulation treats the contaminant as if it were an ideal gas with a molal heat capacity equal to that of air. Water condensation effects are ignored.

NDEN = 0; "nonisothermal" mode. The simulation treats the contaminant as if it were an ideal gas with the heat capacity indicated by CPK and CPP. Water condensation effects are taken into account as appropriate.

NDEN > 0; "isothermal" mode. NDEN specifies the number of triples which follow in the next NDEN lines. The triples are used to specify the contaminant concentration as a function of density based on adiabatic mixing with ambient air. The ordered triples represent (in order): (1) the contaminant mole fraction; (2) the contaminant concentration (kg contam/m**3 mix); and (3) the mixture density (kg mixture/m**3 mixture). The ordered triples must go from pure air to pure contaminant (equivalent to an "isothermal" release in DEGADIS).

ERATE

ERATE is the mass evolution (release) rate (kg/s).

```
ELEJET  DIAJET
        ELEJET is the initial jet elevation (m), and DIAJET
        is the initial jet diameter (m).

TEND
        TEND is the duration of the primary release (s).  For
        steady-state releases, set TEND to 0.; to run the
        jet/plume model only, set TEND to a negative number.

DISTMX
        DISTMX is the maximum distance between output points
        in the JETPLU output (m).
```

When the plume reaches ground level, DEGBRIDG takes the
output from the jet/plume model and creates the file
necessary for DEGADIS to complete the simulation.

3.2 Nonjet releases

     DEGINP is the interactive input module which defines a
ground-level, low initial momentum (nonjet) release
simulation.

     Upon completion, DEGINP creates a file like the one
shown below; note that many of the variables were discussed
earlier.

```
                                TITLE1
                                TITLE2
                                TITLE3
                                TITLE4
                                U0, Z0, ZR
                                ISTAB
                                OODIST, AVTIME
                                INDVEL, RML
                                TAMB, PAMB, HUMID, RELHUM
                                ISOFL, TSURF
                                IHTFL, HTCO
                                IWTFL, WTCO
                                GASNAM
                                GASMW, GASTEM, GASRHO
                                CPK, CPP
                                GASULC, GASLLC, GASZZC
                          /     NP
If (ISOFL.NE.0) then |     DEN((J,1),J=1,5)
   (for external     |     DEN((J,2),J=1,5)
     density         |        .
   calculations)     |        .
                     |        .
                     \     DEN((J,NP),J=1,5
                                YCLOW
                                GMASS0
                                NT
```

```
        / PTIME(1),ET(1),R1T(1),PWC(1),PTEMP(1),PFRACV(1)
NT    |  PTIME(2),ET(2),R1T(2),PWC(2),PTEMP(2),PFRACV(2)
of    |     .
these |     .
      |     .
      \  PTIME(NT),ET(NT),R1T(NT),PWC(NT),PTEMP(NT),PFRACV(NT)
                        CHECK4
                        TINP
```

The following description summarizes the use of each variable
not already discussed:

OODIST

        The distance to plume touchdown for jet releases (m).
        For nonjet releases, this is set to zero.

HUMID

        The ambient absolute humidity. Note that the value
        of RELHUM is used to estimate the ambient absolute
        humidity unless RELHUM is equal to 0.0.

ISOFL

        The flag which indicates an "isothermal" simulation
        is being made (if ISOFL is 1).

HTCO

        The heat transfer coefficient if a constant
        coefficient is desired.

IWTFL

        The flag which indicates ground-to-cloud water
        transfer is estimated for the source blanket.

WTCO

        The water transfer coefficient if a constant
        coefficient is desired.

GASTEM

        The temperature of the released contaminant (after
        any depressurization).

GASRHO

        The contaminant density at GASTEM conditions.

NP

        If an "isothermal" simulation is being made (i.e., if
        ISOFL is nonzero), then the next NP lines contain the
        contaminant/air density relationship in tabular form.
        For J ranging from 1 to NP, DEN(1,J) has the
        contaminant mole fraction, DEN(2,J) has the
        contaminant concentration (in kg/m**3), DEN(3,J) has
        the mixture density (in kg/m**3), DEN(4,J) has the
        mixture enthalpy (in J/kg), and DEN(5,J) has the

mixture temperature (in K). Pure ambient air values are input for J=1; pure contaminant values are input for J=NP.

YCLOW

The contaminant mole fraction where the calculations are stopped. (For transient simulations, calculations are carried out to YCLOW/5.)

GMASS0

The initial mass of contaminant gas over the source for transient spills.

NT

The number of times required to describe the source. For J ranging from 1 to NT, ET(J) has the primary source evolution rate (kg/s), R1T(J) has the primary source radius, PWC(J) has the primary source contaminant mass fraction, PTEMP(J) has the primary source temperature, and PFRACV(J) has the primary source liquid mass fraction all evaluated at PTIME(J).

For steady-state releases, NT should be set to 4. Set ET, R1T, PWC, PTEMP, and PFRACV to steady-state values for times of 0.0 and 60230.0 s. For times of 60231.0 and 60232.0 s, set ET and R1T to zero with PWC, PTEMP, and PFRACV still at steady-state values.

CHECK4

CHECK4 is true (T) for steady-state simulations; otherwise, it is false.

TINP

TINP is the time stamp when the input was created.

4. Diagnostic (TRAP) messages

==

This section summarizes only the CHANGES made to TRAP messages.

■ No Changes made.

==

5. Fixes

The DEGADIS code has been updated to be compliant with Intel Visual Fortran Composer V12. The Interface and related statements have been deleted. This includes C Programming related code.