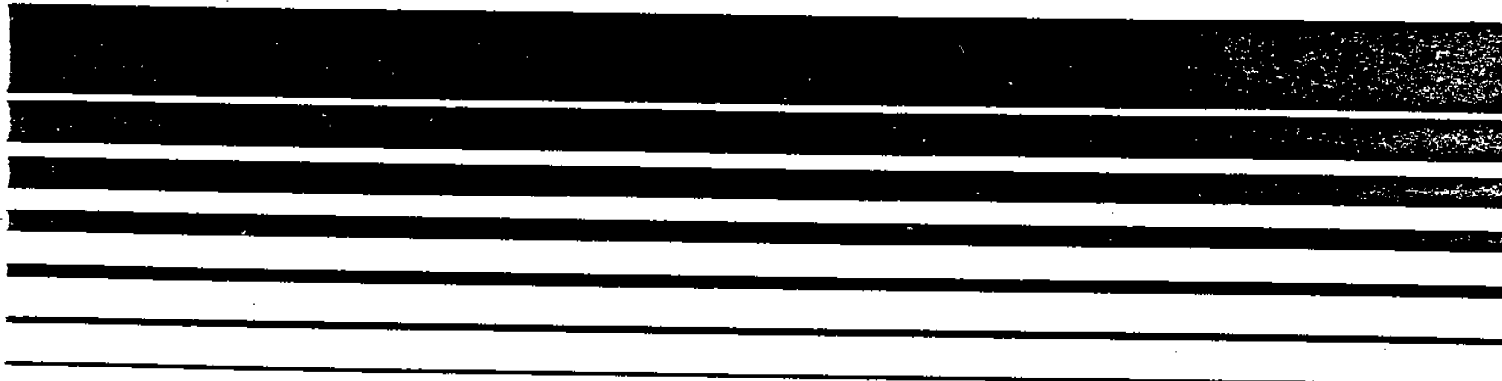**&EPA**

A Dispersion Model For Elevated Dense Gas Jet Chemical Releases

Volume II. User's Guide

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DISCLAIMER

ACKNOWLEDGEMENTS

PREFACE

This version of the elevated dense gas dispersion model, Ooms/DEGADIS, has been developed by Dr. Jerry Havens and Dr. Tom Spicer of the University of Arkansas with the support of funding from the United States Environmental Protection Agency (EPA). It represents intermediate development of a dense gas modeling package which is undergoing further refinement through additional EPA support. While this model has not been extensively tested against field data, and is subject to specific limitations and uncertainties, the EPA is making it publicly available through the National Technical Information Service (NTIS) as an interim research tool pending further model evaluation and development.

The Ooms/DEGADIS model has been written in FORTRAN with specific intent for compilation and execution on a Digital Equipment Corporation VAX computer. Implementation of this model on any other computer system may be attempted at the risk of the user. Considerations for such implementation, however, are discussed in Appendix B of Volume II.

To facilitate dissemination of the model, it is being provided on two PC-compatible diskettes. The model should be uploaded via modem from a PC terminal to a host VAX computer, and several files must then be renamed prior to compilation and execution. Specific information on this process is contained in the file AAREADME.TXT. Print this file and the compilation batch file, BUILD.COM, prior to attempting compilation.

It is the concern of the EPA that this model be applied only within the framework of its intended use. To this end the user is referred to the specific recommendations in Volume I, Section VII for model application. These recommendations take advantage of the fact that, in this version of the Ooms/DEGADIS model, the portion of the model adapted from Ooms and his colleagues can be executed as a standalone model, as can the DEGADIS portion. To begin any particular simulation, it is recommended that the Ooms portion of the model be executed by itself.

This can be accomplished by setting the input variable <TEND> equal to 1. If the output from this simulation predicts that the plume will touch down less than 1 kilometer from the source, the complete Ooms/DEGADIS model may be appropriately applied (set <TEND> equal to zero or greater). If the plume is not predicted to touch down within 1 kilometer, this model should not be used.

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LIST OF SYMBOLS

b_j	characteristic width of plume (radius $= b_j\sqrt{2}$), m
c	local concentration, kg/m^3
c^*	concentration on plume axis, kg/m^3
r	radial distance to jet/plume axis, m
s	distance along plume axis, m
u	local velocity in direction of plume axis, m/s
u_a	wind velocity, m/s
u^*	plume excess velocity at plume axis, $u(r = 0) - u_a\cos\theta$, m/s
x	horizontal coordinate, m
y	vertical coordinate, m
α_1, α_2, α_3	entrainment coefficients
θ	angle between plume axis and horizontal, radius
λ	turbulence Schmidt number, 1.16
ρ	local density, kg/m^3
ρ_a	air density, kg/m^3
ρ^*	plume excess density at plume axis, $\rho(r = 0) - \rho_a$, kg/m^3

SUMMARY

The mathematical modeling techniques used to predict atmospheric dispersion of denser-than-air gases in the Ooms and DEGADIS models are briefly summarized. The Ooms model describes the release and subsequent dilution and trajectory of an elevated gas jet as a gas plume. If the plume falls to ground level, DEGADIS describes the resulting ground-level plume. As well, DEGADIS can be used to describe the release and dilution from a low-momentum, ground-level release. The necessary model-input information to simulate a denser-than-air gas release is summarized. Example simulations of steady-state and transient release are included. Guidelines for installation of the models are included, and a listing of the Ooms and DEGADIS models are included along with a partial list of program variables and diagnostic messages.

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I. MODEL SUMMARIES

This section is intended to summarize the critical components of the formulation of each model and the associated limitations and cautions. The suggested limitations and guidelines are based on the experience gained during the development of the models and verification by comparison with a wide range of denser-than-air gas laboratory and field-scale dispersion tests.

Ooms' Model

Ooms, Mahieu, and Zelis' (1974) model comprises simplified balance equations for mass and momentum to describe the jet illustrated in Figure I.1.
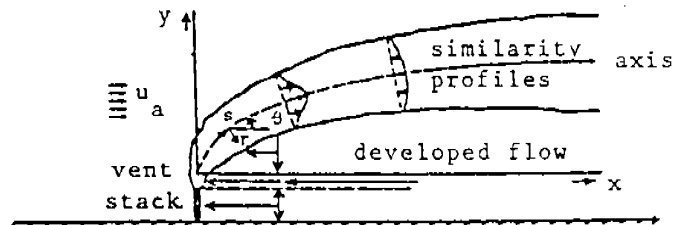
Figure I.1. Schematic diagram of Ooms' model.

Gaussian similarity profiles for velocity, density, and concentration are assumed to apply in the developed jet:

$$u(s,r,\theta) = u_a \cos\theta + u^*(s)\, e^{-r^2/b_j^2(s)} \qquad (I.1)$$

$$\rho(s,r,\theta) = \rho_a + \rho^*(s)\, e^{-r^2/\lambda^2 b_j^2(s)} \qquad (I.2)$$

$$c(s,r,\theta) = c^*(s)\, e^{-r^2/\lambda^2 b_j^2(s)} \qquad (I.3)$$

Balance equations for mass, horizontal and vertical momentum, and energy are integrated over the radius of the plume, and the resulting ordinary differential equations are numerically integrated. Initial conditions are specified at the beginning of the "developed flow" region of the jet (Figure I.1). The trajectory of the jet to the developed flow region is calculated using wind-tunnel data correlations by Kamotani and Greber (1972).

The balance equations for mass and momentum incorporate empirical coefficients for estimating air entrainment. The coefficients α_1, α_2, and α_3 provide for entrainment as follows:

α_1 is the entrainment coefficient for a turbulent free jet. The value 0.057 was incorporated by Ooms, after Albertson, et al. (1950).

α_2 accounts for entrainment into the plume at a sufficiently long distance downwind of the vent where the velocity of the plume approaches the wind velocity. The value 0.5 was incorporated by Ooms, after Richards (1963).

α_3 accounts for entrainment due to atmospheric turbulence. Ooms suggested estimation of the entrainment velocity as $u' = (\epsilon b_j)^{1/3}$, with specification of ϵ (the eddy energy dissipation) as a function of height, wind velocity, and atmospheric stability. The eddy energy dissipation for a neutral atmosphere was recommended by Briggs (1969):

$\epsilon = 0.0677 \ u_a/z \ (m^2/s^3)$ for $z < 300$ m

and for "unstable" and "stable" atmospheres by Kaimal et al. (1976):

$\epsilon = 0.004 \ (m^2/s^3)$ for unstable atmospheres

$\epsilon = 0$ for stable atmospheres

The value 1.0 for α_3 was incorporated by Ooms, after Briggs (1969).

A listing of the code is included in Appendix E. Because the Ooms model equations were derived using the ideal gas equation of state, the current version of the Ooms model code does not account for changes in temperature and density associated with moisture condensation or with contaminant phase changes (contaminant aerosol). Also, the Ooms model will not approach the Gaussian plume model as the density and momentum of the released jet approach ambient values. This is due to the fact that the Ooms model assumes the jet to be radially symmetric at all times which is not true for the Gaussian plume model since σ_y and σ_z are not generally equal. Finally, because the Ooms model code uses fixed-step integration routines, duplicate simulations should be made with different step sizes varying by a factor of about 3 to 5 to ensure the numerical error is sufficiently small. This can be done by adjusting the value of <H> in the input file.

DEGADIS Summary Description

The DEGADIS (DEnse GAs DISpersion) model combines the principal features of the Shell HEGADAS model (Colenbrander, 1980, and Colenbrander and Puttock, 1983) and a box model proposed by van Ulden (1983). DEGADIS was developed for the U.S. Coast Guard and the Gas Research Institute and was designed to model the atmospheric dispersion of denser-than-air gases (Havens and Spicer, 1985, and Spicer and Havens, 1987). The general application of the model involves formation of a "secondary" gas source, the subsequent entrainment of gas from that secondary source by the wind field, and downwind dispersion of the gas plume or cloud. Figure I.2 illustrates the general methodology. The description of the formation and development of the secondary source utilizes a box model. The entrainment from the secondary source and subsequent downwind dispersion utilizes the similarity representations of the cloud concentration and vertical velocity profiles of the HEGADAS model. Denser-than-air gas releases which cannot be represented as

4

Ambient wind (can be zero)

Input to downwind dispersion model

$Q_*(t)$

Frontal entrainment velocity u_e

$T(t)$, $C(t)$, $\rho(t)$

H

u_f

u_f

$R(t)$

$R_p(t)$

q_s

Secondary Source Formation

$$C(x,y,z) = C_C(x) \exp\left[-\left(\frac{|y|-b(x)}{S_y(x)}\right)^2 - \left(\frac{z}{S_z(x)}\right)^{1+\alpha}\right], \quad |y| > b$$

$$C(x,y,z) = C_C(x) \exp\left[-\left(\frac{z}{S_z(x)}\right)^{1+\alpha}\right], \quad |y| \leq b$$

$$u_x = u_0 \left(\frac{z}{z_0}\right)^\alpha$$

- - - ISO CONCENTRATION CONTOURS

FOR $C = C_u$

Downwind Dispersion
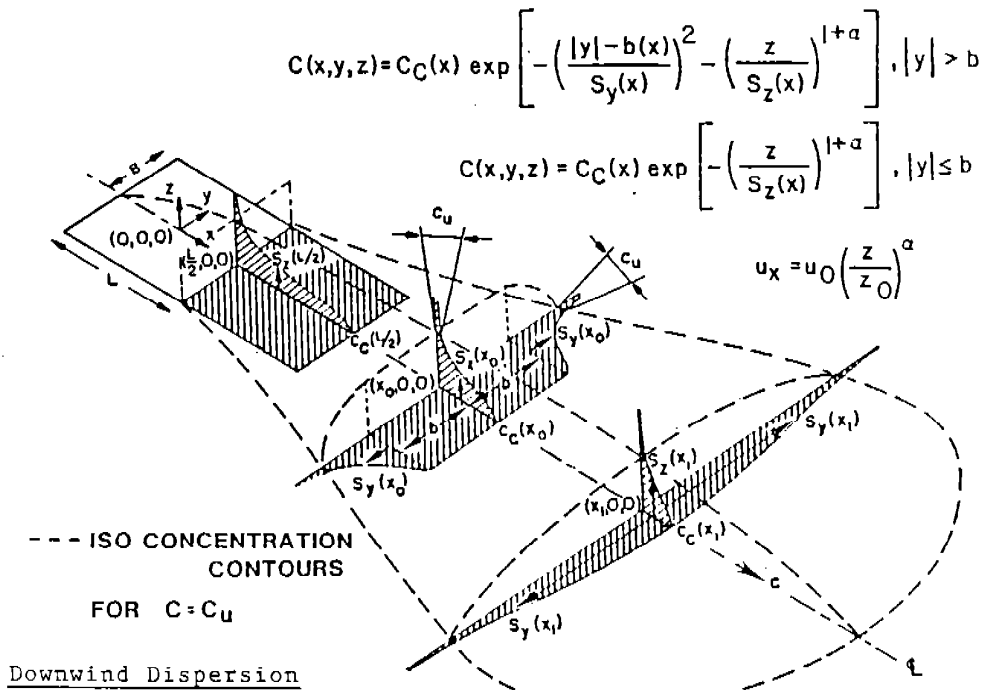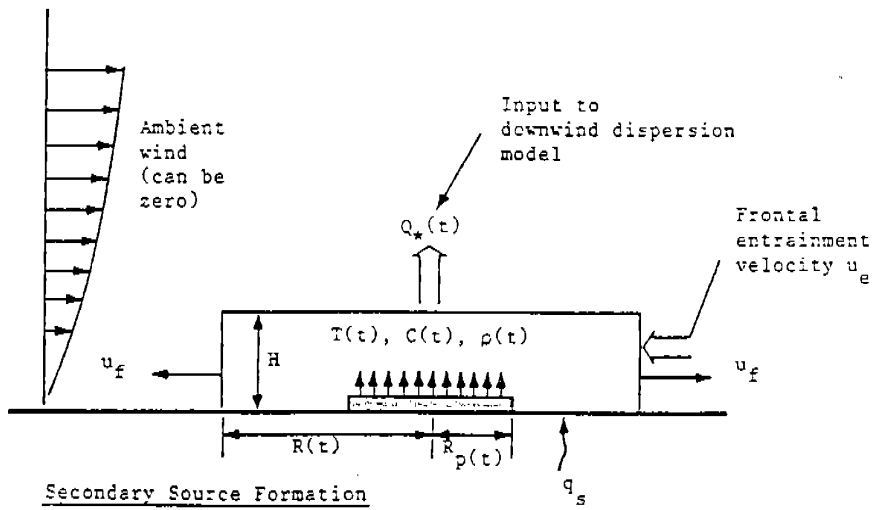
Figure I.2.   Schematic diagram of DEGADIS model.

.steady, continuous releases are modeled as a series of pseudosteady releases. A complete description of DEGADIS can be found in Havens and Spicer (1985) or Spicer and Havens (1987).

Application of the model to releases of a denser-than-air gas in zero wind involves only the box model. The box model treatment of gravity spreading and associated air entrainment is based on parameterization of the laboratory still-air experiments described by Havens and Spicer (1985). For releases in wind, the box model also describes the source development but provides for entrainment of the gas-air source cloud into the ambient wind field.

DEGADIS incorporates heat transfer and water transfer when applicable from the underlying surface to the cloud. Inclusion of these procedures in the model is optional. Effects of heat transfer on both the mean cloud buoyancy and the vertical turbulent mixing (air entrainment) are included while direct effect of water transfer is included only in the mean cloud buoyancy.

DEGADIS is written in Digital Equipment Corporation's VAX/VMS* Fortran (a superset of ANSI Fortran 77); it is composed of six programs which communicate using ASCII files (see Section III and Appendix C). A listing of the code is included as Appendix F, and a partial list of program variables is given in Appendix H. Considerations for installation of DEGADIS are discussed in Appendices A and B. DEGADIS self-diagnostics are listed in Appendix I along with suggested actions. (Appendix D discusses the input information for a standalone DEGADIS simulation.)

As a standalone model, DEGADIS application should be limited to the description of atmospheric dispersion of denser-than-air gas releases at ground level onto flat, unobstructed terrain or water. Because of the assumption of flat, unobstructed terrain, when the surface roughness used in DEGADIS becomes a significant fraction of the depth of the dispersing layer, this assumption may no longer be satisfied. Application to releases from sources above ground level (e.g. overflow from

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dikes) would be expected to give conservative predictions of the downwind hazard zones, but this has not been verified.

Demonstration of DEGADIS has been primarily directed to the prediction of hazard extent defined by gas concentrations in the hydrocarbon flammable limit range (~1 to 20%). Even though the relation between peak gas concentration and time-averaged gas concentration is uncertain, there is some basis for using 2.0 as an estimate of the peak-to-time-averaged-concentration ratio for determining a flammable gas concentration zone. If this assumption is made, the predicted distance to LFL/2 would be the maximum distance at which a flammable gas concentration would be predicted. Based on the simulations of field experiments presented in Havens and Spicer (1985), the average ratio of observed distance to calculated distance for a given time-averaged concentration level (OBS/PRE) ranged from 0.82 to 1.03 for the 2.5% level nine out of ten times (i.e. 90% confidence interval); for the 5% level, the average (OBS/PRE) ranged from 0.73 to 0.96 for a 90% confidence interval. If for a given release scenario the calculated distance to the 2.5% average concentration level was 120 m, the distance to the 2.5% average concentration for nine out of ten realizations of the same release would be expected to range (on the average) between 98 m and 124 m, which would also represent the range of the downwind extent of the flammable gas concentration zone for LNG if the peak-to-average ratio of 2.0 is assumed.

Limitations and Cautions

There are some items which should be considered when using the Ooms and DEGADIS models. As previously stated, because the Ooms model equations were derived using the ideal gas equation of state, the current version of the Ooms model code does not account for changes in temperature and density associated with moisture condensation or with contaminant phase changes (contaminant aerosol). Of course, neither model is currently capable of determining any interactions with obstacles in the flow. Also, the Ooms model will not approach the Gaussian plume model as the density and momentum of the released jet approach ambient values. This is due to the fact that the Ooms model

assumes the jet to be radially symmetric at all times which is not true for the Gaussian plume model since σ_y and σ_z are not generally equal. Finally, because the Ooms model code uses fixed-step integration routines, duplicate simulations should be made with different step sizes varying by a factor of about 3 to 5 to ensure the numerical error is sufficiently small.

The Ooms model portion of the calculation is terminated when $(c/c^*) = 0.1$ at ground level, and the output from the Ooms model is used to establish the initial conditions for DEGADIS. In DEGADIS, the source concentration is set to c^*, and the source radius is set to $\sqrt{2}b_j$. Because the Ooms model calculation is stopped when $(c/c^*) = 0.1$ at ground level, the jet x-direction momentum may still be significant. Because DEGADIS describes low initial momentum releases, care should be taken that the jet x-direction momentum is no longer significant. For cases when the jet x-direction momentum is not significant when $(c/c^*) = 0.1$ at ground level, the method of first-order lines has been proposed to account for the ground interaction (Dodge et al., 1982). This has not been implemented since the maximum concentration as a function of distance may increase over the region of ground interaction for this method (which is physically impossible).

II. MODEL INPUTS

As implemented under VAX/VMS, the Ooms/DEGADIS models use three areas of input information:

- VAX/VMS command procedure for execution
- simulation definition
- numerical parameters.

The VAX/VMS command procedure used to execute Ooms/DEGADIS is generated by OOMS_IN. As well, OOMS_IN is the input module which reads the simulation definition. An example input session is included in Section IV. The numerical parameters (convergence criteria, initial increments, etc.) are supplied to DEGADIS though a series of input files. Although these numerical parameters are easily changed, the user should need to change these only rarely with the exception of the time-sort parameters which are explained in Section IV.

VAX/VMS Command Procedure

The VAX/VMS command procedure generated by OOMS_IN controls the execution of images for the simulation. Image execution follows one of two paths, either for a transient (time-limited) release or for a steady-state release. OOMS_IN will automatically generate the appropriate command procedure; but first, OOMS_IN requires a simulation name be specified. The simulation name must be a valid VAX/VMS file name without a file extension and is designated RUN_NAME. OOMS and DEGADIS will use this file name with standard extensions for input, interprocess communication, and output. Figures II.1 and II.2 show example VAX/VMS command procedures for the run name TEST_S and TEST for steady-state and transient releases, respectively. The directory which contains the executable images of the Ooms model and DEGADIS has been assigned the system logical name SYS$DEGADIS (see Appendix A). The COPY/LOG command simply copies a file from the first argument to the second argument, and the RUN command executes the specified image. Of course, these steps may also be carried out by issuing the commands at a terminal.

```
$ ASSIGN TEST_S.INO FOR001
$ ASSIGN TEST_S.OUT FOR003
$ ASSIGN TEST_S.IND FOR002
$ RUN SYS$DEGADIS:OOMS
$ DEASSIGN FOR001
$ DEASSIGN FOR002
$ DEASSIGN FOR003
$ RUN SYS$DEGADIS:DEGBRIDGE
$ TEST_S
$ COPY/LOG    SYS$DEGADIS:EXAMPLE.ER1    TEST_S.ER1
$ COPY/LOG    SYS$DEGADIS:EXAMPLE.ER2    TEST_S.ER2
$ RUN    SYS$DEGADIS:DEGADIS1
TEST_S
$ RUN    SYS$DEGADIS:SDEGADIS2
TEST_S
$ COPY/LOG    TEST_S.OUT+TEST_S.SCL+TEST_S.SR3 -
TEST_S.LIS
```

Figure II.1.   Example DEGADIS command procedure on VAX/VMS
               for a steady-state simulation named TEST_S.

```
$ ASSIGN TEST.INO FOR001
$ ASSIGN TEST.OUT FOR003
$ ASSIGN TEST.IND FOR002
$ RUN SYS$DEGADIS:OOMS
$ DEASSIGN FOR001
$ DEASSIGN FOR002
$ DEASSIGN FOR003
$ RUN SYS$SYSDEGADIS:DEGBRIDGE
TEST
$ COPY/LOG    SYS$DEGADIS:EXAMPLE.ER1    TEST.ER1
$ COPY/LOG    SYS$DEGADIS:EXAMPLE.ER2    TEST.ER2
$ COPY/LOG    SYS$DEGADIS:EXAMPLE.ER3    TEST.ER3
$ RUN    SYS$DEGADIS:DEGADIS1
TEST
$ RUN    SYS$DEGADIS:DEGADIS2
TEST
$ RUN    SYS$DEGADIS:DEGADIS3
TEST
$ COPY/LOG    TEST.OUT+TEST.SCL+TEST.SR3 -
TEST.LIS
```

Figure II.2.   Example DEGADIS command procedure on VAX/VMS
               for a transient simulation named TEST.

Simulation Definition

OOMS_IN is a method of simulation definition where the user specifies information about the ambient wind field, the properties of the released gas, and some details of the release.

The input is carried out using free-formatted files. The use of this method means that a value of each parameter must be specified in the input file even if it has no meaning for the simulation at hand. As well, this form of input allows the user creating the input file to be able to ignore spacing in the input file. Numbers on a particular line can be separated by commas, spaces, or tabs. Comments may also be included at the end of any line in the input file as long as all required values are given before any comments are included. Lines which are only comments are not allowed. (Sample input files are included in Section IV.)

The ambient wind field is characterized by a known velocity u_0 at a given height z_0, a surface roughness z_R, and the Pasquill stability class or Monin-Obukhov length. The Pasquill stability class is used to estimate values of the lateral similarity parameter coefficients δ and β (along with the averaging time as discussed in Spicer and Havens, 1987) and values of the along-wind similarity coefficients (Beals, 1971). The Monin-Obukhov length λ used by Businger et al. (1971) in their logarithmic velocity profile function ψ (Table II.1) is used to calculate the friction velocity u_*. In addition to these specifications, the ambient temperature, pressure, and humidity must be specified.

The properties of air and the released gas are used to evaluate the mixture density as a function of temperature and composition. The desired released gas properties include the molecular weight MW_c, the release temperature T_0, and two constants q_1 and p_1 which describe the heat capacity according to the equation

$$C_{p_c}(T) = (MW_c)^{-1} \left[3.33 \times 10^4 + q_1 \left[\frac{T^{p_1} - T_0^{p_1}}{T - T_0} \right] \right] \qquad (II.1)$$

TABLE II.1

REPRESENTATIVE MONIN-OBUKHOV LENGTHS AND POWER LAW EXPONENTS
FOR DIFFERENT ATMOSPHERIC STABILITIES

Pasquill Stability Category	Monin-Obukhov Length (λ) as a Function of Surface Roughness z_R (m)	Typical (*) Power Law Exponents α	Corrections to Logarithmic Profiles as Given by Businger (1973)
A	$-11.4\, z_R^{0.10}$	0.108	$\psi = 2 \ln\left[\dfrac{1+a}{2}\right] + \ln\left[\dfrac{1+a^2}{2}\right]$
B	$-26.0\, z_R^{0.17}$	0.112	$\quad - 2 \tan^{-1}(a) + \pi/2$
C	$-123\, z_R^{0.30}$	0.120	with $a = (1 - 15(z/\lambda))^{1/4}$
D	∞	0.142	$\psi = 0$
E	$123\, z_R^{0.30}$	0.203	
F	$26.0\, z_R^{0.17}$	0.253	$\psi = -4.7(z/\lambda)$

(*) calculated for 8 m/s at 10 m with surface roughness of 0.001 m

where C_{p_c} (T) is the mean heat capacity (J/kg K) at temperature T. A constant heat capacity can also be specified as discussed later in this section.

In specifying the details of the release, the user must choose to simulate the release as time-limited (transient) or steady-state. As well, the jet elevation, diameter, and orientation must be specified.

Figure II.3 summarizes the structure of the input file RUN_NAME.IN needed by OOMS_IN. The following description is written for each of the variables in Figure II.3. Variables are written in brackets. After each line of input, an explanation is included. All units are SI (meters, kilograms, second) except as specified.

```
<TITLE1>
<TITLE2>
<TITLE3>
<TITLE4>
<UO>    <ZO>
<ZR>
<INDVEL> <ISTAB> <MOLEN>
<TAMB> <PAMB> <RELHUM>
<TSURF>
<GASNAM>
<GASMW>
<AVTIM>
<JETTEM>
<GASUL> <GASLL> <ZLL>
<INDHT> <CPC> <CPP>
<ERATE>
<JETELE> <JETDIA>
<TEND>
<XO> <H> <DISTA> <DISTAN>
<K1> <K2> <K3>
```

Figure II.3. RUN_NAME.IN structure required by OOMS_IN.

```
<TITLE1>
<TITLE2>
<TITLE3>
<TITLE4>     Each of <TITLE1>, <TITLE2>, <TITLE3>, and <TITLE4> are used
             to keep a title block with the output of the model(s).  Each
             are up to 80 characters long.


<U0>   <Z0>
             <U0> is the ambient wind velocity at <Z0>.


<ZR>         <ZR> is the surface roughness.


<INDVEL>   <ISTAB>   <MOLEN>
             This line is used to specify the ambient velocity profile.
             <INDVEL> is the indicator used to specify whether the
             ambient velocity profile is based on:
             (1) the Pasquill stability category in <ISTAB> using 1
                 for A, 2 for B, etc.;  or
             (2) the Monin-Obukhov length in <MOLEN> (as a real
                 number).  If a Monin-Obukhov length of infinity is
                 desired, input a value of 0.0 for <MOLEN>.
             Note that the Pasquill stability category must be specified
             (regardless of <INDVEL>) since <ISTAB> is used to estimate
             other parameters.


<TAMB>   <PAMB>   <RELHUM>
             This line specifies the ambient air temperature (<TAMB> in
             K), the ambient pressure (<PAMB> in N/m² or atm), and the
             ambient relative humidity (<RELHUM> as a percent).


<TSURF>
             This line specifies the surface temperature (in K).  If the
             value of <TSURF> is below 250 K, <TSURF> is set to <TAMB>.
```

\<GASNAM>

> \<GASNAM> is a user-generated 3-letter name used to
> identify the dispersing gas.

\<GASMW>

> \<GASMW> is the gas molecular weight (kg/kmole).

\<AVTIM>

> \<AVTIM> is the averaging time to be used for this particular
> gas. At present, this parameter is used to estimate the
> value of DELTA in DEGADIS.

\<JETTEM>

> \<JETTEM> is the temperature of the released gas jet (K).

\<GASUL>   \<GASLL>   \<ZLL>

> \<GASUL> and \<GASLL> are the upper and lower limits (in mole
> fraction) used for contour computations at the elevation
> \<ZLL>. Note that the computations will be carried out to
> \<GASLL>/2.

\<INDHT>   \<CPC>   \<CPP>

> \<INDHT> is used to determine whether heat transfer with the
> ground is included in DEGADIS. Heat transfer is not
> included when \<INDHT> is set to zero but is included when
> \<INDHT> is nonzero. \<CPC> and \<CPP> are used to calculate
> the gas heat capacity using the specification in DEGADIS as
> a function of temperature. (If this function is used, the
> average gas temperature is used to specify the mean
> (constant) heat capacity in the Ooms model.) If a constant
> contaminant heat capacity is desired, \<CPP> is set to 1.0
> and \<CPC> is set to the desired heat capacity (in J/kg K).

\<ERATE\>

> \<ERATE\> is the mass evolution rate of the pure contaminant (in kg/s).

\<JETELE\>   \<JETDIA\>

> \<JETELE\> is the initial jet elevation above ground level.
> \<JETDIA\> is the initial diameter of the jet.

\<TEND\>

> \<TEND\> is the duration of the release. For a steady-state case, input 0.0 for \<TEND\>. If the Ooms model is to be run alone, input a negative number for \<TEND\>.

\<X0\>   \<H\>   \<DISTA\>   \<DISTAN\>

> \<X0\> is the starting value for the jet trajectory integration. \<H\> is the step size for the Ooms model. \<DISTA\> is the downwind distance to the first output value. \<DISTAN\> is the distance between output points in the Ooms model.

\<K1\>   \<K2\>   \<K3\>

> \<K1\>, \<K2\>, and \<K3\> are the parameters used to specify the initial jet direction as follows:

> \<K1\> is used for horizontal jets directed upwind (-1) and downwind (1); \<K1\>=0 for other orientations.

> \<K2\> is used for vertical jets directed upward (+1) and downward (-1); \<K2\>=0 for other orientations.

> \<K3\> is used for horizontal jets directed transverse to the left (-1) and to the right (+1); \<K3\>=0 for other orientations.

> Note that only one of \<K1\>, \<K2\>, or \<K3\> can be nonzero at any time.

Appendix G contains program listings for OOMS_IN and DEGBRIDGE.
(DEGBRIDGE takes the output from the Ooms model and creates the file
necessary for DEGADIS to complete the calculations as needed.)

III. MODEL IMPLEMENTATION

The models described in Section I have been implemented in VAX/VMS Fortran (a superset of Fortran 77) in the codes OOMS and DEGADIS. DEGADIS is comprised of six separate programs as follows:

(*) DEGADISIN   is the interactive input module which defines the simulation.

(*) DEGADIS1   determines α and describes the gas source for transient and steady-state releases.

(*) DEGADIS2   describes the pseudosteady-state downwind dispersion of the released gas.

(*) DEGADIS3   sorts the results of DEGADIS2 for a transient release at given times.

(*) DEGADIS4   sorts the results of DEGADIS2 for a transient release at given positions.

(*) SDEGADIS2   describes the steady-state downwind dispersion of the released gas.

As indicated in Figures II.1 and II.2, a steady-state release is simulated by executing OOMS, DEGADISIN, DEGADIS1, and SDEGADIS2, while a time-limited (transient) release is simulated by executing OOMS, DEGADISIN, DEGADIS1, DEGADIS2, and DEGADIS3.

IV. EXAMPLE SIMULATION

The example simulation conditions shown in Table IV.1 for the accidental release of methylisocyanate (MIC) on December 3, 1984, in Bhopal, India, were reported by Singh (1986). To simulate this release. the MIC was assumed to be released as a pure, ambient temperature gas at a steady rate of 6.72 kg/s. For the lowest concentration of interest, the lethal concentrations to 50% of laboratory animals exposed to MIC (LC_{50}) for one and two hours are about 30 and 20 ppm, respectively.

TABLE IV.1

EXAMPLE SIMULATION RELEASE CONDITIONS

Mass of MIC released	40 tons
Duration of release	90 min
Vent elevation	33 m
Vent diameter	0.2 m
Wind velocity at 10 m	2.9 m/s
Atmospheric stability	E/F

The input file used to simulate the release conditions of Table IV.1 as a steady-state release is shown in Figure IV.1. Note that comments can be included at the end of each line as long as the specified values are entered on the line first; as well, comments can appear at the end of the file after all values have been entered. A surface roughness of 0.1 m has been used. (Note that the surface roughness should not be larger than the depth of the denser-than-air gas layer in DEGADIS; for this case, the value of S_z at the beginning of the steady-state DEGADIS calculation was 33.8 m.) Also, an averaging time of 3600 s has been used to correspond with the averaging time for the LC_{50}; note that the

concentrations of 30 ppm (CASULO.00003 mole fraction) and 20 ppm (GASLL=0.00002 mole fraction) are to be used to calculate concentration contours in DEGADIS. The fact that this is a steady-state simulation is indicated by the value of TEND (0.0). Finally, the jet is assumed to be oriented vertically upward since K1, K2, and K3 are all set to 0.

Note that the Ooms/DEGADIS model can be executed interactively or in batch mode. An example batch command file to run the model under VMS is shown in Figure IV.2 for the example simulation called EXAMPLE. (The logical symbol SYS$DEGADIS: is assigned to the directory which contains the executable image of the model.) Note that any file name may be used; the same file name will be used throughout the simulation with different extensions for internal files used by the model. Upon completion of the simulation, the output of the model is in the file with the original name and extension LIS; for this example, the output file will be EXAMPLE.LIS. To run the model interactively, the same lines shown in Figure IV.2 should be entered at the terminal.

Several lines of output are written to the terminal during the execution of the model. (In batch mode, the same lines are written to the batch log file.) As discussed in Section II.1, the program OOMS_IN reads the input file (EXAMPLE.IN in this case) and generates the input file to the OOMS program; when OOMS_IN finishes, OOMS_IN writes the line "OOMS_IN - beginning command file". At this point, the OOMS program begins; several lines of output are generated showing the values of various parameters calculated by the program. When OOMS finishes, DEGBRIDGE begins; DEGBRIDGE writes the line "DEGBRIDGE - beginning DEGBRIDGE". DEGBRIDGE takes the output of OOMS and generates the necessary input file for DEGADIS. When DEGBRIDGE finishes, the standard DEGADIS procedure begins with the copying of the ER1 and ER2 numerical parameter files. DEGADIS generates several lines of output showing the values of various numerical parameters calculated by the model. The last step of the model is to generate the LIS file from the output files of OOMS and DEGADIS.

For the example case above, the OOMS calculations are terminated at 540 m when the lower edge of the plume reaches ground level. At this

point, the centerline concentration (c^*) is 2.83 x 10^{-3} kg/m^3. From
this point, the DEGADIS calculation begins; the initial concentration
used in DEGADIS is taken to be 2.83 x 10^{-3} kg/m^3 (from OOMS) and the
value of S_z at the downwind edge of the DEGADIS source is 33.8 m. The
output of DEGADIS for this example case shows the 30 ppm level reaches
5.76 km and the 20 ppm level reaches 7.22 km. Note that the downwind
distance used in DEGADIS is measured from the DEGADIS source.
Therefore, the distances predicted by the OOMS/DEGADIS model to the 30
and 20 ppm concentration levels for the example case are 6.30 km and
7.76 km, respectively. The complete output listing for this example
simulation can be found in Appendix J. Note that the "width at z=" to
some appropriate mole percent value actually refers to the distance to
that isopleth concentration from the plume centerline (i.e., half-width).

The OOMS code can be run (without DEGADIS) using OOMSIN by specifying
a TEND which is less than zero. For this case, the input file is
identical to the example case shown in Figure IV.1 except that TEND is set
equal to -1. As before, the OOMS calculations are terminated at 540 m
when the boundary of the cloud first reaches ground level.

Simulation of the release of an impure dense gas can be performed by
adjusting the molecular weight and heat capacity inputs to the program.
The molecular weight should be the equivalent molecular weight of the
mixture at the release point, and the heat capacity inputs should be those
of the initial mixture. Concentration (mole fraction) values output by
the program should then be multiplied by the initial mole fraction of
contaminant in the released mixture to obtain actual mole fraction values.

This is a steady-state test simulation of the OOMS and DEGADIS models.
    Methylisocyanate (MIC) release


```
2.9  10.                        UO, ZO
0.1                             ZR
1  6   0.                       INDVEL, ISTAB, MOLEN
298.  1.  50.                   TAMB, PAMB, RELHUM
298.                            TSURF
MIC                             GASNAM
57.                             GASMW
3600.                           AVTIM - based on 1 hr toxic levels
298.                            JETTEM
0.00003   0.00002  0.5          GASUL, GASLL, ZLL
0  2000.  1.                    INDHT,  CPC, CPP
6.72                            ERATE
33.  0.2                        JETELE, JETDIA
0.0                             TEND
1.  1.   10.  10.               XO, H, DISTA, DISTAN
0   0   0                       K1, K2, K3
```

Since ONLY one of {K1, K2, or K3} MUST be nonzero, OOMS_IN checks these values
to ensure that these conditions are met. If they are not met, OOMS_IN forces
one of {K1, K2, or K3} to be 1; if all are zero, the Jet is assumed to be
oriented vertically upward.

This is the end of the file. Any comments can be included here since the
file is not read after the line for K1 et al. above has been read.

Figure IV.1. Listing of EXAMPLE.IN.


```
$RUN SYS$DEGADIS:OOMS_IN
EXAMPLE
```


Figure IV.2. Example command file used to
              simulate the EXAMPLE simulation.

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van Ulden, A. P., "A New Bulk Model for Dense Gas Dispersion: Two-Dimensional Spread in Still Air," I.U.T.A.M. Symposium on Atmospheric Dispersion of Heavy Gases and Small Particles, Delft University of Technology, The Netherlands, August 29-September 2. 1983.

APPENDIX A

INSTALLATION ON VAX/VMS

DEGADIS was developed under VAX/VMS V3.5 and VAX-11 Fortran V3.5 although there should be no installation difficulty for VAX/VMS V4.0 or later.

The directory which contains the Fortran source code for DEGADIS must be equivalenced with the logical name SYS$DEGADIS:. If the full directory specification is DQA0:[HACS.DEGADIS], issue the VAX/VMS command:

$ ASSIGN DQA0:[HACS.DEGADIS] SYS$DEGADIS:

with either the /PROCESS, /GROUP, or /SYSTEM qualifier (/SYSTEM is recommended). Once this assignment is made, the files must be compiled and linked to form DEGADISIN, DEGADIS1, DEGADIS2, DEGADIS3, DEGADIS4, and SDEGADIS2 according to the specifications in Appendix C. The process which compiles and links DEGADIS must have READ, WRITE, and EXECUTE access privileges to SYS$DEGADIS while only READ and EXECUTE access privileges are needed to execute the existing models.

The process for compilation and linking on the VAX is provided in the batch file BUILD.COM. To execute, SUBMIT this file to the batch queue on the VAX computer. The resulting files will be executable according to the instructions in section II of this User's Guide.

APPENDIX B
CONSIDERATIONS FOR INSTALLATION OTHER
THAN VAX/VMS

There are two types of problems which may occur when attempting to install DEGADIS on a different computer or operating system. The first source of difficulty is the use of non-standard ANSI Fortran 77 language elements. The second source of difficulty is the use of external VAX/VMS routines in DEGADIS.

The following list is a collection of the VAX-11 Fortran extensions which have been used in DEGADIS:

(*) In-line comments--An exclamation mark (!) is used to include comments at the end of a valid statement.

(*) Special characters--The underscore (_) is used in variable names.

(*) DO loops--DO loops are used with the structure:

    DO v = e1,e2[,e3]

            .

            .

            .

    END DO

where v is a variable name and e1, e2, and e3 are numeric expressions. The numeric expressions have the standard Fortran 77 meaning.

(*) INCLUDE statements--INCLUDE statements simply allow other source files to be inserted in the routine being compiled at this point in the source. The system table '($SSDEF)' is used to check the status of returning system routines.

(*) OPEN keyword NAME--The OPEN keyword NAME specifies the file name to be opened.

(*) Fortran descriptors--The Q descriptor obtains the integer number of characters remaining in the input record during a READ operation. The dollar sign ($) descriptor suppresses the carriage return at the end of a line on output.

(*) Continuation lines--Continuation lines have been expressed by using either a nonblank character in column 6 or by beginning the line with a tab and a number in the next column.

(*) Concatenation of character strings--Character strings are concatenated using two slashes (//).

The following VAX/VMS subroutines have been used in DEGADIS:

(*) SECNDS

TIME = SECNDS(TIME0)

SECNDS returns to TIME the difference between the number of seconds after midnight on the system clock and the value of TIME0.

(*) LIB$DATE_TIME

ISTAT = LIB$DATE_TIME (STRING)

LIB$DATE_TIME returns a 24-character ASCII string with the system date and time. ISTAT is an integer variable which accepts the return status.

(*) LIB$DO_COMMAND

ISTAT = LIB$DO_COMMAND (STRING)

LIB$DO_COMMAND issues the command STRING (a character string) to VAX/VMS. If the command is not issued, ISTAT contains the failure code. If the command is issued, the calling process is terminated.

APPENDIX C

DEGADIS IMPLEMENTATION

DEGADIS has been implemented in VAX/VMS Fortran (a superset of Fortran 77). DEGADIS is comprised of six separate programs as follows:

(*) DEGADISIN   is the interactive input module which defines the simulation.

(*) DEGADIS1   determines α and describes the gas source for transient and steady-state releases.

(*) DEGADIS2   describes the pseudosteady-state downwind dispersion of the released gas.

(*) DEGADIS3   sorts the results of DEGADIS2 for a transient release for specified times.

(*) DEGADIS4   sorts the results of DEGADIS2 for a transient release for specified positions.

(*) SDEGADIS2   describes the steady-state downwind dispersion of the released gas.

As indicated in Figures II.1 and II.2, a steady-state release is simulated by executing DEGADISIN, DEGADIS1, and SDEGADIS2, while a transient release is simulated by executing DEGADISIN, DEGADIS1, DEGADIS2, and DEGADIS3 (and DEGADIS4 as desired).

Input Module--DEGADISIN

DEGADISIN is the interactive input module which defines the simulation; DEGADISIN is composed of two subroutines (Figure C.1):

(*) DEGADISIN   contains the program overhead and generates the command file RUN_NAME.COM which can be used to control simulation execution (F-38).

(*) IOT   contains the interactive question-and-answer sequence which defines the simulation; IOT also creates the file RUN_NAME.INP (F-75).

An example of a DEGADISIN query sequence is included in Appendix D. As this information is gathered, it is written to the file RUN_NAME.INP. Once DEGADISIN is completed, RUN_NAME.INP may be edited to correct minor input mistakes. If major revisions are necessary, the recommended practice is to execute DEGADISIN again.

Once the information required by DEGADISIN has been entered properly, DEGADIS may be executed using the command procedure generated by DEGADISIN under the file name RUN_NAME.COM. If DEGADIS is not to be run using this command file, the user must enter the simulation name (RUN_NAME) after each of the programs are begun. As well, the user must provide copies of the numerical parameter files.

```
+----------------+       +----------------+
|                |       |                |
|   DEGADISIN    |-------|      IOT       |
|                |       |                |
|     F-38       |       |     F-75       |
+----------------+       +----------------+
```
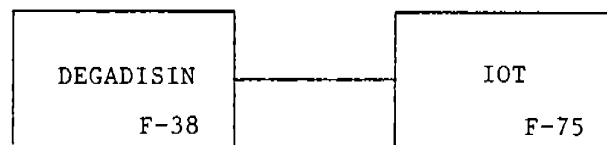
Figure C.1. DEGADISIN flowchart.

```
                          TITLE(1)
                          TITLE(2)
                          TITLE(3)
                          TITLE(4)
                          U0, Z0, ZR
                          ISTAB
                          DELTA, BETA, ML
                          SIGX_COEFF, SIGX_POW, SIGX_MIN_DIST
                          TAMB, PAMB, HUMID
                          ISOFL, TSURF
                          IHTFL, HTCO
                          IWTFL, WTCO
                          GAS_NAME
                          GAS_MW, GAS_TEMP, GAS_RHOE
                          GAS_CPK, GAS_CPP
                          GAS_UFL, GAS_LFL, GAS_ZSP
                        ⎧ NP
If (ISOFL≠0) then       │ DEN((J,1),J=1,5)
(for                    │ DEN((J,2),J=1,5)
external density        ⎨    .
calculations)           │    ..
                        │    .
                        ⎩ DEN((J,NP),J=1,5)
                          CCLOW
                          GMASSO
                          NT
                        ⎧ PTIME(1),ET(1),R1T(1),PWC(1),PTEMP(1),PFRACV(1)
                        │ PTIME(2),ET(2),R1T(2),PWC(2),PTEMP(2),PFRACV(2)
                        │    .
NT of these             ⎨    .
                        │    .
                        │ PTIME(NT),ET(NT),R1T(NT),PWC(NT),PTEMP(NT),PFRACV(NT)
                        ⎩ CHECK1, CHECK2, AGAIN, CHECK3, CHECK4, CHECK5
                          TINP
for steady-state          ESS, SLEN, SWID
  only
```

Figure C.2. Structure for free-formatted RUN_NAME.INP file.

Source Module--DEGADIS1

DEGADIS1 estimates values for the friction velocity and ambient wind profile power α and characterizes the primary gas source for the remainder of the model; DEGADIS1 is composed of the following subroutines (Figure C.3):

```
┌─────────────┐        ┌─────────────┐
│  DEGADIS1   ├────┬───┤     IO      │
│    F-13     │    │   │    F-73     │
└─────────────┘    │   └─────────────┘
┌─────────────┐    │   ┌─────────────┐
│   AFGEN     │    ├───┤   ESTRT1    │
│    F-3      │    │   │    F-49     │
└─────────────┘    │   └─────────────┘        ┌─────────────┐
┌─────────────┐    │   ┌─────────────┐     ┌──┤    RTMI     │
│   GAMMA     │    ├───┤    ALPH     ├─────┤  │   F-119     │
│    F-58     │    │   │    F-5      │     │  └─────────────┘
└─────────────┘    │   └─────────────┘     │  ┌─────────────┐
┌─────────────┐    │   ┌─────────────┐     └──┤    PSIF     │
│   RIPHIF    │    ├───┤     SZF     │        │    F-98     │
│    F-108    │    │   │   F-182     │        └─────────────┘
└─────────────┘    │   └─────────────┘
┌─────────────┐    │   ┌─────────────┐
│   RKGST     │    ├───┤    SRC1     │
│    F-111    │    │   │   F-140     │
└─────────────┘    │   └─────────────┘
┌─────────────┐    │   ┌─────────────┐
│  SURFACE    │    ├───┤    NOBL     │
│   F-180     │    │   │    F-92     │
└─────────────┘    │   └─────────────┘
┌─────────────┐    │   ┌─────────────┐
│   TPROP     │    ├───┤    CRFG     │
│   F-184     │    │   │    F-8      │
└─────────────┘    │   └─────────────┘
┌─────────────┐    │   ┌─────────────┐
│   TRAP      │    ├───┤    HEAD     │
│   F-207     │    │   │    F-63     │
└─────────────┘    │   └─────────────┘
┌─────────────┐    │   ┌─────────────┐
│   AFGEN2    │    └───┤   TRANS1    │
│    F-4      │        │   F-199     │
└─────────────┘        └─────────────┘
```
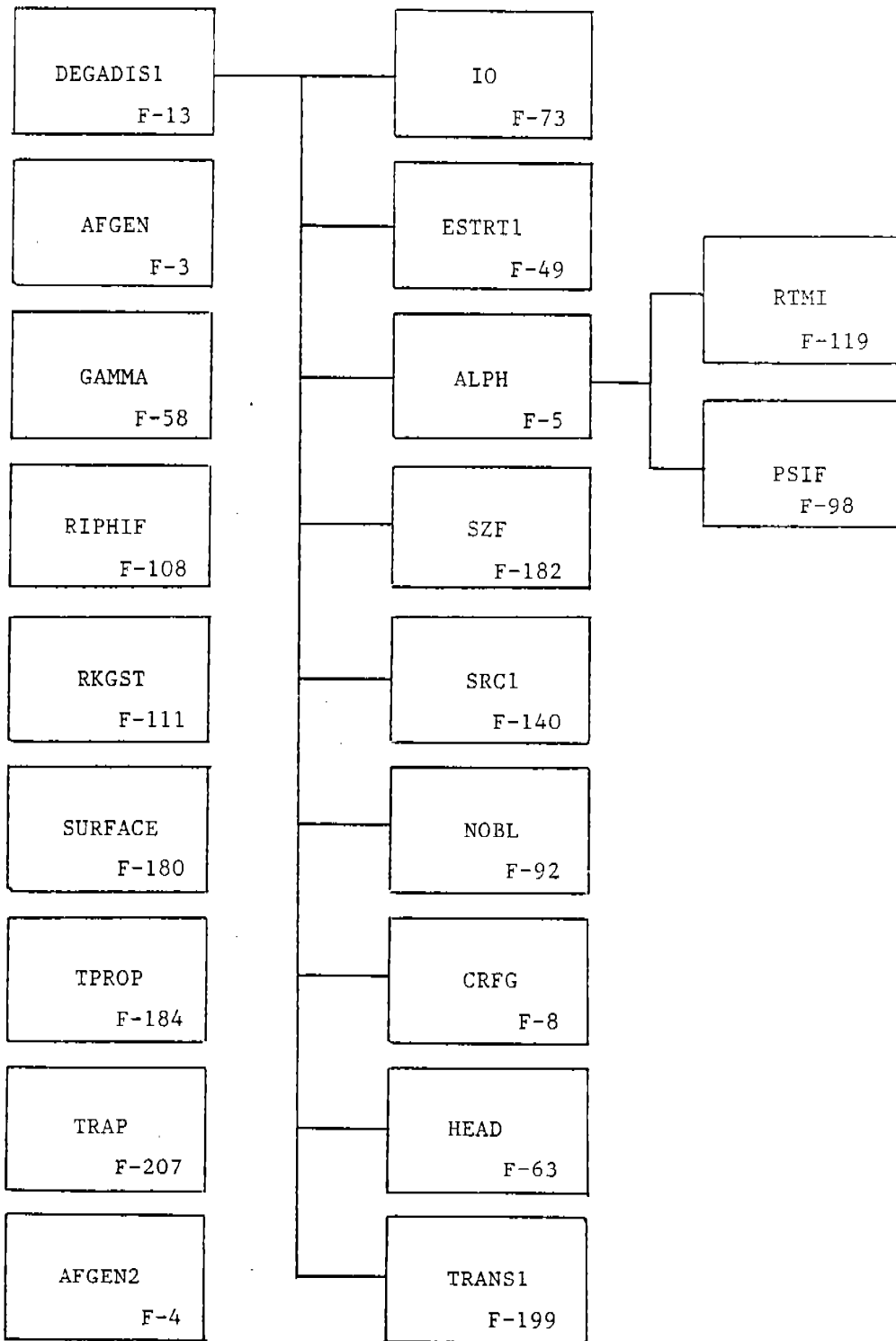
Figure C.3.   DEGADIS1 flowchart.

(*) AFGEN   is a utility which linearly interpolates between a pair of points based on a list of supplied values (F-3).

(*) AFGEN2   is a utility which linearly interpolates between a pair of points based on a list of supplied values (F-4).

(*) ALPH   estimates the ambient wind profile power α by minimizing the integral of the difference between an ambient logarithmic velocity profile and the assumed power law velocity profile (F-5).

(*) CRFG   creates a table of calculated values which will describe the secondary gas source for the downwind dispersion calculations (F-8).

(*) DEGADIS1   contains the program overhead and sequentially calls the routines required to estimate the ambient wind profile power α and to characterize the primary gas source (F-14).

(*) ESTRT1   recovers the numerical parameters contained in the file RUN_NAME.ER1 (F-49).

(*) GAMMA   is a utility function that calculates the gamma function of the argument (i.e. $\Gamma(x)$) (F-58).

(*) HEAD   writes a formatted output heading to the file RUN_NAME.SCL (F-63).

(*) IO   recovers the simulation definition contained in RUN_NAME.INP (F-73).

(*) NOBL   estimates gas source behavior when no gas blanket is
                    present (F-92).

(*) PSIF   calculates the ψ function in the logarithmic velocity
                    profile (F-98).

(*) RIPHIF   is a series of utilities which calculates the
                    Richardson number and the value of $\phi(Ri)$ (F-108).

(*) RKGST   is a utility routine which performs numerical
                    integration of a specified system of equations using
                    a variable-step, modified fourth-order Runge-Kutta
                    method (F-111).

(*) RTMI   is a utility routine which solves the roots of an
                    equation by the Milne method set up by ALPH (F-119).

(*) SRC1   contains the ordinary differential equations which
                    describe the gas blanket formed as a result of the
                    primary gas source (F-140).

(*) SURFACE   is a utility routine which estimates heat and water
                    transfer rates across the bottom surface of the gas
                    layer (F-180).

(*) SZF   estimates the value of S_z if the primary source can
                    just form a gas blanket over the source (F-182).

(*) TPROP   is a series of utility routines which estimate the
                    thermodynamic properties of a given gas mixture
                    (F-184).

(*) TRANS1   writes the information to continue the next
                    simulation step to the file RUN_NAME.TR2 (F-199).

(*) TRAP   is a utility included for program diagnostics
                        (F-207).

As input, DEGADIS1 requires two files:

(*) RUN_NAME.ER1   contains various numerical parameters.
                    For most simulations, a copy of the
                    SYS$DEGADIS:EXAMPLE.ER1 file will be adequate. (See
                    Figure II.1 or II.2.) A copy of
                    SYS$DEGADIS:EXAMPLE.ER1 is included in Figure C.4.

(*) RUN_NAME.INP   contains the simulation definition as discussed in
                    Appendix D. The format of RUN_NAME.INP is shown in
                    Figure C.2.

As output, DEGADIS1 generates the following files:

(*) RUN_NAME.SCD   contains the calculated values which describe the
                    secondary gas source. It is generated by SRC1 and
                    NOBL and is then read by CRFG; it is a temporary
                    file.

(*) RUN_NAME.SCL   is the listed output which describes the input
                    information for the simulation and the calculated
                    secondary gas source. It is written by HEAD and
                    CRFG.

(*) RUN_NAME.TR2   contains the information to continue the next
                    simulation step.

```
!This is an example of how to set up and use the run parameter
! input files.  Comment lines start with an exclamation mark(!)
! in the first column.  The only restrictions for data input are
! as follows:
!              1) The data must be entered in the same order
!                 all of the time.
!              2) Only the number must be between columns 10 and 20.
!              3) Always include the decimal point in the number
!
! Column layout:
!23456789012345678901234567890
!--------1---------2---------3
!         I          I
STPIN      0.01      MAIN - RKGST - INITIAL STEP SIZE
ERBND      0.0025    MAIN - RKGST - ERROR BOUND
STPMX      5.12      MAIN - RKGST - MAXIMUM STEP SIZE
WTRG       1.        MAIN - RKGST - WEIGHT FOR RG
WTTM       1.        MAIN - RKGST - WEIGHT FOR Total Mass
WTYA       1.        MAIN - RKGST - WEIGHT FOR ya
WTYC       1.        MAIN - RKGST - WEIGHT FOR yc
WTEB       1.        MAIN - RKGST - WEIGHT FOR Energy Balance
WTmB       1.        MAIN - RKGST - WEIGHT FOR Momentum Balance
WTuh       1.        MAIN - RKGST - WEIGHT FOR Ueff*Heff
XLI        0.05      ALPH - LOWER LIMIT OF SEARCH FOR ALPHA
XRI        0.40      ALPH - UPPER LIMIT OF SEARCH FOR ALPHA
EPS        0.001     ALPH - ERROR BOUND USED BY 'RTMI'
ZLOW       0.01      ALPHI - maximum BOTTOM HEIGHT FOR FIT OF ALPHA
!
STPINZ     -0.02     ALPHI - INITIAL RKGST STEP <0.
!
ERBNDZ     0.005     ALPHI - ERROR BOUND FOR RKGST
!
STPMXZ     -0.04     ALPHI - MAXIMUM STEP FOR RKGST <0.
!
! Note that comment lines can be mixed with the numbers.
!
SRCOER     0.007     SRC10 - OUTPUT Error criterion
SRCSS      5.2       SRC10 - min time for Steady; STPMX
SRCcut     .00001    SRC10 - min height for blanket
htcut      .0        SRC1 - min height for blanket heat transfer
ERNOBL     1.0005    NOBL - CONVERGENCE ratio
NOBLPT     100.      NOBL - NUMBER OF POINTS
!                           USED ON THE LAST PORTION OF THE SOURCE
!
crfger     0.008     error criterion in building GEN3 vectors
!
epsilon    0.59      epsilon USED IN AIR ENTRAINMENT SPECIFICATION
!
! /SPRD_CON/
!
ce         1.15      constant in gravity slumping equation
```

Figure C.4.   SYS$DEGADIS:EXAMPLE.ER1 listing.

```
delrhomin  0.025     stop cloud spread if delrho<delrhomin
!
!
! /SZFC/
!
szstp0     0.01      SZF - Initial step size
szerr      0.001     SZF - Error criterion
szstpmx    5.0       SZF - Maximum step size [=] m
szsz0      0.01      SZF - Initial Value of dellay*Ueff*Heff
!
!
!     /ALPHcom/
!
ialpfl     1.        ALPHI - calculation flag; 0) alpha=alpco; 1)1/(1+z); 2)1
alpco      0.2       ALPHI - Value for alpha if IALPFL = 0
!
!
!     /PHIcom/
!
iphifl     3.        PHIF - calc flag
dellay     2.15      Raito of Hl/Heff
!
!
!
!     /VUcom/
!
vua        1.3       Constant Av in source model
vub        1.2       Constant Bv in source model
vuc        20.0      Constant Ev in source model
vud        .64       Constant Dv in source model
vudelta    0.20      Constant DELTAv in source model
!
! End-of-File
```

Figure C.4. (concluded)

Pseudosteady-State Module--DEGADIS2

DEGADIS2 performs the downwind dispersion portion of the calculation
for each of several observers released successively over the transient
source described by DEGADIS1. (Note that the routines INCGAMMA, GAMMA,
and SERIES are linked in DEGADIS2 but never are called in DEGADIS2.)
DEGADIS2 is composed of the following subroutines (Figure C.5):

(*) AFGEN   is a utility which linearly interpolates between a
pair of points based on a list of supplied values
(F-3).

(*) AFGEN2   is a utility which linearly interpolates between a
pair of points based on a list of supplied values
(F-4).

(*) DEGADIS2   contains the program overhead and sequentially calls
the routines to recover the information generated in
DEGADIS1, recover the numerical parameter file
RUN_NAME.ER2, and perform the simulation (F-23).

(*) ESTRT2   recovers the numerical parameters contained in the
file RUN_NAME.ER2, particularly the number of
observers NOBS (F-53).

(*) OB   contains the ordinary differential equations which
average the gas source for each observer (F-95).

(*) PSS   contains the ordinary differential equations which
describe the portion of the downwind dispersion
calculation when $b > 0$ (F-99).

(*) PSSOUT   governs the output of calculated points to the file
RUN_NAME.PSD when PSS is active (F-102).

```
┌─────────────────┐      ┌─────────────────┐
│  DEGADIS2       ├──┬───┤  STRT2          │
│    F-22         │  │   │    F-173        │
└─────────────────┘  │   └─────────────────┘
                     │
┌─────────────────┐  │   ┌─────────────────┐
│  AFGEN          │  ├───┤  ESTRT2         │
│    F-3          │  │   │    F-53         │
└─────────────────┘  │   └─────────────────┘

┌─────────────────┐  │   ┌─────────────────┐
│  AFGEN2         │  ├───┤  SSSUP          │
│    F-4          │  │   │    F-164        │
└─────────────────┘  │   └───────┬─────────┘
                     │           │
┌─────────────────┐  │           │   ┌─────────────────┐
│  RIPHIF         │  │           ├───┤  TUPF           │
│    F-108        │  │           │   │    F-217        │
└─────────────────┘  │           │   └─────────────────┘
                     │           │
┌─────────────────┐  │           │   ┌─────────────────┐
│  RKGST          │  │           ├───┤  OB             │
│    F-111        │  │           │   │    F-95         │
└─────────────────┘  │           │   └─────────────────┘
                     │           │
┌─────────────────┐  │           │   ┌──────────┐  ┌──────────┐
│  SURFACE        │  │           ├───┤  PSS     ├──┤  PSSOUT  │
│    F-180        │  │           │   │   F-99   │  │   F-102  │
└─────────────────┘  │           │   └──────────┘  └──────────┘
                     │           │
┌─────────────────┐  │           │   ┌──────────┐  ┌──────────┐
│  TPROP          │  │           └───┤  SSG     ├──┤  SSGOUT  │
│    F-184        │  │               │   F-153  │  │   F-156  │
└─────────────────┘  │               └──────────┘  └──────────┘
                     │
┌─────────────────┐  │
│  TRAP           │  │
│    F-207        │  │
└─────────────────┘  │
                     │
┌─────────────────┐  │   ┌─────────────────┐
│  TS             │  └───┤  TRANS2         │
│    F-216        │      │    F-202        │
└─────────────────┘      └─────────────────┘

┌─────────────────┐
│  UIT            │
│    F-222        │
└─────────────────┘
```
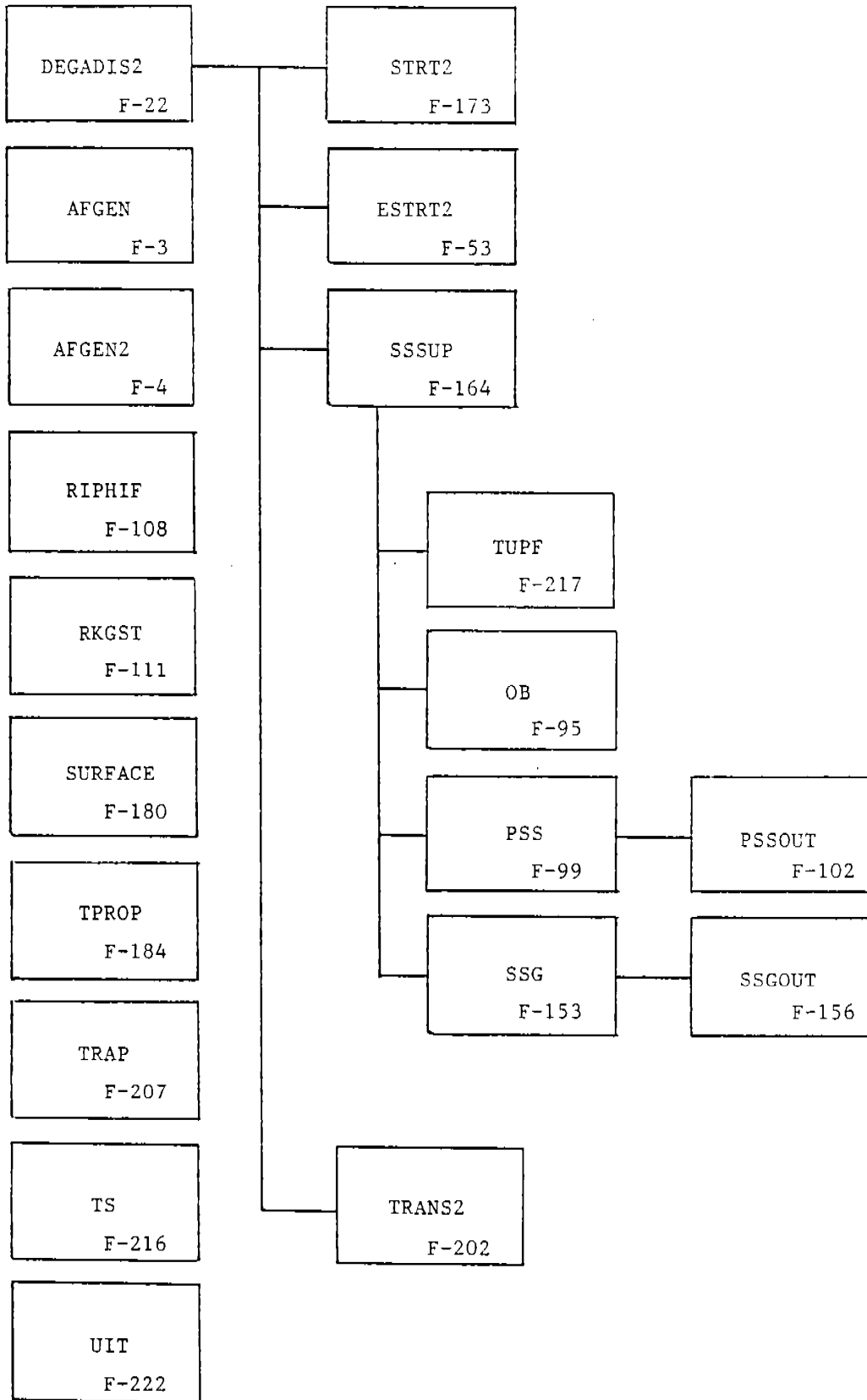
Figure C.5. DEGADIS2 flowchart.

(*) RIPHIF   is a series of utilities which calculates the
                    Richardson number and the value of $\phi(Ri)$ (F-108).

(*) RKGST   is a utility routine which performs numerical
                    integration of a specified system of equations using
                    a modified fourth-order Runge-Kutta method (F-111).

(*) SSG   contains the ordinary differential equations which
                    describe the portion of the downwind dispersion
                    calculation when b = 0 (F-153).

(*) SSGOUT   governs the output of calculated points to the file
                    RUN_NAME.PSD when SSG is active (F-156).

(*) SSSUP   is a supervisor routine which controls the averaging
                    of the source for each observer, the portion of the
                    downwind dispersion calculation when b > 0, and the
                    portion of the downwind dispersion calculation when
                    b = 0 (F-164).

(*) STRT2   recovers the information generated in DEGADIS1
                    contained in the file RUN_NAME.TR2 (F-173).

(*) SURFACE   is a utility routine which estimates heat and water
                    transfer rates across the bottom surface of the gas
                    layer (F-180).

(*) TPROP   is a series of utility routines which estimate the
                    thermodynamic properties of a given gas mixture
                    (F-184).

(*) TRANS2   writes the information necessary for DEGADIS3 to the
                    file (RUN_NAME.TR3) (F-202).

(*) TRAP   is a utility included for program diagnostics
                   (F-207).

(*) TS   calculates the time when a given observer will be at
                   a given downwind distance (F-216).

(*) TUPF   contains the two routines which determine the
                   intersection of the upwind/downwind edge of the
                   secondary gas source with a given observer (F-217).

(*) UIT   is a series of routines to calculate observer
                   position and velocity as a function of time (F-222).

As input, DEGADIS2 requires two files:

(*) RUN_NAME.ER2   contains the various numerical parameters,
                   particularly the number of observers NOBS. For most
                   simulations, a copy of the SYS$DEGADIS:EXAMPLE.ER2
                   file will be adequate. (See Figure II.1 or II.2.) A
                   copy of SYS$DEGADIS:EXAMPLE.ER2 is included in Figure
                   C.6.

(*) RUN_NAME.TR2   contains the basic simulation definition as well as
                   calculated secondary source parameters.

DEGADIS2 generates the following output files:

(*) RUN_NAME.OBS   contains a summary of the source parameters for each
                   observer.

```
! This is an example for an 'ER2' run parameter file.
! The same rules apply as for the 'ER1' files.
!
!2345678901234567890123456789012345678901234567890
!---------1---------2---------3
!
! These values are in common area /ERROR/
!
*   SYOER       0.0         SSSUP - RKGST - INITIAL SY
    ERRO        0.005       SSSUP - RKGST(OBS) - ERROR BOUND
    SZOER       0.01        SSSUP - RKGST(OBS) - INITIAL SZ
    WTAIO       1.0         SSSUP - RKGST(OBS) - WEIGHT FOR AI
    WTQOO       1.0         SSSUP - RKGST(OBS) - WEIGHT FOR Q
    WTSZO       1.0         SSSUP - RKGST(OBS) - WEIGHT FOR SZ
*   ERRP        0.003       SSSUP - RKGST(PSS) - ERROR BOUND
*   SMXP        10.         SSSUP - RKGST(PSS) - MAXIMUM STEP
*   WTSZP       1.0         SSSUP - RKGST(PSS) - WEIGHT FOR SZ
*   WTSYP       1.0         SSSUP - RKGST(PSS) - WEIGHT FOR SY
*   WTBEP       1.0         SSSUP - RKGST(PSS) - WEIGHT FOR BEFF
*   WTDH        1.0         SSSUP - RKGST(PSS) - WEIGHT FOR DH
*   ERRG        0.003       SSSUP - RKGST(SSG) - ERROR BOUND
*   SMXG        10.         SSSUP - RKGST(SSG) - MAXIMUM STEP SIZE
    ERTDNF      0.0005      TDNF - CONVERGENCE CRITERION
    ERTUPF      0.0005      TUPF - CONVERGENCE CRITERION
*   WTRUH       1.0         SSSUP - RKGST(SSG) - WEIGHT FOR RUH
*   WTDHG       1.0         SSSUP - RKGST(SSG) - WEIGHT FOR DH
    !
    ! These values are in common area /STP/
    !
    STPO        0.05        SSSUP - RKGST(OBS) - INITIAL STEP
*   STPP        0.05        SSSUP - RKGST(PSS) - INITIAL STEP
*   ODLP        0.06        SSSUP - RKGST(PSS) - RELATIVE OUTPUT DELTA
*   ODLLP       80.         SSSUP-RKGST(PSS)-MAXIMUM DISTANCE BETWEEN OUTPUTS(m)
*   STPG        0.05        SSSUP - RKGST(SSG) - INITIAL STEP
*   ODLG        0.045       SSSUP - RKGST(SSG) - RELATIVE OUTPUT DELTA
*   ODLLG       80.         SSSUP-RKGST(SSG)-MAXIMUM DISTANCE BETWEEN OUTPUTS(m)
    !
    ! The last variable NOBS is in /CNOBS/
    !
    ! Note: it is read in as a real value even though it is integer type
    !       in the program.
    !
    NOBS        30.
    !
    !
    !
    ! End-of-File
*used by steady-state simulation
```

Figure C.6.   SYS$DEGADIS:EXAMPLE.ER2 listing.

(*) RUN_NAME.PSD   contains the calculated downwind dispersion parameters for each observer. DEGADIS3 and DEGADIS4 sort this information to determine the downwind concentration profiles as a function of position and time.

(*) RUN_NAME.TR3   contains the simulation definition and the number of each record type written to RUN_NAME.PSD.

Time Sort Modules--DEGADIS3 and DEGADIS4

DEGADIS3 sorts the downwind dispersion calculation for each of several observers for concentration information at several given times; the along-wind dispersion correction is then applied as desired. DEGADIS3 uses the following subroutines (Figure C.7).

(*) DEGADIS3   contains the program overhead and sequentially calls the routines to recover the information generated in DEGADIS2, recover the numerical parameter file RUN_NAME.ER3, sort and apply the along-wind dispersion correction to the results of DEGADIS2, and output the results (F-28).

(*) ESTRT3   recovers the numerical parameters contained in the file RUN_NAME.ER3, particularly the time sort parameters (F-57).

(*) GAMMA   is a utility function that calculates the gamma function of the argument (i.e. $\Gamma(x)$) (F-58).

(*) GETTIM   sets the default time sort parameters as needed (F-60).

(*) INCGAMMA   is a utility function that calculates the incomplete gamma function of the two arguments (F-69).
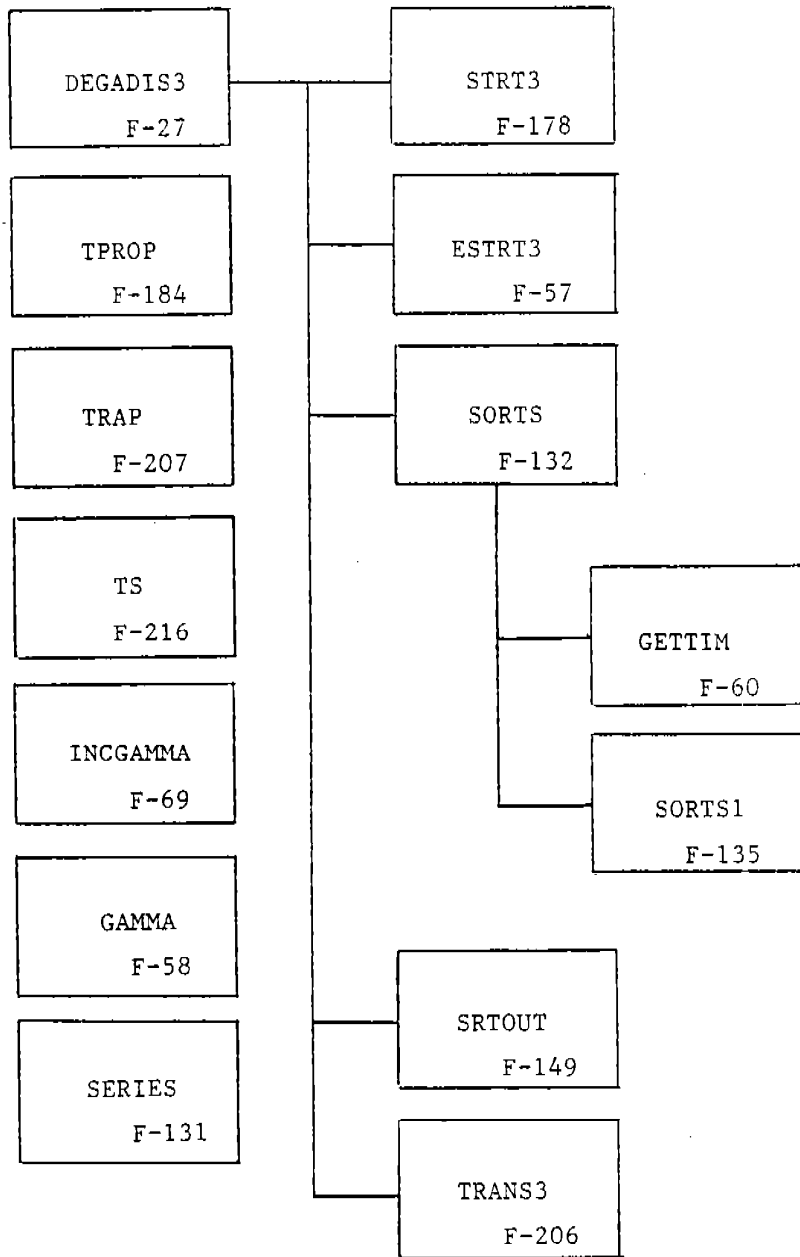
Figure C.7. DEGADIS3 flowchart.

(*) SERIES   evaluates a series needed to estimate the mass of gas above a given concentration level (F-131).

(*) SORTS   recovers the information in RUN_NAME.PSD and arranges the information according to the time sort parameters in the file RUN_NAME.ER3 (F-132).

(*) SORTS1   applies the along-wind dispersion correction to the time-sorted information (F-135).

(*) SRTOUT   generates the formatted output file RUN_NAME.SR3 (F-149).

(*) STRT3   recovers the information generated in DEGADIS2 contained in the file RUN_NAME.TR3 (F-178).

(*) TPROP   is a series of utility routines which estimate the thermodynamic properties of a given gas mixture (F-184).

(*) TRANS3   writes RUN_NAME.TR4 which contains the necessary information to recover the other output files for this simulation (F-206).

(*) TRAP   is a utility included for program diagnostics (F-207).

(*) TS   calculates the time when a given observer will be at a given downwind distance (F-216).

As input, DEGADIS3 requires three files:

(*) RUN_NAME.ER3   contains various numerical parameters including the
                    time sort parameters and the flag which dictates
                    whether the along-wind dispersion correction is
                    applied. A copy of SYS$DEGADIS:EXAMPLE.ER3 file uses
                    the default time sort parameters and includes the
                    along-wind dispersion correction which should apply
                    for most simulations. (See Figure II.2.) A copy of
                    SYS$DEGADIS:EXAMPLE.ER3 is included in Figure C.8.

(*) RUN_NAME.PSD   contains the calculated downwind dispersion
                    parameters for each observer. DEGADIS3 sorts this
                    information to determine the downwind concentration
                    profiles as a function of position at a given time.

(*) RUN_NAME.TR3   contains the number of each record type written to
                    RUN_NAME.PSD as well as the simulation definition.

As output, DEGADIS3 generates two new files:

(*) RUN_NAME.SR3   is the formatted output list of the time-sorted
                    concentration parameters. Concentration contours are
                    generated for the specified upper and lower
                    flammability at the specified height entered in
                    DEGADISIN or OOMS_IN. An example is included in
                    Section IV.

(*) RUN_NAME.TR4   contains the necessary information to recover the
                    other output files to facilitate further processing.

```
! This is an example for an 'ER3' run parameter file.
! The same rules apply as for the 'ER1' files.
!
!23456789012345678901234567890
!--------1---------2---------3
!
! These values are in common area /ERROR/
!
ERT1      20.       FIRST SORT TIME
ERDT      5.        SORT TIME DELTA
ERNTIM    20.       NUMBER OF TIMES FOR THE SORT
!
!    Note: ERNTIM is entered as a real variable even though
!          it is an integer type variable in the program.
!
! The value of CHECK5 determines whether the above sort parameters
!    are used.  CHECK5 is initialized through the passed transfer
!    files to .FALSE.  CHECK5 is set to .TRUE. if a real value of 1.
!    is passed in this file.
!
CHECK5     0.       USE THE DEFAULT TIME PARAMETERS
!CHECK5     1.       USE THE TIME PARAMETERS GIVEN ABOVE
!
!
sisx_flag  1.       correction for x-direction dispersion is to be made
!sisx_flag  0.        no correction for x-direction dispersion
!
!
!
! End-of-File
####
```

Figure C.8.   SYS$DEGADIS:EXAMPLE.ER3 listing.

DEGADIS4 sorts the downwind dispersion calculation for each of several observers for concentration information at several given positions; the along-wind dispersion correction is then applied as desired. DEGADIS4 uses the following subroutines (Figure C.9):

(*) DEGADIS4   contains the program overhead and sequentially calls the routines to recover the information generated in DEGADIS2, recover the numerical parameter file RUN_NAME.ER3, sort and apply the along-wind dispersion correction to the results of DEGADIS2, and output the results (F-33).

(*) DOSOUT   generates the formatted output file RUN_NAME.SR4 (F-44).

(*) ESTRT3   recovers the numerical parameters contained in the file RUN_NAME.ER3, particularly whether the x-direction dispersion correction is to be applied (F-57).

(*) GAMMA   is a utility function that calculates the gamma function of the argument (i.e. $\Gamma(x)$) (F-58).

(*) GETTIMDOS   sets the time sort parameters as required to output the concentration time history at the desired positions (F-62).

(*) INCGAMMA   is a utility function that calculates the incomplete gamma function of the two arguments (F-69).

(*) SERIES   evaluates a series needed to estimate the mass of gas above a given concentration level (F-131).
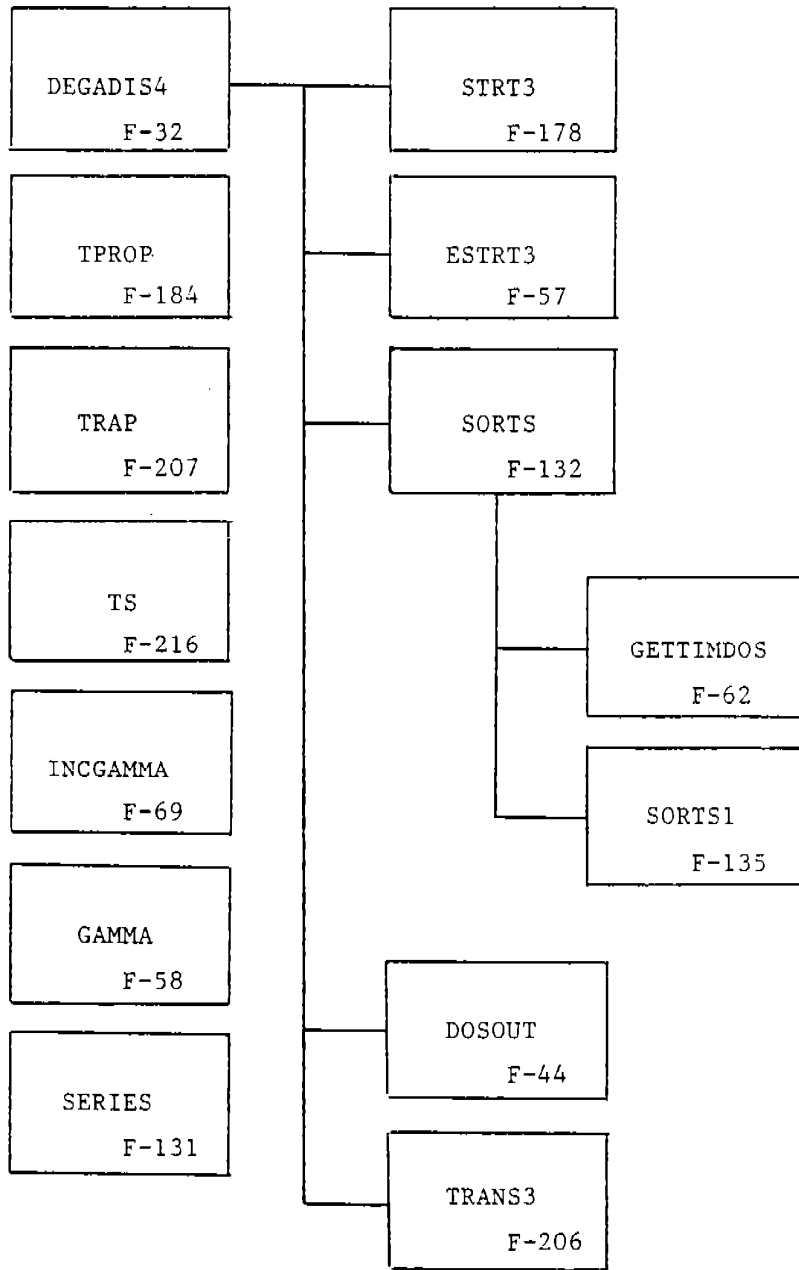
Figure C.9. DEGADIS4 flowchart.

(*) SORTS   recovers the information in RUN_NAME.PSD and arranges the information according to the time sort parameters (F-132).

(*) SORTS1   applies the x-direction dispersion correction to the time-sorted information (F-135).

(*) STRT3   recovers the information generated in DEGADIS2 contained in the file RUN_NAME.TR3 (F-178).

(*) TPROP   is a series of utility routines which estimate the thermodynamic properties of a given gas mixture (F-184).

(*) TRANS3   writes RUN_NAME.TR4 which contains the necessary information to recover the other output files for this simulation (F-206).

(*) TRAP   is a utility included for program diagnostics (F-207).

(*) TS   calculations the time when a given observer will be at a given downwind distance (F-216).

As input, DEGADIS4 requires three files and input from the terminal:

(*) RUN_NAME.ER3   contains the flag which dictates whether the x-direction dispersion correction is applied. A copy of SYS$DEGADIS:EXAMPLE.ER3 file includes the x-direction dispersion correction which should apply for most simulations. (See Figure II.2.) A copy of SYS$DEGADIS:EXAMPLE.ER3 is included in Figure C.8.

(*) RUN_NAME.PSD   contains the calculated downwind dispersion parameters for each observer. DEGADIS4 sorts this information to determine the downwind concentration time histories at the desired positions.

(*) RUN_NAME.TR3   contains the number of each record type written to RUN_NAME.PSD as well as the simulation definition.

(*) terminal input   DEGADIS4 prompts the user for the file name to be used for this run. In addition, DEGADIS4 requests the number of downwind distances (JDOS). For each downwind distance, DEGADIS4 asks for the x-position (DOSDISX(I)). Four positions are allowed for each downwind distance (DOSDISY(IJ,I) and DOSDISZ(IJ,I) for IJ=1 to 4). If fewer than four positions are desired, negative values are entered for the first position which is not desired. A summary of this input information is included in Figure C.10. Note that the same information can be put in a command file for batch processing. As well, the same information can be put in a file which can be associated with FOR005.DAT so that a file can be used for input.

```
                            RUN_NAME
                            JDOS
                         ⎧  DOSDISX(I)
                         ⎪ ⎧DOSDISY(1,I),DOSDISZ(1,I)
        FOR I=1 TO JDOS ⎨ ⎪DOSDISY(2,I),DOSDISZ(2,I)
                         ⎪*⎨DOSDISY(3,I),DOSDISZ(3,I)
                         ⎩ ⎩DOSDISY(4,I),DOSDISZ(4,I)
```

*Note that if fewer than four positions are desired, negative values are entered for the first position which is not desired.

Figure C.10. Structure of input for DEGADIS.

As output, DEGADIS4 generates two new files:

(*) RUN_NAME.SR4   is the formatted output list of the sorted
                   concentration time histories. An example is included
                   in Section IV.

(*) RUN_NAME.TR4   contains the necessary information to recover the
                   other output files to facilitate further processing.

Steady-State Module--SDEGADIS2

SDEGADIS2 is a simplification of DEGADIS2 which uses many of the
same subroutines. SDEGADIS2 performs the downwind dispersion portion of
the calculation for a steady-state source described by DEGADIS1.
SDEGADIS2 is composed of the following subroutines (Figure C.11):

(*) AFGEN   is a utility which linearly interpolates between a
                   pair of points based on a list of supplied values
                   (F-3).

(*) GAMMA   is a utility function that calculates the gamma
                   function of the argument (i.e. $\Gamma(x)$) (F-58).

(*) ESTRT2SS   recovers a subset of the numerical parameters
                   contained in the file RUN_NAME.ER2 as indicated in
                   Figure C.6 (F-55).

(*) INCGAMMA   is a utility function that calculates the incomplete
                   gamma function of the two arguments (F-69).

(*) PSS   is the same subroutine used in DEGADIS2; it contains
                   the ordinary differential equations which describe
                   the downwind dispersion calculation when $b > 0$
                   (F-99).
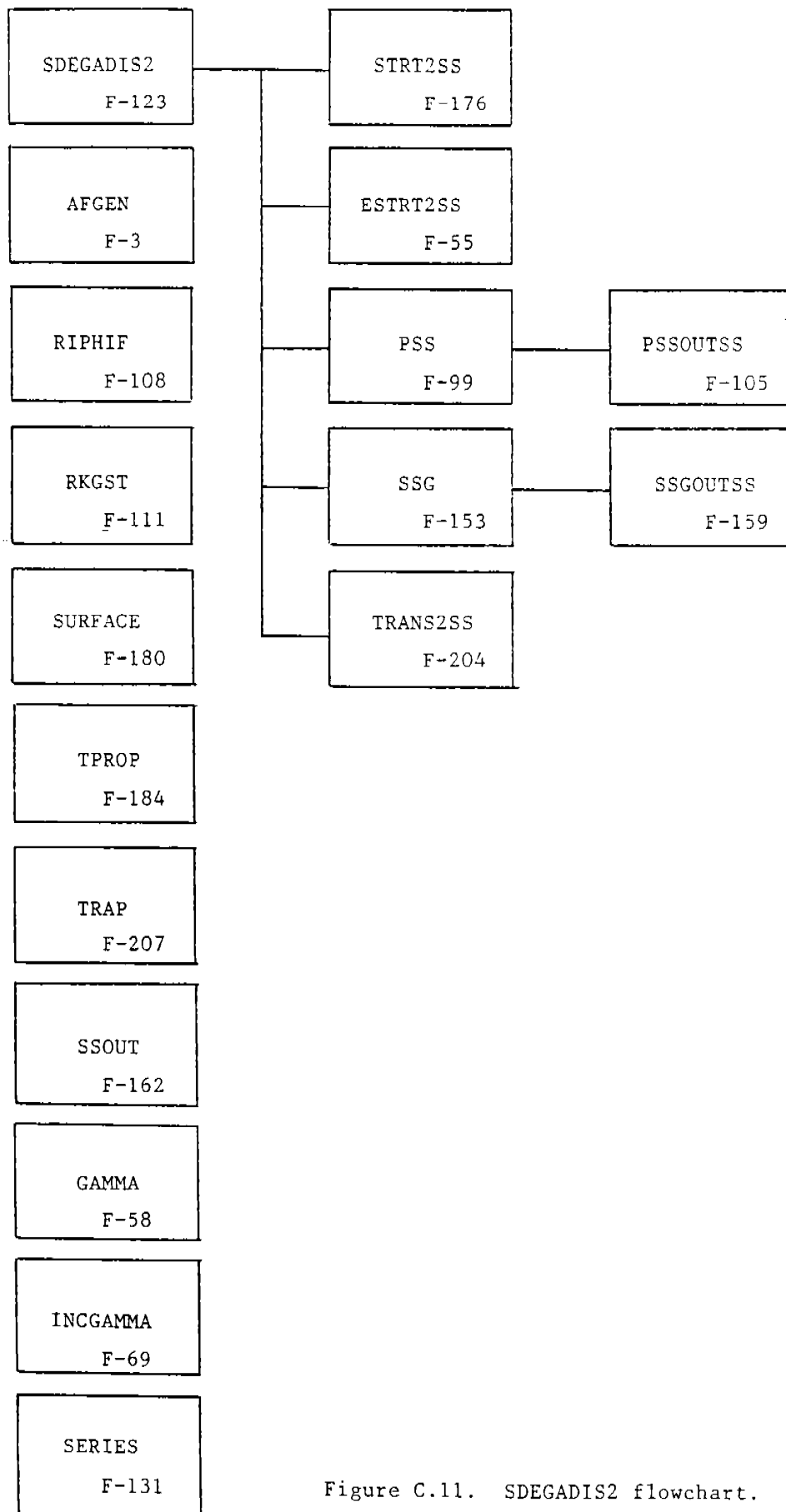
Figure C.11.   SDEGADIS2 flowchart.

(*) PSSOUTSS   governs the output of calculated points to the file RUN_NAME.SR3 when PSS is active (F-105).

(*) RIPHIF   is a series of utilities which calculates the Richardson number and the value of $\phi(Ri)$ (F-108).

(*) RKGST   is a utility routine which performs numerical integration of a specified system of equations using a modified fourth-order Runge-Kutta method (F-111).

(*) SDEGADIS2   contains the program overhead and sequentially calls the routines to recover the information generated in DEGADIS1, recover the numerical parameters file RUN_NAME.ER2, and perform the steady-state simulation (F-123).

(*) SERIES   evaluates a series needed to estimate the mass of gas above a given concentration level (F-131).

(*) SSG   is the same subroutine used in DEGADIS2; it contains the ordinary differential equations which describe the downwind dispersion calculation when b = 0 (F-153).

(*) SSGOUT   governs the output of calculated points to the file RUN_NAME.SR3 when SSG is active (F-156).

(*) SSOUT   writes RUN_NAME.SR3 and calculates the concentration contours (F-162).

(*) STRT2SS   recovers a subset of the information generated in DEGADIS1 contained in the file RUN_NAME.TR2 (F-176).

(*) SURFACE is a utility routine which estimates heat and water transfer rates across the bottom surface of the gas layer (F-180).

(*) TPROP is a series of utility routines which estimate the thermodynamic properties of a given gas mixture (F-184).

(*) TRANS2SS writes RUN_NAME.TR3 (F-204).

(*) TRAP is a utility included for program diagnostics (F-207).

As input, SDEGADIS2 requires two files:

(*) RUN_NAME.ER2 contains various numerical parameters; the steady-state simulation requires only part of these. For most simulations, a copy of the SYS$DEGADIS:EXAMPLE.ER2 file will be adequate. See Figure II.1. A copy of SYS$DEGADIS:EXAMPLE.ER2 is included in Figure C.6.

(*) RUN_NAME.TR2 contains the basic simulation definition as well as calculated secondary source parameters; the steady-state simulation requires only part of these.

As output, SDEGADIS2 generates the following files:

(*) RUN_NAME.SR3   is the formatted output list of the downwind
concentration parameters. Concentration contours are
generated for the specified upper and lower
flammability at the specified height entered in
DEGADISIN.

(*) RUN_NAME.TR3   contains the necessary information to recover the
other output files to facilitate further processing.

APPENDIX D

DEGADIS EXAMPLE SIMULATION

In 1980, the U.S. Department of Energy sponsored at China Lake, California, a series of nine LNG releases referred to as the Burro series of experiments (Koopman et al., 1982). The release condition (Table D.1) for the numerical examples in this Appendix are those of Burro 9 which was modeled both as a steady-state and transient (time-limited) release. As suggested by the Shell Maplin Sands LNG releases (Blackmore et al., 1982), the liquid source diameter was determined using a boiling rate of 0.085 kg/m^2 for LNG on water.

TABLE D.1
SUMMARY OF BURRO 9 TEST CONDITIONS
USED IN EXAMPLE SIMULATIONS

Source Rate:	130.0 kg/s
Source Radius:	22.06 m
Wind Speed:	6.5 m/s at 8.0 m
Atmospheric Stability:	C (Pasquill)
Monin-Obukhov Length:	-140. m
Surface Roughness:	2.05×10^{-4} m
Air Temperature:	35.4°C
Atmospheric Humidity:	12.5%
Surface Temperature:	310K

Example Input Sessions

The input procedures for simulation of the transient release (RUN_NAME=BURRO9) and the steady-state release (RUN_NAME=BURRO9S) are very similar. Therefore, only the specification of the source rate and extent have been included for the transient release. In the point-by-point discussion of the input procedure, note the following:

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

(*) The file name specification RUN_NAME must satisfy system restrictions.

(*) When DEGADISIN requests the user to choose an option, all acceptable 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 parentheses.

(*) For numerical responses, a comma, space, tab, or line terminator (carriage return) may separate the numbers.

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

Notes on Steady-State Simulation of BURRO9

①   Begin the input procedure by execution of DEGADISIN.

②   The file name specification must follow system restrictions. The DEGADIS model uses this file name along with various file extensions for input and output.

③   The Title Block is used to carry any desired comments such as information on the specification of certain parameters.

④   The wind field parameters include the wind velocity (m/s) at a specified height (m) and the surface roughness (m).

⑤   The Pasquill stability class is used to generate estimates of other atmospheric parameters which follow.

⑥   The averaging time is used to determine the value of δ (DELTA) in the lateral dispersion coefficient specification. Changes to the values of δ are calculated assuming that the effect of averaging time only influences the lateral plume meander of a steady-state release. Note that DEGADIS does not currently evaluate time-averaged concentrations for time-limited releases.

⑦   The current settings of pertinent atmospheric parameters are displayed in this list. If any of these are to be changed, the first letter of the parameter to be changed is entered. Note that the default--indicated by <N>--is No for no changes.

⑧   The Monin-Obukhov length (Length in the list) is to be changed, so L is entered in response to the prompt.

⑨   The list is redisplayed to verify the change and to request any further changes. The (default) response of No causes the program to go to the next question.

⑩   The ambient temperature and pressure are entered.

⑪   DEGADISIN calculates the ambient air density for the given input parameters.

(1) $ RUN SYS$DEGADIS:DEGADISIN

                    DEnse GAs DISpersion Model input module.

(2) Enter the simulation name : [DIR]RUNNAME BURRO9S
         INPUT MODULE -- DEGADIS MODEL

     ****
(3)   Enter Title Block -- up to 4 lines of 80 characters
         To stop, type '//'
     Steady-state simulation of BURRO 9
     //
(4)   ENTER WIND PARAMETERS -- UO (m/s), ZO (m), and ZR(m)
         UO -- Wind velocity at reference height ZO
         ZR -- Surface Roughness
     6.5,8.,2.05E-4

(5)   Enter the Pasquill stability class: (A,B,C,D,E,F) <D> C
(6) Enter the averaging time (s) for estimating DELTA: 0.

(7) The values for the atmospheric parameters are set as follows:
     DELTA: 0.1090
     BETA: 0.8940
     Monin-Obukhov length: -9.3344 m
     Sigma X Coefficient: 0.0200
     Sigma X Power: 1.2200
     Sigma X Minimum Distance: 130.0000 m
     Do you wish to change any of these?
(8) (No,Delta,Beta,Length,Coefficient,Power,Minimum) <N> L
     Note: For infinity, ML = 0.0
     Enter the desired Monin-Obukhov length: (m) -140.

(9) The values for the atmospheric parameters are set as follows:
     DELTA: 0.1090
     BETA: 0.8940
     Monin-Obukhov length: -140.0000 m
     Sigma X Coefficient: 0.0200
     Sigma X Power: 1.2200
     Sigma X Minimum Distance: 130.0000 m
     Do you wish to change any of these?
     (No,Delta,Beta,Length,Coefficient,Power,Minimum) <N>

(10) Enter the ambient temperature(C) and pressure(atm): 35.4,0.94

     The ambient humidity can be entered as Relative or Absolute.
     Enter either R or A <R or a>:
     Enter the relative humidity (%): 12.5

(11) Ambient Air density is   1.0720   kg/m**3

(12) If the release is isothermal, respond "Y". A positive response causes DEGADISIN to ask for a list of concentration, density, and mole fraction points for the gas mixture. The default response is negative.

(13) If the release is simulated as adiabatic, the default negative response is chosen. For inclusion of heat transfer effects, the surface temperature and the method of calculating the heat transfer coefficient must be specified.

(14) Water transfer to the source blanket (if present) can be included in the calculation.

(15) Enter the three-letter designation of the diffusing gas. The properties of LNG as methane, LPG as propane, and NH_3 (ammonia) are included among others.

(16) A list of the properties for the specified gas (if available) is given. If any of the parameters are to be changed, the first letter of the parameter to be changed in the list is given to the prompt. Here, the level at which the flammability contours are calculated is changed from 0.5 m to 1.0 m.

(17) The gas property list is displayed again. The default response is no change.

(18) The lowest concentration of interest is the concentration at which the calculations are stopped.

(12) Is this an Isothermal spill? <y or N>

(13) Is heat transfer to be included in the calculations <y or N> Y
Enter the surface temperature [=] K : 310.
Do you want to use the built in correlation, the LLNL correlation, or
enter a particular value?
(Corr,LLNLcorr,Value) <C>

(14) Is water transfer to be included in the source <y or N>

(15) Enter the code name of the diffusing species: LNG

(16) The characteristics for the gas are set as follows:
Molecular weight: 16.04
Storage temperature [K]:   111.70
Density at storage temperature, PAMB [kg/m**3]:   1.6845
Mean Heat capacity constant   5.60000E-08
Mean Heat capacity power   5.0000
Upper Flammability Limit [mole frac]   0.15000
Lower Flammability Limit [mole frac]   5.00000E-02
Height of Flammability Limit [m]   0.50000
Do you wish to change any of these? (No,Mole,Temp,Den,Heat,Power,Upper,Lower,Z) <N> Z
Enter the desired Height for the flammable limit calculations: 1.

(17) The characteristics for the gas are set as follows:
Molecular weight: 16.04
Storage temperature [K]:   111.70
Density at storage temperature, PAMB [kg/m**3]:   1.6845
Mean Heat capacity constant   5.60000E-08
Mean Heat capacity power   5.0000
Upper Flammability Limit [mole frac]   0.15000
Lower Flammability Limit [mole frac]   5.00000E-02
Height of Flammability Limit [m]   1.0000
Do you wish to change any of these? (No,Mole,Temp,Den,Heat,Power,Upper,Lower,Z) <N>

(18)   The suggested LOWEST CONCENTRATION OF INTEREST (gas_lfl/2.)
     is 1.52452E-02 kg/m**3. Enter the desired value: 0.015

(19) The BURRO9 case is for a release of "pure" (undiluted) LNG. For diluted releases, DEGADIS requires the mass fraction of the contaminant and the mixture temperature.

(20) If a steady-state release is to be simulated, type "Y" to the prompt. For a steady simulation, the steady-state mass evolution rate (kg/s) and primary source extent (m) are required.

(21) A note about the numerical parameter files is included. These files contain various constant values used in the programs to which the user has access without recompiling the programs. Access is granted as a convenience.

(22) DEGADISIN will generate a command procedure suitable for running the model under VMS.

(23) If so desired, DEGADISIN will initiate the command procedure under VMS. If not, the program returns to the operating system.

Specification of source parameters.

(19)   Is this a release of pure (P) or diluted (d) material specified above? <P or d>

(20)   Is this a Steady state simulation? <y or N> Y

Enter the desired evolution rate [=] kg/sec : 130.
Enter the desired source radius [=] m : 22.06

(21)   In addition to the information just obtained, DEGADIS
requires a series of numerical parameter files which use
the same name as [DIR]RUNNAME given above.

For convenience, example parameter files are included for
each step. They are:
          EXAMPLE.ER1 and
          EXAMPLE.ER2
 Note that each of these files can be edited during the course of the
simulation if a parameter proves to be out of specification.

(22)   Do you want a command file to be generated to execute the procedure? <Y or n>
The command file will be generated under the file name:
          BURRO9S.com

(23)   Do you wish to initiate this procedure? <y or N>
$

Notes on Transient Simulation of BURRO9

Beginning with the specification of the source rate and extent, the responses to all of the previous questions except the simulation name (RUN_NAME) are the same for the steady-state case and are not repeated.

(19)   The BURRO9 case is for a release of "pure" (undiluted) LNG. For diluted releases, DEGADIS requires the mass fraction of the contaminant and the mixture temperature.

(20)   The default response is for a transient release.

(21)   An initial mass of gas can be specified over the source. This can be used to model aboveground releases such as the Thorney Island Trials.

(22)   The transient source description consists of ordered triples of time, evolution rate, and source radius for pure sources. For diluted sources, values of evolution rate, source radius, contaminant mass fraction, and source temperature must be specified as functions of time.

(23)   An input file can be used to enter the data triples to avoid typing errors or to use as output from another model such as a liquid spreading model. The file format is the same as the terminal entry format.

(24)   The first item is the number of triples used in the description followed by the triples with the last two values showing no gas present.

(25)   A note about the numerical parameter files is included. These files contain various constant values used in the programs to which the user has access without recompiling the programs. Access is granted as a convenience.

(26)   DEGADISIN will generate a command procedure suitable for running the model under VMS.

(27)   If so desired, DEGADISIN will initiate the procedure under VMS. If not, the program returns to the operating system.

(19)   Is this a release of pure (P) or diluted (d) material specified above? <P or d>

(20)   Is this a Steady state simulation? <y or N>

(21)   Enter the initial mass of pure gas over the source. (kg)
       (Positive or zero): 0.

(22)   Source Description

       The description of the primary source mass
       evolution rate E and radius R1 for a transient
       release is input by ordered triples as follows:

            first point   -- t=0, E(t=0), R1(t=0) (initial, nonzero values)
            second point   -- t=t1, E(t=t1), R1(t=t1)
                 .
                 .
                 .

            last nonzero point -- t=TEND, E(t=TEND), R1(t=TEND)
            next to last point -- t=TEND+1., E=0., R1=0.
            last point   -- t=TEND+2., E=0., R1=0.

       Note: the final time (TEND) is the last time when E and R1 are non-zero.

(23)   Do you have an input file for the Source Description? [y or N]

       Enter the number of triples (max= 30) starting with t=0. and ending
       with t=TEND+2. for the source description: 4

(24)   . Enter TIME (sec), EVOLUTION RATE (kg/s), and POOL RADIUS (m)
       0.,130.,22.06
       80.,130.,22.06
       81.,0.,0.
       82.,0.,0.

(25)   In addition to the information just obtained, DEGADIS
       requires a series of numerical parameter files which use
       the same name as [DIR]RUNNAME given above.

           For convenience, example parameter files are included for
       each step. They are:
               EXAMPLE.ER1,
               EXAMPLE.ER2, and
               EXAMPLE.ER3
        Note that each of these files can be edited during the course of the
       simulation if a parameter proves to be out of specification.

(26)   Do you want a command file to be generated to execute the procedure? <Y or n>
       The command file will be generated under the file name:
               BURRO9.com

(27)   Do you wish to initiate this procedure? <y or N>
       $

The generated INP files for BURRO9S and BURRO9 are shown in Figures
IV.1 and IV.2. If necessary, the user may edit the INP file before
beginning the simulation. The generated command procedures are shown in
Figures D.1 and D.2.

Example Simulation Output

After proper completion of the model, BURRO9.LIS and BURRO9S.LIS
contain the output listing for the transient and steady-state releases,
respectively. A discussion of the steady-state and transient simulation
listings follows. Because of the similarities between the steady-state
and transient simulation listings, the first portion of the transient
simulation is not included.

Steady-state simulation of BURRO 9

```
    6.500000        8.000000       2.0500000E-04
       3
    0.1090000       0.8940000       -140.0000
    2.0000000E-02   1.220000        130.0000
    308.5500        0.9400000       5.1530502E-03
       0    310.0000
       1   0.0000000E+00
       0   0.0000000E+00
LNG
    16.04000        111.7000        1.684480
    5.6000000E-08   5.000000
    0.1500000       5.0000000E-02   1.000000
    1.5000000E-02
    0.0000000E+00
       4
    0.0000000E+00   130.0000        22.06000    1.000000    111.7000    1.000000
    6023.000        130.0000        22.06000    1.000000    111.7000    1.000000
    6024.000        0.0000000E+00   0.0000000E+00   1.000000    111.7000    1.000000
    6025.000        0.0000000E+00   0.0000000E+00   1.000000    111.7000    1.000000
 F F F F T F
20-OCT-1987 14:09:42.08
    130.0000        44.12000        17.32598
```

Figure D.1.   BURRO9S.INP listing.

Time-limited simulation of BURRO 9

```
      6.500000        8.000000       2.0500000E-04
          3
      0.1090000       0.8940000      -140.0000
      2.0000000E-02   1.220000        130.0000
       308.5500       0.9400000       5.1530502E-03
        0    310.0000
        1   0.0000000E+00
        0   0.0000000E+00
LNG
       16.04000        111.7000        1.684480
      5.6000000E-08    5.000000
      0.1500000        5.0000000E-02   1.000000
      1.5000000E-02
      0.0000000E+00
          4
      0.0000000E+00   130.0000        22.06000        1.000000   111.7000   1.000000
       80.00000       130.0000        22.06000        1.000000   111.7000   1.000000
       81.00000       0.0000000E+00   0.0000000E+00   1.000000   111.7000   1.000000
       82.00000       0.0000000E+00   0.0000000E+00   1.000000   111.7000   1.000000
      F F F F F F
20-OCT-1987 14:13:26.51
```

Figure D.2.   BURRO9.INP listing.

Notes on Steady-State Simulation of BURRO9

(1) The date and time DEGADISIN was run are included.

(2) The input information gathered by DEGADISIN is repeated to assist in documentation of the simulations. Included here are the Title Block and the atmospheric conditions.

① Data input on   20-OCT-1987 14:09:42.08
Source program run on   20-OCT-1987 14:14:46.01

```
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
X                                                                                               X
X     NOTE:                                                                                     X
X     -----                                                                                     X
X                                                                                               X
X     >    All Calculations are limited to circular liquid sources.                             X
X                                                                                               X
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
```

② TITLE BLOCK

Steady-state simulation of BURRO 9

Wind velocity at reference height	6.50	m/s
Reference height	8.00	m
Surface roughness length	2.050E-04	m
Pasquill Stability class	C	
Monin-Obukhov length	-140.	m
Gaussian distribution constants Delta	0.10900	m
Beta	0.89400	
Wind velocity power law constant Alpha	0.10632	
Friction velocity	0.21878	m/s
Ambient Temperature	308.55	K
Surface Temperature	310.00	K
Ambient Pressure	0.940	atm
Ambient Absolute Humidity	5.153E-03	kg/kg BDA
Ambient Relative Humidity	12.50	%

Adiabatic Mixing:	Mole fraction	CONCENTRATION OF C kg/m**3	GAS DENSITY kg/m**3	Enthalpy J/kg	Temperature K
	0.00000	0.00000	1.07203	0.00000E+00	308.55
	0.00896	0.00538	1.07502	-2043.4	306.53
	0.01786	0.01078	1.07800	-4086.7	304.53
	0.02668	0.01621	1.08097	-6130.1	302.56
	0.04411	0.02717	1.08689	-10217.	298.67
	0.06128	0.03825	1.09279	-14304.	294.87

③ Continuing with the input information, the contaminant gas properties are output.

④ The specification of the mass evolution rate, source radius, contaminant mass fraction, and source temperature are output. For a steady-state release, there is no initial mass in the cloud, and the source parameters are held constant for an arbitrarily large period of time.

⑤ Finally, certain numerical parameters and calculation flags are displayed. Some of these are set in DEGADISIN while others are set in the numerical parameter files.

0.08653	0.05508	1.10163	-20434.	259.38
0.11121	0.07217	1.11034	-26564.	283.??
0.14325	0.09537	1.12198	-34737.	276.57
0.17435	0.11903	1.13358	-42911.	270.28
0.22661	0.16005	1.14325	-57214.	262.00
0.26935	0.19598	1.15282	-69474.	254.87

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0.88801	1.25418	1.53887	-3.33068E+05	132.99
0.92334	1.37336	1.57857	-3.55545E+05	126.35
0.96575	1.53473	1.63269	-3.84152E+05	118.34
1.00000	1.68448	1.68448	-4.08672E+05	111.70

③ Specified Gas Properties:

Molecular weight:	16.040
Storage temperature:	111.70 K
Density at storage temperature and ambient pressure:	1.6845 kg/m**3
Mean heat capacity constant:	5.60000E-08
Mean heat capacity power:	5.0000
Upper mole fraction contour:	0.15000
Lower mole fraction contour:	5.00000E-02
Height for isopleths:	1.0000 m

④ Source input data points

Initial mass in cloud: 0.00000E+00

Time	Contaminant Mass Rate	Source Radius	Contaminant Mass Fraction	Temperature	Enthalpy
s	kg/s	m	kg contam/kg mix	K	J/kg
0.00000E+00	130.00	22.060	1.0000	111.70	-4.08672E+05
6023.0	130.00	22.060	1.0000	111.70	-4.08672E+05
6024.0	0.00000E+00	0.00000E+00	1.0000	111.70	-4.08672E+05
6025.0	0.00000E+00	0.00000E+00	1.0000	111.70	-4.08672E+05

⑤ Calculation procedure for ALPHA: 1

Entrainment prescription for PHI: 3

Layer thickness ratio used for average depth: 2.1500

Air entrainment coefficient used: 0.590

(6) A summary of the calculated secondary source parameters is included. The secondary source gas radius and height are output as functions of time along with other secondary parameters including the source mass flux (Qstar), the vertical concentration distribution parameter at the downwind edge (SZ(x = L/2.)), the contaminant mole fraction (Mole frac C), the gas mixture density (Density), and the Richardson number based on the cloud spreading velocity (Rich No.).

(7) For a steady-state release, the source calculations are terminated after the calculated parameters are no longer changing as a function of time. A summary of the steady-state secondary source is included.

(8) The downwind portion of the calculations is included. The distance downwind of the source is given in the first column. Columns 2 through 6 contain the mole fraction, contaminant concentration, mixture density, ratio of $(\rho - \rho_a)/c_c$ (Gamma), and mixture temperature on the centerline of the gas cloud at ground level. Columns 7 through 9 contain the contour shape parameters b (Half Width), S_z, and S_y. Finally, columns 10 and 11 contain the width from the centerline to the indicated concentration levels at the indicated height. Note that the output is prematurely terminated. Output actually continues until the centerline, ground-level concentration drops below the lowest concentration of interest.

Gravity slumping velocity coefficient used: 1.150

NON Isothermal calculation

Heat transfer calculated with correlation: 1

Water transfer not included

(6)   *****   CALCULATED SOURCE PARAMETERS   *****

Time sec	Gas Radius m	Height m	Qstar kg/m**2/s	SZ(x=L/2.) m	Mole frac C	Density kg/m**3	Temperature K	Rich No.
0.000000E+00	22.0600	1.103030E-05	6.818148E-02	0.417234	1.00000	1.67985	112.008	0.756144
1.60000	22.4197	1.511141E-02	6.761492E-02	0.424343	0.998022	1.66763	113.004	0.756144
3.52000	23.1805	2.896016E-02	6.658905E-02	0.440051	0.994459	1.64163	115.114	0.756144
4.48000	23.6237	3.352411E-02	6.604830E-02	0.448937	0.992791	1.62802	116.227	0.756144
5.12000	23.9315	3.581163E-02	6.573497E-02	0.455514	0.991825	1.61802	117.033	0.756144
6.40000	24.5615	3.841195E-02	6.514826E-02	0.468544	0.990368	1.59944	118.528	0.756144
7.04000	24.8777	3.878484E-02	6.494597E-02	0.475763	0.989921	1.59919	119.334	0.756144
8.96000	25.3717	3.822614E-02	6.489014E-02	0.489967	0.989604	1.56839	120.946	0.756144
15.3600	25.1948	3.796661E-02	6.520404E-02	0.489793	0.989842	1.56810	120.946	0.756144

(7) Source strength [kg/s] :   130.00   Equivalent Primary source radius [m] :   22.060
Equivalent Primary source length [m] :   44.120   Equivalent Primary source half-width [m] :   17.326

Secondary source concentration [kg/m**3] :   1.5397   Secondary source SZ [m] :   0.48979

Contaminant flux rate: 5.11989E-02

Secondary source mass fractions... contaminant: 0.981864   air: 1.80427E-02
          Enthalpy: -3.86753E+05   Density: 1.5681

Secondary source length [m] :   50.390   Secondary source half-width [m] :   19.788

(8)

Distance (m)	Mole Fraction	Concentration (kg/m**3)	Density (kg/m**3)	Gamma	Temperature (K)	Half Width (m)	Sz (m)	Sy (m)	Width at z= 1.00 m to:	
									5.00 mole% (m)	15.0 mole% (m)
25.2	0.990	1.54	1.5681	0.322	121.	19.8	0.489	6.538E-06	19.8	19.8
25.8	0.984	1.52	1.5523	0.316	123.	18.7	0.490	1.43	20.6	19.3
29.2	0.962	1.44	1.5139	0.308	128.	17.9	0.490	3.75	22.7	20.5
31.6	0.945	1.38	1.4982	0.309	131.	17.8	0.490	4.79	23.9	21.0
34.8	0.923	1.30	1.4651	0.302	136.	17.9	0.495	5.93	25.3	21.7
38.0	0.897	1.22	1.4261	0.289	143.	18.0	0.503	6.93	26.6	22.3

(6) A summary of the calculated secondary source parameters is
included. The secondary source gas radius and height are output
as functions of time along with other secondary parameters
including the source mass flux (Qstar), the vertical concentration
distribution parameter at the downwind edge (SZ(x = L/2.)), the
contaminant mole fraction (Mole frac C), the gas mixture density
(Density), and the Richardson number based on the cloud spreading
velocity (Rich No.). Note that only a portion of the output is
shown. The source calculation ends when all the primary and
secondary source gas has been taken up in the atmospheric flow.

⑥   ✗✗✗✗✗   CALCULATED SOURCE PARAMETERS   ✗✗✗✗✗

Time sec	Gas Radius m	Height m	Qstar kg/m✗✗2/s	SZ(x=L/2.) m	Mole frac C	Density kg/m✗✗3	Temperature K	Rich No.
0.000000E+00	22.0600	1.103030E-05	6.818148E-02	0.417234	1.00000	1.67985	112.008	0.756144
1.250000E-03	22.0600	2.356897E-05	6.818144E-02	0.417234	1.00000	1.67985	112.008	0.756144
2.500000E-03	22.0600	3.610756E-05	6.818139E-02	0.417234	1.00000	1.67985	112.008	0.756144
3.750000E-03	22.0601	4.864604E-05	6.818133E-02	0.417234	1.00000	1.67985	112.008	0.756144
5.000000E-03	22.0601	6.118439E-05	6.818126E-02	0.417234	1.00000	1.67985	112.008	0.756144
6.250000E-03	22.0601	7.372261E-05	6.818118E-02	0.417234	0.999999	1.67985	112.008	0.756144

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81.3600	14.8348	2.780102E-02	0.109961	0.606779	0.981068	1.24567	153.291	0.756144
81.5200	12.0742	2.360015E-02	0.125116	0.589908	0.979136	1.19431	160.121	0.756144
81.6800	8.90169	1.823564E-02	0.143168	0.529419	0.977271	1.13949	168.066	0.756144
81.8400	5.27878	1.147265E-02	0.160261	0.386511	0.975869	1.07404	178.501	0.756144
81.8600	4.74160	1.039801E-02	0.183404	0.399503	0.975860	1.06443	180.113	0.000000E+00
81.9600	2.08103	4.857970E-03	0.172351	0.189777	0.975860	1.00028	191.664	0.000000E+00
82.0100	0.828913	2.052904E-03	0.162497	8.258369E-02	0.975860	0.943090	203.237	0.000000E+00
82.0325	0.296554	7.756192E-04	0.153897	3.261293E-02	0.975860	0.893179	214.645	0.000000E+00
82.0337	0.267955	7.042261E-04	0.153154	2.975642E-02	0.975860	0.888863	215.686	0.000000E+00
82.0350	0.245386	6.008303E-04	0.152315	2.748155E-02	0.975860	0.883995	216.873	0.000000E+00
82.0378	0.245386	1.021048E-04	0.148447	2.748155E-02	0.975860	0.861546	222.516	0.000000E+00
82.0383	0.245386	1.192880E-05	0.144329	2.748155E-02	0.975860	0.837649	228.849	0.000000E+00
82.0384	0.245386	4.982423E-06	0.142887	2.748155E-02	0.975860	0.829278	231.150	0.000000E+00

(7) An indication of the constants used in the x-direction dispersion correction is included. The output will also indicate if the x-direction dispersion correction was not applied.

(8) The concentration field is shown for different times after the beginning of the spill. Unless otherwise specified, DEGADIS will choose default values for the time to output the concentration field. If other times are desired, DEGADIS3 can be executed again after the appropriate changes to RUN_NAME.ER3 have been made. See Appendix C for details.

(9) The downwind portion of the calculations is included. The distance downwind of the source is given in the first column. Columns 2 through 6 contain the mole fraction, contaminant concentration, mixture density, ratio of $(\rho - \rho_a)/c_c$ (Gamma), and mixture temperature on the centerline of the gas cloud at ground level. Columns 7 through 9 contain the contour shape parameters b (Half Width), S_z, and S_y. Finally, columns 10 and 11 contain the width from the centerline to the indicated concentration levels at the indicated height. Note that the output is prematurely terminated.

Sorted values for each specified time.

⑦ X-Direction correction was applied.
    Coefficient: 2.00000E-02
    Power: 1.2200
    Minimum Distance: 130.00   m

⑧   Time after beginning of spill   14.00000   sec

⑨
Distance (m)	Mole Fraction	Concentration (kg/m**3)	Density (kg/m**3)	Gamma	Temperature (K)	Half Width (m)	Sz (m)	Sy (m)	Width at z= 1.00 m to: 5.00 mole% (m)	15.0 mole% (m)
36.4	0.929	1.06	1.2102	0.130	176.	16.0	0.594	6.25	24.3	20.9
50.9	0.737	0.759	1.2468	0.230	187.	16.2	0.651	9.77	28.5	22.7
65.7	0.521	0.456	1.2105	0.304	215.	16.4	0.647	12.7	29.6	
80.7	0.248	0.174	1.1286	0.324	263.	12.0	0.761	14.0	20.7	

For the UFL of   15.000   mole percent, and the LFL of   5.0000   mole percent:

The mass of contaminant between the UFL and LFL is: 120.85   kg.
The mass of contaminant above the LFL is: 786.92   kg.

    Time after beginning of spill   25.00000   sec

Distance (m)	Mole Fraction	Concentration (kg/m**3)	Density (kg/m**3)	Gamma	Temperature (K)	Half Width (m)	Sz (m)	Sy (m)	Width at z= 1.00 m to: 5.00 mole% (m)	15.0 mole% (m)
35.5	0.940	1.07	1.1932	0.113	178.	16.3	0.626	6.03	24.6	21.5
50.0	0.788	0.826	1.2255	0.186	185.	16.4	0.701	9.66	29.4	24.2
64.8	0.670	0.662	1.2472	0.265	192.	17.6	0.744	12.7	34.1	26.8
79.8	0.592	0.544	1.2182	0.269	205.	19.0	0.775	15.3	38.1	28.6
95.0	0.520	0.446	1.1846	0.253	220.	20.0	0.825	17.8	41.3	29.3
110.	0.429	0.341	1.1567	0.249	236.	20.8	0.903	20.1	43.6	29.0

In addition to the output of the concentration field at specified times (using DEGADIS3), DEGADIS allows output of concentration time histories at specified positions using DEGADIS4 for transient releases. (Specifics about DEGADIS4 and its input requirements are included in Appendix C.) DEGADIS4 can be executed interactively or in batch mode. An example DEGADIS4 interactive run and output follow.

Notes on Using DEGADIS4

① DEGADIS4 can be run interactively as demonstrated here or in batch mode by supplying the same responses demonstrated here. DEGADIS4 sends the output to RUN_NAME.SR4.

② The RUN_NAME of the transient simulation is used here.

③ The number of downwind positions where output is desired is entered here. For each downwind distance, questions 4 and 5 are required.

④ The x-coordinate is the downwind distance from the source where output is desired.

⑤ At each downwind distance, DEGADIS4 asks for the y- and z-coordinates desired. DEGADIS4 automatically supplies information about the centerline concentration ($y = 0$ and $z = 0$). Note that negative numbers signal that no more positions are desired for this particular downwind distance.

① $ RUN SYS$DEGADIS:DEGADIS4
② Enter the file name used for this run: BURRO9
③ Enter the number of downwind distances desired:
   max of   10 downwind distances; 4 positions at each distance
   1

④ enter the x coordinate:
   100.
⑤   enter the y and z coordinate pairs at this distance:
   0., 1...
   30., 1.
   -1.,-1...
    ti: 17.000   tf: 98.562   dt: 2.0000   dist: 100.00
   FORTRAN STOP
   $

Notes in DEGADIS4 Output

①   DEGADIS4 indicates the constants used in the x-direction dispersion correction. The user has the option of not making the x-direction dispersion correction if desired by making the appropriate changes to RUN_NAME.ER3. See Appendix C.

②   At each downwind distance specified, the concentration profile parameters are output as a function of time. Note that part of the output has been removed.

① X-Direction correction was applied.
    Coefficient: 2.00000E-02
    Power: 1.2200
    Minimum Distance: 130.00   m

② Centerline values for the position -->
x: 100.00   m

| Time | Mole Fraction | Concentration | Density | Gamma | Temperature | Half Width | Sz | Sy | Width at z= 1.00 m to: | |
| | | | | | | | | | 5.00 mole% | 15.0 mole% |
(s)		(kg/m**3)	(kg/m**3)		(K)	(m)	(m)	(m)	(m)	(m)
19.0	0.283	0.210	1.1320	0.300	259.	15.3	0.891	17.5	30.8	
21.0	0.385	0.302	1.1522	0.264	242.	18.5	0.861	18.3	37.7	
23.0	0.465	0.382	1.1713	0.260	229.	20.0	0.846	18.5	41.3	27.4
25.0	0.491	0.411	1.1755	0.251	225.	20.2	0.850	18.5	42.2	29.3
27.0	0.500	0.421	1.1759	0.246	224.	20.4	0.858	18.6	42.7	30.2
29.0	0.502	0.423	1.1770	0.248	224.	20.6	0.868	18.7	43.2	30.7
31.0	0.507	0.429	1.1780	0.246	223.	20.7	0.875	18.7	43.4	31.2
33.0	0.511	0.435	1.1795	0.246	222.	20.6	0.877	18.7	43.4	31.4
35.0	0.512	0.435	1.1791	0.245	222.	20.6	0.876	18.6	43.4	31.4
37.0	0.511	0.433	1.1781	0.245	222.	20.6	0.876	18.7	43.4	31.3
39.0	0.512	0.435	1.1794	0.246	222.	20.6	0.878	18.6	43.4	31.4
89.0	0.512	0.434	1.1779	0.243	222.	20.7	0.875	18.7	43.4	31.4
91.0	0.511	0.434	1.1783	0.244	222.	20.6	0.876	18.7	43.4	31.4
93.0	0.511	0.433	1.1778	0.245	222.	20.6	0.876	18.7	43.4	31.3
95.0	0.485	0.401	1.1678	0.239	227.	20.9	0.893	19.2	44.0	31.1

③ DEGADIS4 outputs the concentration time history at the off-centerline positions specified.

③

Time	Mole fraction at: y= 0.00000E+00 m z= 1.0000 m	Mole fraction at: y= 30.000 m z= 1.0000 m	Mole fraction at: y= -1.0000 m z= -1.0000 m	Mole fraction at: y= 0.00000E+00 m z= 0.00000E+00 m
(s)				
17.00000	0.0000000E+00	0.0000000E+00		
19.00000	0.1060624	5.4025235E-02		
21.00000	0.1424979	9.8715379E-02		
23.00000	0.1730387	0.1328462		
25.00000	0.1860092	0.1447582		
27.00000	0.1921793	0.1513815		
29.00000	0.1952771	0.1557802		
31.00000	0.2000309	0.1600196		
33.00000	0.2026532	0.1617373		
35.00000	0.2026345	0.1614892		
37.00000	0.2019068	0.1608861		
39.00000	0.2030946	0.1616422		

●
●
●

89.00000	0.2021314	0.1614686		
91.00000	0.2021210	0.1613367		
93.00000	0.2015993	0.1608710		
95.00000	0.1926055	0.1577260		

APPENDIX E

OOMS' MODEL CODE LISTING

APPENDIX F
DEGADIS CODE LISTING

APPENDIX H
PARTIAL LISTING OF PROGRAM VARIABLES

Variable	Data Type	Symbol	Units	Comments
AGAIN	LOGICAL			Local communications in SSSUP
ALEPH	REAL			Collection of constants to calculate observer position and velocity
ALPHA	REAL	α	n/a	Power law velocity profile power
ALPHA1	REAL	$(1.0 + \alpha)$	n/a	
BETA	REAL	β	n/a	Lateral similarity power
CCLOW	REAL		kg/m^3	Lowest mixture concentration of interest
CHECK1	LOGICAL			Unused logical flag
CHECK2	LOGICAL			When true, release type without a liquid source
CHECK3	LOGICAL			Local communications flag used in DEGADIS1
CHECK4	LOGICAL			When true, steady-state simulation
CHECK5	LOGICAL			When true, user sets time-sort parameters
DELTA	REAL	δ	$m^{1-\beta}$	Lateral similarity coefficient
DEN(1,I)	REAL	y_c	mole fraction	Contaminant mole fraction
DEN(2,I)	REAL	c_c	kg/m^3	Contaminant concentration for the given mole fraction

Variable	Data Type	Symbol	Units	Comments
DEN(3,I)	REAL	ρ	kg/m^3	Mixture density for the given mole fraction
DEN(4,I)	REAL	h	J/kg	Mixture enthalpy for the given mole fraction
DEN(5,I)	REAL	T	K	Mixture temperature for the given mole fraction
EMAX	REAL		kg/s	Maximum of secondary source mass evolution rate
ESS	REAL	E	kg/s	Steady-state release rate
ET(I)	REAL	E(t)	kg/s	Source mass evolution rate as a function of time PTIME(I)
G	REAL	g	m/s^2	Acceleration due to gravity
GAMMAF	REAL	$\Gamma(1/(1+\alpha))$	n/a	
GAS_CPK	REAL	q_1	$J/kmol\ K^{p_1-1}$	Constant for contaminant heat capacity
GAS_CPP	REAL	p_1	n/a	Power for contaminant heat capacity
GAS_LFL	REAL		mole fraction	Lower contaminant concentration level for estimating contours
GAS_MW	REAL	MW_C	kg/kmol	Contaminant molecular weight
GAS_NAME	CHARACTER*3			Name of contaminant
GAS_RHOE	REAL	ρ_0	kg/m^3	Saturated vapor density of contaminant at T_0
GAS_TEMP	REAL	T_0	K	Contaminant storage temperature
GAS_UFL	REAL		mole fraction	Upper contaminant concentration level for estimating contours

Variable	Data Type	Symbol	Units	Comments
GAS_ZSP	REAL		m	Height for estimating contours
GMASS0	REAL		kg	Initial mass of gas over the primary source
HTCO	REAL	h_0	J/m^2sK	Constant coefficient when IHTFL=-1
		v_H	m/s	LLNL heat transfer velocity when IHTFL=2
HUMID	REAL		kg water/ kg dry air	Ambient absolute humidity
IHTFL	INTEGER			Heat transfer flag: IHTFL=-1 constant coefficient IHTFL=0 no heat transfer IHTFL=1 DEGADIS correlation IHTFL=2 LLNL correlation
ISOFL	INTEGER			Isothermal release when ISOFL=1
ISTAB	INTEGER			Pasquill atmospheric stability indicator (ISTAB=1 for A, (ISTAB=2 for B, etc.)
IWTFL	INTEGER			Water transfer flag IWTFL=-1 constant coefficient IWTFL=0 no water transfer IWTFL=1 DEGADIS correlation
K	REAL	k	n/a	von Karman's constant, 0.35
LUNLOG	INTEGER			Fortran logical unit number which acts as a simulation log
MAXNOB	INTEGER			Maximum number of observers
ML	REAL	λ	m	Monin-Obukhov length
NOBS	INTEGER			Number of observers for the pseudosteady-state simulation

Variable	Data Type	Symbol	Units	Comments
NREC(I,1)	INTEGER			Number of records generated in PSSOUT for observer I
NREC(I,2)	INTEGER			Number of records generated in SSGOUT for observer I
PAMB	REAL	p	atm	Ambient pressure
POUND	CHARACTER*4			Character string to signal end of data ('// ')
POUNDN	REAL			Numerical value to signal end of data (-1.E-20)
QSTR(1,I)	REAL	t	s	Independent variable time for ordered pairs QSTR
QSTR(2,I)	REAL	Q_*	kg/m^{2}s	Atmospheric takeup rate as a function of time
RADG(1,I)	REAL	t	s	Independent variable time for ordered pairs RADG
RADG(2,I)	REAL	R	m	Secondary source radius as a function of time
RELHUMID	REAL		%	Ambient relative humidity
RHOA	REAL	ρ_a	kg/m^3	Ambient air density
RM	REAL	R_m	m	Radius at EMAX (when secondary source mass evolution rate is a maximum)
RMAX	REAL	R_{max}	m	Maximum secondary source radius
RT2	REAL	$\sqrt{2}.$	n/a	Constant
R1SS	REAL	R_p	m	Steady-state primary source radius

Variable	Data Type	Symbol	Units	Comments
R1T(I)	REAL	R_p	m	Primary source radius as a function of time PTIME(I)
SIGX_COEFF	REAL			Along-wind similarity coefficient
SIG_MIN_DIST	REAL		m	Minimum distance to apply x-direction dispersion correction
SIGX_POW	REAL		n/a	Along-wind similarity power
SLEN	REAL	L	m	Steady-state source length
SQPIO2	REAL	$\sqrt{\pi/2}$.	n/a	Constant
SQRTPI	REAL	$\sqrt{\pi}$	n/a	Constant
SRCDEN(1,I)	REAL	t	s	Independent variable time for ordered pairs SRCDEN
SRCDEN(2,I)	REAL	ρ	kg/m^3	Secondary source density as a function of time
SRCENTH(1,I)	REAL	t	s	Independent variable time for ordered pairs SRCENTH
SRCENTH(2,I)	REAL	h	J/kg	Secondary source enthalpy as a function of time
SRCWA(1,I)	REAL	t	s	Independent variable time for ordered pairs SRCWA
SRCWA(2,I)	REAL	w_a	mass fraction	Secondary source air mass fraction as a function of time
SRCWC(1,I)	REAL	t	s	Independent variable time for ordered pairs SRCWC

Variable	Data Type	Symbol	Units	Comments
SRCWC(2,I)	REAL	w_c	mass fraction	Secondary source contaminant mass fraction as a function of time
SWID	REAL		m	Steady-state source half-width
SZM	REAL	S_{z0m}	m	Value of S_{z0} at EMAX (when secondary source mass evolution rate is a maximum)
TAMB	REAL	T	K	Ambient temperature
TEND	REAL		s	Termination time of secondary source
TINP	CHARACTER*24			Time DEGADISIN was executed
TITLE(1:4)	CHARACTER*80			Text title block 4 lines of 80 spaces
TO(I)	REAL		s	Time of release for observer I
TSURF	REAL	T_s	K	Surface temperature
USTAR	REAL	u_*	m/s	Friction velocity
UO	REAL	u_0	m/s	Ambient velocity at height z_0
WTCO	REAL	F	$kg/m^2 s$	Mass transfer coefficient when IWTFL=-1
XV(I)	REAL	x_v	m	Virtual source position for estimation of S_y in SSG
ZO	REAL	z_0	m	Height for velocity u_0
ZR	REAL	z_R	m	Roughness length

APPENDIX I

DEGADIS DIAGNOSTIC MESSAGES

To assist the user in determining the source of any problems, a diagnostic procedure has been included in DEGADIS. The subroutine TRAP is meant to cause an orderly termination of the program for many detected errors. It performs two basic functions: TRAP displays an error code and a single line diagnostic message giving the reason for premature termination, and TRAP forces an output of the COMMON area data sets to the file TRAP.DBG.

The first three lines sent to the execution log (default=TERMINAL) include the TRAP introductory lines and the error code number:

  The best laid plans of mice and men . . .

  You have entered a TRAP--THE LAND OF NO RETURN

  CODE: NN

where NN represents the code of the error message which follows in the log. The error message begins with the name of the calling routine.

The following is a list of the error codes, error messages, and suggested actions for each problem.

Code: 1
    DEGADIS1? Source integration has returned IHLF=NN

Action: This error occurs during integration of the equations which describe the gas source. IHLF is an error code returned by the integration package RKGST.
    When IHLF=11, more than 10 bisections of the initial increment of the independent variable were necessary to make an integration step within the specified error. Reduce the initial step size of the independent variable (STPIN in the ER1 file). If this does not work, it will be necessary to either increase the error criteria for all of the dependent variables being integrated (ERBND in the ER1 file) or increase the error criteria for the variable violating the criteria by decreasing the error weight for that variable (one of the following: WTRG, WTTM, WTYA, WTYC, WTEB, WTMB, or WTUH in the ER1 file).
    When IHLF=12, the initial increment of the independent variable (STPIN) is 0. Correct the ER1 file and execute the program again.

When IHLF=13, the initial increment of the independent variable (STPIN) is not the same sign as the difference between the upper bound of the interval and the lower bound of the interval. STPIN must be positive. Correct the ER1 file and execute the program again.

Code: 2
Reserved

Code: 3
    SZF? Local integration failed; IHLF=NN

Action: This error occurs during estimation of SZ over the source when no gas is present. IHLF is an error code returned by the integration package RKGST.
    When IHLF=11, more than 10 bisections of the initial increment of the independent variable were necessary to make an integration step within the specified error. Reduce the initial step size of the independent variable (SZSTPO in the ER1 file). If this does not work, increase the error criteria for all of the dependent variables being integrated (SZERR in the ER1 file).
    When IHLF=12, the initial increment of the independent variable (SZSTPO) is 0. Correct the ER1 file and execute the program again.
    When IHLF=13, the initial increment of the independent variable (SZSTPO) is not the same sign as the difference between the upper bound of the interval and the lower bound of the interval. SZSTPO must be positive. Correct the ER1 file and execute the program again.

Code: 4
    SURFACE? Negative QRTE for positive DELTA_T.

Action: This is a diagnostic message indicating an error in estimation of the heat capacity. Check the input to the model and execute the program again.

Code: 5
    CRFG? More points for GEN3 were needed.

Action: The COMMON area /GEN3/ stores representative values of the calculated source parameters. If this message occurs, relax the CRFG error criteria (CRFGER) in the ER1 file. If this is a common problem, the length of the /GEN3/ vectors can be increased by changing the value of MAXL in DEGADIS1.DEC and reinstalling DEGADIS.

Code: 6
    TUPF?   Observer calculations--TUPF failed

Action: The trial-and-error search associated with finding the upwind
edge of the gas source for an observer failed. Often this problem can
be avoided by adding one or two additional observers to the present
number of observers (which changes the conditions for the trial and
error).   Another possibility is to increase the error criteria for this
function (ERTUPF) in the ER2 file.

Code: 7
    TDNF?   Observer calculations--TDNF failed

Action: The trial-and-error search associated with finding the downwind
edge of the gas source for an observer failed. Often this problem can
be solved by adding one or two additional observers to the present
number of observers (which changes the conditions for the trial and
error). Another possibility is to increase the error criteria for this
function (ERTDNF) in the ER2 file.

Code: 8
    SSSUP?   Observer Integration failed, IHLF=NN

Action: This error occurs during integration of the five differential
equations which average the source for each observer. IHLF is an error
code returned by the integration package RKGST.
    When IHLF=11, more than 10 bisections of the initial increment of
the independent variable were necessary to make an integration step
within the specified error. Reduce the initial step size of the
independent variable (STP0 in the ER2 file). If this does not work, it
will be necessary to either increase the error criteria for all of the
dependent variables being integrated (ERR0 in the ER2 file) or increase
the error criteria for the variables violating the criteria by
decreasing the error weight for that variable (one of the following:
WTAIO, WTQOO, or WTSZO in the ER2 file).
    When IHLF=12, the initial increment of the independent variable
(STP0) is 0. Correct the ER2 file and execute the program again.
    When IHLF=13, the initial increment of the independent variable
(STP0) is not the same sign as the difference between the upper bound of
the interval and the lower bound of the interval. STP0 must be
positive. Correct the ER2 file and execute the program again.

Code: 9
    SSSUP/SDEGADIS2? Pseudosteady Integration failed, IHLF=NN

Action: This error occurs during integration of the four differential
equations describing the portion of the downwind calculation when b > 0.
The routine calling TRAP is SSSUP if a transient simulation is being
executed; if a steady-state simulation is being executed, the calling
routine is SDEGADIS2. IHLF is an error code returned by the integration
package RKGST.
    When IHLF=11, more than 10 bisections of the initial increment of
the independent variable were necessary to make an integration step
within the specified error. Reduce the initial step size of the
independent variable (STPP in the ER2 file). If this does not work, it
will be necessary to either increase the error criteria for all of the
dependent variables being integrated (ERRP in the ER2 file) or increase
the error criteria for the variable violating the criteria by decreasing
the error weight for that variable (one of the following: WTSZP, WTSYP,
WTBEP, or WTDH in the ER2 file).
    When IHLF=12, the initial increment of the independent variable
(STPP) is 0. Correct the ER2 file and execute the program again.
    When IHLF=13, the initial increment of the independent variable
(STPP) is not the same sign as the difference between the upper bound of
the interval and the lower bound of the interval. STPP must be
positive. Correct the ER2 file and execute the program again.

Code: 10
    SSSUP/SDEGADIS2? Gaussian Integration fail, IHLF=nn

Action: This error occurs during integration of the differential
equations describing the portion of the downwind calculation when b=0.
The routine calling TRAP is SSSUP if a transient simulation is being
executed; if a steady-state simulation is being executed, the calling
routine is SDEGADIS2. IHLF is an error code returned by the integration
package RKGST.
    When IHLF=11, more than 10 bisections of the initial increment of
the independent variable were necessary to make an integration step
within the specified error. Reduce the initial step size of the
independent variable. (STPG in the ER2 file). If this does not work,
it will be necessary to either increase the error criteria for all of
the dependent variables being integrated (ERRG in the ER2 file) or
increase the error criteria for the variable violating the criteria by
decreasing the error weight for that variable (either WTRUH or WTDHG in
the ER2 file).
    When IHLF=12, the initial increment of the independent variable
(STPG) is 0. Correct the ER2 file and execute the program again.
    When IHLF=13, the initial increment of the dependent variable (STPG)
is not the same sign as the difference between the upper bound of the
interval and the lower bound of the interval. STPG must be positive.
Correct the ER2 file, and execute the program again.

Code: 11
    SSSUP/SDEGADIS2 Total No. of Records exceeds 120,000

Action: This is an arbitrary stopping point for the process in order to
keep a runaway simulation from filling up disk space. Relax the output
specification (ODLP, ODLLP, ODLG, or, DLLG) in the ER2 file in order to
generate less output if the input parameters are valid.

Code: 12
Reserved

Code: 13
Reserved

Code: 14
Reserved

Code: 15
Reserved

Code: 16
    PSSOUT/PSSOUTSS? PSS started with B < 0.

Action: This condition is checked at the beginning of the downwind
calculation in order to confirm proper handling of the movement to the
Gaussian phase of the downwind calculation. Check the initial
conditions and execute the program again.

Code: 17
    TPROP/ADDHEAT? Enthalpy out of bounds

Action: Diagnostic message indicating that an enthalpy lower than the
adiabatic mixing enthalpy was passed to ADDHEAT. Check the input
conditions and execute the program again.

Code: 18
    ALPH? ALPHA integration failed, IHLF=NN

Action: The integration which determines the integral least squares fit
for ALPHA has failed. Note that small values of the Monin-Obukhov
length (ML < O(1m)) in combination with stable atmospheric conditions
may cause this failure. IHLF is an error code returned by the
integration package RKGST.
    When IHLF=11, more than 10 bisections of the initial increment of
the independent variable were necessary to make an integration step
within the specified error. Reduce the absolute value of the initial
step size of the independent variable (STPINZ in the ER1 file). If this
does not work, it will be necessary to increase the error criteria
(ERBNDZ in the ER1 file).
    When IHLF=12, the initial increment of the independent variable
(STPINZ) is 0. Correct the ER1 file and execute the program again.
    When IHLF=13, the initial increment of the independent variable
(STPINZ) is not the same sign as the difference between the upper bound
of the interval and the lower bound of the interval. STPINZ must be
negative. Correct the ER1 file and execute the program again. This
error will also occur if the surface roughness ZR is greater than the
reference height Z0.

Code: 19
    ALPH? RTMI has failed to locate ALPHA IERR:NN

Action: The search procedure which determines ALPHA has failed. This
error may be the result of an unusual velocity specification such as
small values of the Monin-Obukhov length (ML < O(1.m)) or small
reference heights (Z0 < O(10. * ML)). IERR is an error code returned
by the routine RTMI.
    When IERR=1, the search for ALPHA failed after a specified number of
iterations. Increase the error bound used by RTMI (EPS in the ER1
file).
    When IERR=2, the basic assumption that the function which governs
the search for ALPHA changes sign over the specified interval is false.
Increase the search interval by decreasing the lower bound of ALPHA (XLI
in the ER1 file) and increasing the upper bound (XRI in the ER1 file).

Code: 20
    ESTRT? Premature EOF in RUN_NAME.ER1 or RUN_NAME.ER2

Action: The portion of the program which reads ER1 and ER2 files
encountered an end-of-file mark before all of the information had been
read. Confirm these files and execute the program again. If necessary,
copy and edit the appropriate EXAMPLE file and execute the program
again.

Code: 21
   ESTRT1/ESTRT2/ESTRT2SS/ESTRT3?   DECODE failed.

Action: The portion of the program which reads the ER1, ER2, or the ER3
file failed to understand a numerical entry.   The numbers must appear in
columns 11-20 of the line with no alphabetic characters in the field.
(Note that exponential notation is not allowed.)   This restriction does
not apply to comment lines which have an exclamation point (!) in the
first column.

Code: 22
   ESTRT1?   The parameter file RUN_NAME.ER1 was not found.

Action: The ER1 file was not found for the current simulation
(RUN_NAME).   Copy the file EXAMPLE.ER1 to RUN_NAME.ER1 and edit it as
necessary.   Execute the program again.

Code: 23
   SORTS1?   Fewer than 3 points sorted for any time.

Action: Only one or two simulation points were applicable for the sort
times specified.   There are three possible causes for this condition:
   (1) if this message appears when the sort times are defaulted
(CHECK5 is set to 0. in the ER3 file), the number of observers will
probably have to be increased to give a good resolution of the downwind
concentration field.   (The number of observers is NOBS in the ER2 file
with a maximum (MAXNOB) given in DEGADIS2.DEC.).   As a rule of thumb,
one gets good resolution of the downwind concentration field if the
ratio: (secondary source duration / number of observers) is less than
about 10 seconds (or 20 at most).
   (2) The sort times specified in the ER3 file were before the
simulation had developed significantly.   This is only applicable when
the user is specifying the sort times (i.e. when CHECK5 is set to 1. in
the ER3 file).   Increase the time of the first sort (ERT1), and rerun
the program.
   (3) The sort times specified in the ER3 file were after the gas was
below the lowest concentration of interest.   This is only applicable
when the user is specifying the sort times (i.e. when CHECK5 is set to
1. in the ER3 file).   Increase the time of the first sort (ERT1), and
rerun the program.   If additional results are desired for later times,
restart the simulation and specify a lower concentration of interest in
the input step (lower CCLOW in DEGADISIN).

Code: 24
   TPROP?   Trial and error loop compromised.

Action: TPROP estimates the temperature of a mixture based upon the
composition and enthalpy of the mixture.   Ensure the properties for the
diffusing species are entered correctly and execute the simulation
again.

Code: 25
    TPROP? Isothermal density loop compromised.

Action: This error should never occur, but if it does, rebuild the model from the original files and run the simulation over.

Code: 26
    TPROP? Invalid entry flag in ADIABAT.

Action: This is a programming diagnostic and should never occur. If it does, rebuild the model from the original files.

Code: 27
Reserved

Code: 28
    TPROP? IGEN request too large in SETDEN.

Action: The subroutine SETDEN (in TPROP) performs a series of adiabatic mixing calculations with a specified gas mixture and ambient air and places the result in the array DEN(5,IGEN). This error indicates more points are needed in DEN than were originally requested. Increase the allocation for DEN by changing the value of IGEN in DEGADISIN.DEC and reinstalling DEGADIS.

Code: 29
    PHIF? Flag IPHIFL is out of bounds.

Action: Proper values of IPHIFL are integers between 1 and 5 inclusive. Although values of IPHIFL are entered in the ER1 file as real numbers, they should be in this range. Check the ER1 file and execute the program again.

Code: 30
    SSSUP/SDEADIS2? Concentration greater than RHOE.

Action: If the concentration of the contaminant becomes greater than the pure component density for an isothermal simulation, this error will occur. However, this situation should never occur. Check the input conditions and execute the program again.

<u>Code:</u> 31
    SSSUP? Concentration greater than RHOE.

<u>Action:</u> If the concentration of the contaminant becomes greater than
the pure component density for an isothermal simulation, this error will
occur. However, this situation should never occur. Check the input
conditions and execute the program again.

<u>Code:</u> 32
    PSS? Sz convergence failure.

<u>Action:</u> This is a programming diagnostic and should never occur. If it
does, check the input conditions and execute the program again.

<u>Code:</u> 33
    SSG? Sz convergence failure.

<u>Action:</u> This is a programming diagnostic and should never occur. If it
does, check the input conditions and execute the program again.

APPENDIX J

OOMS/DEGADIS

EXAMPLE SIMULATION OUTPUT

(corresponds to example in Section IV of this volume)

o DOWNWIND DISTANCE TO FIRST PRINTOUT = 10.0 M
o DISTANCE BETWEEN PRINTOUTS = 10.0 M
o AMBIENT AIR DENSITY = 1.18 KG/M**3
o DISPERSION JET DENSITY = 2.33 KG/M**3
o AMBIENT TEMPERATURE = 298.0 DEG CELSIUS
o INITIAL JET TEMPERATURE = 298.0 DEG CELSIUS
o INITIAL JET DIAMETER = 20.0 CM
o INITIAL JET FLOWRATE = 0.2880E+01 M**3/S
o DEPTH OF SECTOR = 1000.0 M
o DISTANCE FROM THE CENTERLINE TO THE JET ORIGIN
  IN THE Y DIRECTION = 0.0 M
o DISTANCE FROM THE SECTOR SURFACE TO THE JET ORIGIN
  IN THE Z DIRECTION = 967.0 M
o MEAN VELOCITY OF THE WIND = 5.8 M/S
o ORIENTATION OF THE JET
  VERTICAL UPWARD
o ENTRAINMENT COEFFICIENTS
  ALFA 1= 0.0570
  ALFA 2= 0.5000
  ALFA 3= 1.0000

JET DEVELOPMENT:

X (METERS)	Z (METERS)	CONCENTRATION(CL) (KG/M**3)
10.7135	41.490	0.8797E-01
20.5632	43.195	0.5794E-01
30.5399	44.208	0.4645E-01
40.5174	44.875	0.4044E-01
50.5074	45.317	0.3688E-01
60.5036	45.592	0.3470E-01
70.5026	45.727	0.3343E-01
80.5025	45.738	0.3275E-01
90.5019	45.631	0.3173E-01
100.4995	45.415	0.3030E-01
110.4947	45.104	0.2859E-01
120.4870	44.711	0.2673E-01
130.4765	44.254	0.2485E-01
140.4635	43.743	0.2302E-01
150.4483	43.192	0.2128E-01
160.4313	42.609	0.1967E-01
170.4129	42.002	0.1820E-01
180.3933	41.377	0.1685E-01
190.3729	40.738	0.1564E-01
200.3519	40.088	0.1453E-01
210.3304	39.432	0.1354E-01
220.3084	38.769	0.1264E-01
230.2861	38.102	0.1182E-01
240.2637	37.432	0.1108E-01
250.2412	36.759	0.1040E-01
260.2185	36.085	0.9788E-02
270.1957	35.409	0.9226E-02
280.1729	34.733	0.8712E-02
290.1501	34.055	0.8239E-02
300.1269	33.377	0.7804E-02
310.1037	32.698	0.7403E-02
320.0805	32.018	0.7032E-02
330.0573	31.338	0.6688E-02

340.0341	30.657	0.6369E-02
350.0109	29.974	0.6072E-02
360.9853	29.222	0.5768E-02
370.9618	28.537	0.5511E-02
380.9381	27.851	0.5271E-02
390.9146	27.163	0.5045E-02
400.8907	26.473	0.4834E-02
410.8668	25.781	0.4635E-02
420.8429	25.086	0.4447E-02
430.8186	24.389	0.4270E-02
440.7942	23.690	0.4103E-02
450.7694	22.987	0.3945E-02
460.7444	22.281	0.3795E-02
470.7195	21.571	0.3653E-02
480.6941	20.857	0.3518E-02
490.6682	20.138	0.3390E-02
500.6421	19.415	0.3267E-02
510.6154	18.686	0.3151E-02
520.5886	17.952	0.3040E-02
530.5610	17.211	0.2933E-02
540.5332	16.464	0.2832E-02

****

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U O A _ D E G A D I S   M O D E L   O U T P U T   - -   V E R S I O N   2.0   ******************

******************* 17-MAR-1988 10:42:30.90 *******************

Data input on   17-MAR-1988 10:42:27.45
Source program run on   17-MAR-1988 10:42:30.90

NOTE:

> All Calculations are limited to circular liquid sources.

TITLE BLOCK

Steady-state simulation test OOMS-DEGADIS MIC release (Bhopal)

Wind velocity at reference height   2.90   m/s
Reference height   10.00   m

Surface roughness length   0.100   m

Pasquill stability class   F

Monin-Obukhov length   17.5   m
Gaussian distribution constants   Delta   0.03600   m
                                   Beta   0.89400

Wind velocity power law constant   Alpha   0.44905
Friction velocity   0.13910   m/s

Ambient Temperature   298.00   K

Surface Temperature   298.00   K
Ambient Pressure   1.000   atm
Ambient Absolute Humidity   1.009E-02 kg/kg BDA
Ambient Relative Humidity   50.00   %

Adiabatic Mixing: Mole fraction CONCENTRATION OF C   GAS DENSITY   Enthalpy   Temperature
                                      kg/m**3   kg/m**3   J/kg   K
                   0.00000   0.00000   1.17737   0.00000E+00   298.00
                   0.06729   0.15688   1.25501   0.00000E+00   298.00
                   0.14408   0.33590   1.34362   0.00000E+00   298.00

                   0.23254   0.54213   1.44569   0.00000E+00   298.00
                   0.33555   0.78227   1.56454   0.00000E+00   298.00
                   0.45702   1.06543   1.70469   0.00000E+00   298.00

                   0.60239   1.40431   1.87241   0.00000E+00   298.00
                   0.77950   1.81714   2.07674   0.00000E+00   298.00
                   1.00000   2.33112   2.33112   0.00000E+00   298.00

Specified Gas Properties:

  Molecular weight: 57.000
  Storage temperature: 298.00   K
  Density at storage temperature and ambient pressure: 2.3311   kg/m**3
  Mean heat capacity constant: 80700.
  Mean heat capacity power: 1.0000
  Upper mole fraction contour: 3.00000E-05
  Lower mole fraction contour: 2.00000E-05
  Height for isopleths: 0.50000   m

Source input data points

         Initial mass in cloud: 0.00000E+00

Time   Contaminant   Source Radius   Contaminant   Temperature   Enthalpy
            Mass Rate   Mass Fraction
  s   kg/s   m   kg contam/kg mix   K   J/kg
0.00000E+00 6.7200   15.893   2.34446E-03   298.00   0.00000E+00
6023.0   6.7200   15.893   2.34446E-03   298.00   0.00000E+00
6024.0   0.00000E+00   0.00000E+00   2.34446E-03   298.00   0.00000E+00
6025.0   0.00000E+00   0.00000E+00   2.34446E-03   298.00   0.00000E+00

Calculation procedure for ALPHA: 1

Entrainment prescription for PHI: 3

Layer thickness ratio used for average depth: 2.1500

Air entrainment coefficient used: 0.590

Gravity slumping velocity coefficient used: 1.150

NON Isothermal calculation

Heat transfer calculated with correlation: 1

Water transfer not included

CALCULATED SOURCE PARAMETERS

*****

Time sec	Gas Radius m	Height m	Qstar kg/m**2/s	SZ(x=L/2.) m	Mole frac C	Density kg/m**3	Temperature K	Rich No.
0.000000E+00	15.8926	1.100000E-05	1.491725E-04	1.83550	1.185348E-03	1.17873	298.000	0.756144
7.68000	15.8926	23.1214	1.491725E-04	29.8055	1.185348E-03	1.17873	298.000	0.756144

Source strength [kg/s] : 6.7200
Equivalent Primary source length [m] : 31.785

Equivalent Primary source radius [m] : 15.893
Equivalent Primary source half-width [m] : 12.482

Secondary source concentration [kg/m**3] : 2.76350E-03
Secondary source SZ [m] : 29.806

Contaminant flux rate: 6.65150E-03

Secondary source mass fractions... contaminant: 2.344463E-03 air: 0.98769
Enthalpy: 0.00000E+00   Density: 1.1787

Secondary source length [m] : 31.785   Secondary source half-width [m] : 12.482

Distance (m)	Mole Fraction	Concentration (kg/m**3)	Density (kg/m**3)	Gamma	Temperature (K)	Half Width (m)	Sz (m)	Sy (m)	Width at z= 0.50 m to: 2.000E-03mole% (m)	3.000E-03mole% (m)
15.9	1.185E-03	2.763E-03	1.1787	0.495	298.	12.5	29.8	3.000E-02	12.5	12.5
16.7	1.185E-03	2.763E-03	1.1787	0.495	298.	11.9	29.8	0.727	13.3	13.3
19.1	1.185E-03	2.762E-03	1.1787	0.495	298.	11.2	29.8	1.45	14.2	14.0
22.3	1.184E-03	2.760E-03	1.1787	0.495	298.	10.7	29.8	2.05	14.8	14.6
28.7	1.182E-03	2.756E-03	1.1787	0.495	298.	9.93	29.8	2.91	15.8	15.5
35.1	1.181E-03	2.754E-03	1.1787	0.495	298.	9.35	29.9	3.56	16.5	16.2
41.5	1.179E-03	2.749E-03	1.1787	0.495	298.	8.87	29.9	4.11	17.2	16.7
67.1	1.173E-03	2.735E-03	1.1787	0.495	298.	7.36	30.1	5.81	19.1	18.5
79.9	1.169E-03	2.725E-03	1.1787	0.495	298.	6.75	30.1	6.50	19.9	19.2
92.7	1.165E-03	2.716E-03	1.1787	0.495	298.	6.20	30.2	7.12	20.5	19.8
105.	1.161E-03	2.706E-03	1.1787	0.495	298.	5.70	30.3	7.69	21.2	20.4
118.	1.157E-03	2.697E-03	1.1787	0.495	298.	5.23	30.3	8.22	21.8	20.9
131.	1.153E-03	2.688E-03	1.1787	0.495	298.	4.78	30.4	8.72	22.3	21.4
144.	1.149E-03	2.678E-03	1.1787	0.495	298.	4.37	30.5	9.19	22.9	21.9
157.	1.145E-03	2.669E-03	1.1787	0.495	298.	3.97	30.6	9.64	23.3	22.4
169.	1.141E-03	2.660E-03	1.1787	0.495	298.	3.59	30.6	10.1	23.8	22.8
182.	1.137E-03	2.651E-03	1.1787	0.495	298.	3.22	30.7	10.5	24.3	23.2
195.	1.133E-03	2.642E-03	1.1787	0.495	298.	2.87	30.8	10.9	24.7	23.6
208.	1.129E-03	2.633E-03	1.1787	0.495	298.	2.54	30.8	11.3	25.1	24.0
221.	1.126E-03	2.624E-03	1.1787	0.495	298.	2.21	30.9	11.6	25.5	24.3
233.	1.122E-03	2.615E-03	1.1787	0.495	298.	1.89	31.0	12.0	25.9	24.7
246.	1.118E-03	2.607E-03	1.1787	0.495	298.	1.58	31.1	12.3	26.3	25.0
259.	1.114E-03	2.598E-03	1.1787	0.495	298.	1.29	31.1	12.7	26.7	25.4
272.	1.111E-03	2.589E-03	1.1786	0.495	298.	0.993	31.2	13.0	27.0	25.7
285.	1.107E-03	2.581E-03	1.1786	0.495	298.	0.709	31.3	13.3	27.4	26.0
297.	1.103E-03	2.572E-03	1.1786	0.495	298.	0.431	31.3	13.6	27.7	26.3
310.	1.100E-03	2.564E-03	1.1786	0.495	298.	0.160	31.4	13.9	28.0	26.6

26.7	28.1	14.1	31.5	0.000E+00	298.	0.495	1.1786	2.555E-03	1.096E-03	323.
27.4	28.9	14.5	31.6	0.000E+00	298.	0.495	1.1786	2.468E-03	1.059E-03	342.
28.1	29.7	15.0	31.7	0.000E+00	298.	0.495	1.1785	2.386E-03	1.024E-03	361.
29.0	30.7	15.6	31.9	0.000E+00	298.	0.495	1.1785	2.280E-03	9.779E-04	387.
29.5	31.2	15.8	31.9	0.000E+00	298.	0.495	1.1785	2.230E-03	9.564E-04	400.
30.4	32.1	16.4	32.1	0.000E+00	298.	0.495	1.1784	2.135E-03	9.157E-04	425.
31.3	33.1	17.0	32.3	0.000E+00	298.	0.495	1.1784	2.047E-03	8.779E-04	451.
32.1	34.0	17.6	32.4	0.000E+00	298.	0.495	1.1783	1.964E-03	8.426E-04	477.
33.0	35.0	18.2	32.6	0.000E+00	298.	0.495	1.1783	1.888E-03	8.097E-04	502.
33.9	35.9	18.8	32.8	0.000E+00	298.	0.495	1.1783	1.816E-03	7.788E-04	528.
34.7	36.8	19.3	32.9	0.000E+00	298.	0.495	1.1782	1.748E-03	7.499E-04	553.
35.5	37.7	19.9	33.1	0.000E+00	298.	0.495	1.1782	1.685E-03	7.226E-04	579.
36.3	38.6	20.5	33.3	0.000E+00	298.	0.495	1.1782	1.625E-03	6.970E-04	605.
37.1	39.5	21.1	33.5	0.000E+00	298.	0.495	1.1781	1.569E-03	6.728E-04	630.
37.9	40.4	21.6	33.6	0.000E+00	298.	0.495	1.1781	1.515E-03	6.499E-04	656.
38.7	41.2	22.2	33.8	0.000E+00	298.	0.495	1.1781	1.465E-03	6.283E-04	681.
39.5	42.1	22.8	34.0	0.000E+00	298.	0.495	1.1781	1.417E-03	6.077E-04	707.
40.2	42.9	23.3	34.2	0.000E+00	298.	0.495	1.1780	1.371E-03	5.882E-04	733.
41.0	43.7	23.9	34.4	0.000E+00	298.	0.495	1.1780	1.328E-03	5.697E-04	758.
41.7	44.5	24.5	34.6	0.000E+00	298.	0.495	1.1780	1.287E-03	5.521E-04	784.
42.5	45.3	25.0	34.8	0.000E+00	298.	0.495	1.1780	1.248E-03	5.353E-04	809.
43.2	46.1	25.6	35.0	0.000E+00	298.	0.495	1.1780	1.211E-03	5.193E-04	835.
43.9	46.6	26.1	35.2	0.000E+00	298.	0.495	1.1779	1.175E-03	5.040E-04	861.
44.9	48.1	27.0	35.5	0.000E+00	298.	0.495	1.1779	1.124E-03	4.823E-04	899.
45.9	49.2	27.8	35.8	0.000E+00	298.	0.495	1.1779	1.077E-03	4.621E-04	937.
46.9	50.4	28.6	36.1	0.000E+00	298.	0.495	1.1779	1.033E-03	4.431E-04	976.
47.9	51.5	29.4	36.5	0.000E+00	298.	0.494	1.1779	9.913E-04	4.252E-04	1.014E+03
48.9	52.5	30.3	36.8	0.000E+00	298.	0.494	1.1778	9.522E-04	4.084E-04	1.053E+03
49.8	53.6	31.1	37.1	0.000E+00	298.	0.494	1.1778	9.153E-04	3.926E-04	1.091E+03
50.7	54.7	31.9	37.4	0.000E+00	298.	0.494	1.1778	8.805E-04	3.777E-04	1.129E+03
51.6	55.7	32.7	37.8	0.000E+00	298.	0.494	1.1778	8.477E-04	3.636E-04	1.168E+03
52.5	56.7	33.5	38.1	0.000E+00	298.	0.494	1.1778	8.167E-04	3.503E-04	1.206E+03
53.4	57.7	34.3	38.4	0.000E+00	298.	0.494	1.1778	7.873E-04	3.377E-04	1.245E+03
54.2	58.7	35.1	38.8	0.000E+00	298.	0.494	1.1777	7.594E-04	3.257E-04	1.283E+03
55.1	59.6	35.9	39.1	0.000E+00	298.	0.494	1.1777	7.330E-04	3.144E-04	1.321E+03
55.9	60.6	36.7	39.5	0.000E+00	298.	0.494	1.1777	7.079E-04	3.036E-04	1.360E+03
56.7	61.5	37.5	39.8	0.000E+00	298.	0.494	1.1777	6.840E-04	2.934E-04	1.398E+03
57.4	62.4	38.3	40.2	0.000E+00	298.	0.494	1.1777	6.613E-04	2.837E-04	1.437E+03
58.2	63.3	39.1	40.5	0.000E+00	298.	0.494	1.1777	6.397E-04	2.744E-04	1.475E+03
59.2	64.5	40.2	41.0	0.000E+00	298.	0.494	1.1777	6.124E-04	2.627E-04	1.526E+03
60.1	65.6	41.2	41.5	0.000E+00	298.	0.494	1.1777	5.869E-04	2.517E-04	1.577E+03
61.1	66.7	42.3	42.0	0.000E+00	298.	0.494	1.1776	5.628E-04	2.414E-04	1.629E+03
62.0	67.8	43.3	42.4	0.000E+00	298.	0.494	1.1776	5.401E-04	2.317E-04	1.680E+03
62.8	68.9	44.4	42.9	0.000E+00	298.	0.494	1.1776	5.188E-04	2.225E-04	1.731E+03
63.7	69.9	45.4	43.4	0.000E+00	298.	0.494	1.1776	4.986E-04	2.139E-04	1.782E+03
64.5	70.9	46.5	43.9	0.000E+00	298.	0.494	1.1776	4.796E-04	2.057E-04	1.833E+03
65.2	71.9	47.5	44.4	0.000E+00	298.	0.494	1.1776	4.616E-04	1.980E-04	1.885E+03
66.0	72.9	48.5	44.9	0.000E+00	298.	0.494	1.1776	4.446E-04	1.907E-04	1.936E+03

66.7	73.8	49.6	45.4	0.000E+00	298.	0.494	1.1776	4.284E-04	1.838E-04	1.987E+03
67.4	74.7	50.6	45.9	0.000E+00	298.	0.494	1.1776	4.131E-04	1.772E-04	2.038E+03
68.1	75.6	51.6	46.4	0.000E+00	298.	0.494	1.1776	3.986E-04	1.710E-04	2.089E+03
68.9	76.7	52.9	47.0	0.000E+00	298.	0.494	1.1776	3.815E-04	1.636E-04	2.153E+03
69.7	77.7	54.2	47.6	0.000E+00	298.	0.494	1.1775	3.654E-04	1.567E-04	2.217E+03
70.4	78.7	55.5	48.3	0.000E+00	298.	0.494	1.1775	3.502E-04	1.502E-04	2.281E+03
71.0	79.7	56.7	48.9	0.000E+00	298.	0.494	1.1775	3.360E-04	1.441E-04	2.345E+03
71.7	80.6	58.0	49.5	0.000E+00	298.	0.494	1.1775	3.226E-04	1.384E-04	2.409E+03
72.3	81.5	59.3	50.2	0.000E+00	298.	0.494	1.1775	3.100E-04	1.329E-04	2.473E+03
72.8	82.4	60.5	50.8	0.000E+00	298.	0.493	1.1775	2.980E-04	1.278E-04	2.537E+03
73.4	83.2	61.8	51.4	0.000E+00	298.	0.493	1.1775	2.867E-04	1.230E-04	2.601E+03
73.8	84.0	63.0	52.1	0.000E+00	298.	0.493	1.1775	2.760E-04	1.184E-04	2.665E+03
74.3	84.8	64.3	52.7	0.000E+00	298.	0.493	1.1775	2.659E-04	1.141E-04	2.729E+03
74.7	85.7	65.8	53.5	0.000E+00	298.	0.493	1.1775	2.545E-04	1.092E-04	2.806E+03
75.1	86.5	67.3	54.2	0.000E+00	298.	0.493	1.1775	2.438E-04	1.046E-04	2.883E+03
75.5	87.3	68.8	55.0	0.000E+00	298.	0.493	1.1775	2.337E-04	1.002E-04	2.960E+03
75.8	88.0	70.3	55.8	0.000E+00	298.	0.493	1.1775	2.242E-04	9.617E-05	3.037E+03
76.0	88.7	71.7	56.5	0.000E+00	298.	0.493	1.1775	2.153E-04	9.233E-05	3.113E+03
76.2	89.3	73.2	57.3	0.000E+00	298.	0.493	1.1775	2.068E-04	8.872E-05	3.190E+03
76.3	89.9	74.7	58.1	0.000E+00	298.	0.493	1.1775	1.989E-04	8.531E-05	3.267E+03
76.4	90.5	76.2	58.8	0.000E+00	298.	0.493	1.1775	1.914E-04	8.208E-05	3.344E+03
76.4	91.0	77.6	59.6	0.000E+00	298.	0.493	1.1775	1.843E-04	7.903E-05	3.421E+03
76.3	91.4	79.1	60.4	0.000E+00	298.	0.492	1.1775	1.775E-04	7.615E-05	3.497E+03
76.2	91.8	80.5	61.1	0.000E+00	298.	0.492	1.1775	1.712E-04	7.341E-05	3.574E+03
76.0	92.2	82.0	61.9	0.000E+00	298.	0.492	1.1774	1.651E-04	7.082E-05	3.651E+03
75.7	92.5	83.5	62.7	0.000E+00	298.	0.492	1.1774	1.594E-04	6.836E-05	3.728E+03
75.4	92.8	84.9	63.4	0.000E+00	298.	0.492	1.1774	1.539E-04	6.602E-05	3.805E+03
75.0	93.0	86.4	64.2	0.000E+00	298.	0.492	1.1774	1.487E-04	6.380E-05	3.881E+03
74.5	93.2	87.8	64.9	0.000E+00	298.	0.492	1.1774	1.438E-04	6.168E-05	3.958E+03
74.0	93.3	89.3	65.7	0.000E+00	298.	0.492	1.1774	1.391E-04	5.967E-05	4.035E+03
73.3	93.4	90.7	66.5	0.000E+00	298.	0.492	1.1774	1.346E-04	5.775E-05	4.112E+03
72.7	93.4	92.1	67.2	0.000E+00	298.	0.492	1.1774	1.304E-04	5.592E-05	4.189E+03
71.9	93.4	93.6	68.0	0.000E+00	298.	0.491	1.1774	1.263E-04	5.418E-05	4.265E+03
71.0	93.3	95.0	68.7	0.000E+00	298.	0.491	1.1774	1.224E-04	5.252E-05	4.342E+03
70.1	93.2	96.4	69.5	0.000E+00	298.	0.491	1.1774	1.187E-04	5.092E-05	4.419E+03
69.1	93.0	97.9	70.2	0.000E+00	298.	0.491	1.1774	1.152E-04	4.940E-05	4.496E+03
67.9	92.8	99.3	71.0	0.000E+00	298.	0.491	1.1774	1.118E-04	4.795E-05	4.573E+03
66.7	92.5	101.	71.7	0.000E+00	298.	0.491	1.1774	1.085E-04	4.656E-05	4.649E+03
65.4	92.2	102.	72.5	0.000E+00	298.	0.491	1.1774	1.054E-04	4.522E-05	4.726E+03
63.9	91.8	104.	73.2	0.000E+00	298.	0.491	1.1774	1.024E-04	4.394E-05	4.803E+03
62.3	91.4	105.	74.0	0.000E+00	298.	0.491	1.1774	9.959E-05	4.272E-05	4.880E+03
60.6	90.9	106.	74.7	0.000E+00	298.	0.490	1.1774	9.685E-05	4.154E-05	4.957E+03
58.8	90.4	108.	75.5	0.000E+00	298.	0.490	1.1774	9.422E-05	4.041E-05	5.033E+03
56.7	89.7	109.	76.2	0.000E+00	298.	0.490	1.1774	9.170E-05	3.933E-05	5.110E+03
54.6	89.1	111.	76.9	0.000E+00	298.	0.490	1.1774	8.927E-05	3.829E-05	5.187E+03
52.2	88.4	112.	77.7	0.000E+00	298.	0.490	1.1774	8.694E-05	3.729E-05	5.264E+03
49.5	87.6	113.	78.4	0.000E+00	298.	0.490	1.1774	8.469E-05	3.613E-05	5.341E+03

5.417E+03	3.540E-05	8.253E-05	1.1774	0.490	298.	0.000E+00	79.1	115.	86.7	46.6
5.494E+03	3.451E-05	8.046E-05	1.1774	0.489	298.	0.000E+00	79.9	116.	85.8	43.4
5.571E+03	3.365E-05	7.845E-05	1.1774	0.489	298.	0.000E+00	80.6	118.	84.8	39.7
5.648E+03	3.282E-05	7.653E-05	1.1774	0.489	298.	0.000E+00	81.3	119.	83.7	35.6
5.725E+03	3.203E-05	7.467E-05	1.1774	0.489	298.	0.000E+00	82.1	120.	82.6	30.6
5.801E+03	3.126E-05	7.287E-05	1.1774	0.489	298.	0.000E+00	82.8	122.	81.3	24.5
5.878E+03	3.052E-05	7.115E-05	1.1774	0.489	298.	0.000E+00	83.5	123.	80.0	15.8
5.955E+03	2.980E-05	6.948E-05	1.1774	0.489	298.	0.000E+00	84.3	125.	78.6	
6.032E+03	2.911E-05	6.786E-05	1.1774	0.488	298.	0.000E+00	85.0	126.	77.1	
6.109E+03	2.844E-05	6.631E-05	1.1774	0.488	298.	0.000E+00	85.7	127.	75.5	
6.185E+03	2.780E-05	6.480E-05	1.1774	0.488	298.	0.000E+00	86.4	129.	73.8	
6.262E+03	2.717E-05	6.335E-05	1.1774	0.488	298.	0.000E+00	87.1	130.	71.9	
6.339E+03	2.657E-05	6.195E-05	1.1774	0.488	298.	0.000E+00	87.9	131.	70.0	
6.416E+03	2.599E-05	6.059E-05	1.1774	0.488	298.	0.000E+00	88.6	133.	67.9	
6.493E+03	2.542E-05	5.927E-05	1.1774	0.488	298.	0.000E+00	89.3	134.	65.7	
6.569E+03	2.488E-05	5.800E-05	1.1774	0.487	298.	0.000E+00	90.0	136.	63.3	
6.646E+03	2.435E-05	5.676E-05	1.1774	0.487	298.	0.000E+00	90.7	137.	60.7	
6.723E+03	2.384E-05	5.557E-05	1.1774	0.487	298.	0.000E+00	91.4	138.	57.9	
6.800E+03	2.334E-05	5.441E-05	1.1774	0.487	298.	0.000E+00	92.1	140.	54.8	
6.877E+03	2.286E-05	5.329E-05	1.1774	0.487	298.	0.000E+00	92.8	141.	51.5	
6.953E+03	2.239E-05	5.220E-05	1.1774	0.486	298.	0.000E+00	93.5	142.	47.8	
7.030E+03	2.194E-05	5.114E-05	1.1774	0.486	298.	0.000E+00	94.2	144.	43.6	
7.107E+03	2.150E-05	5.013E-05	1.1774	0.486	298.	0.000E+00	94.9	145.	38.9	
7.184E+03	2.107E-05	4.913E-05	1.1774	0.486	298.	0.000E+00	95.6	147.	33.4	
7.261E+03	2.066E-05	4.817E-05	1.1774	0.486	298.	0.000E+00	96.3	148.	26.5	
7.337E+03	2.026E-05	4.723E-05	1.1774	0.486	298.	0.000E+00	97.0	149.	16.6	
7.414E+03	1.987E-05	4.633E-05	1.1774	0.485	298.	0.000E+00	97.7	151.		
7.491E+03	1.949E-05	4.544E-05	1.1774	0.485	298.	0.000E+00	98.4	152.		
7.568E+03	1.912E-05	4.458E-05	1.1774	0.485	298.	0.000E+00	99.1	153.		
7.645E+03	1.877E-05	4.375E-05	1.1774	0.485	298.	0.000E+00	99.8	155.		
7.721E+03	1.842E-05	4.294E-05	1.1774	0.485	298.	0.000E+00	101.	156.		
7.798E+03	1.808E-05	4.215E-05	1.1774	0.484	298.	0.000E+00	101.	157.		
7.875E+03	1.775E-05	4.139E-05	1.1774	0.484	298.	0.000E+00	102.	159.		
7.952E+03	1.743E-05	4.064E-05	1.1774	0.484	298.	0.000E+00	103.	160.		
8.029E+03	1.712E-05	3.991E-05	1.1774	0.484	298.	0.000E+00	103.	161.		
8.105E+03	1.682E-05	3.921E-05	1.1774	0.484	298.	0.000E+00	104.	163.		
8.182E+03	1.652E-05	3.852E-05	1.1774	0.484	298.	0.000E+00	105.	164.		
8.259E+03	1.623E-05	3.785E-05	1.1774	0.483	298.	0.000E+00	105.	165.		
8.336E+03	1.595E-05	3.719E-05	1.1774	0.483	298.	0.000E+00	106.	167.		
8.413E+03	1.568E-05	3.656E-05	1.1774	0.483	298.	0.000E+00	107.	168.		
8.489E+03	1.541E-05	3.594E-05	1.1774	0.483	298.	0.000E+00	107.	169.		
8.566E+03	1.516E-05	3.533E-05	1.1774	0.482	298.	0.000E+00	108.	171.		
8.643E+03	1.490E-05	3.474E-05	1.1774	0.482	298.	0.000E+00	109.	172.		
8.720E+03	1.466E-05	3.417E-05	1.1774	0.482	298.	0.000E+00	109.	173.		
8.797E+03	1.442E-05	3.361E-05	1.1774	0.482	298.	0.000E+00	110.	175.		
8.873E+03	1.418E-05	3.306E-05	1.1774	0.482	298.	0.000E+00	111.	176.		
8.950E+03	1.395E-05	3.253E-05	1.1774	0.481	298.	0.000E+00	111.	177.		

9.027E+03	1.373E-05	3.201E-05	1.1774	0.481	298.	0.000E+00	112.	179.
9.104E+03	1.351E-05	3.150E-05	1.1774	0.481	298.	0.000E+00	113.	180.
9.181E+03	1.330E-05	3.100E-05	1.1774	0.481	298.	0.000E+00	113.	181.
9.257E+03	1.309E-05	3.052E-05	1.1774	0.481	298.	0.000E+00	114.	183.
9.334E+03	1.289E-05	3.005E-05	1.1774	0.480	298.	0.000E+00	115.	184.
9.411E+03	1.269E-05	2.958E-05	1.1774	0.480	298.	0.000E+00	115.	185.
9.488E+03	1.250E-05	2.913E-05	1.1774	0.480	298.	0.000E+00	116.	187.
9.565E+03	1.231E-05	2.869E-05	1.1774	0.480	298.	0.000E+00	117.	188.
9.641E+03	1.212E-05	2.826E-05	1.1774	0.479	298.	0.000E+00	117.	189.
9.718E+03	1.194E-05	2.784E-05	1.1774	0.479	298.	0.000E+00	118.	191.
9.795E+03	1.176E-05	2.742E-05	1.1774	0.479	298.	0.000E+00	119.	192.
9.872E+03	1.159E-05	2.702E-05	1.1774	0.479	298.	0.000E+00	119.	193.
9.949E+03	1.142E-05	2.663E-05	1.1774	0.478	298.	0.000E+00	120.	195.
1.003E+04	1.126E-05	2.624E-05	1.1774	0.478	298.	0.000E+00	121.	196.
1.010E+04	1.109E-05	2.586E-05	1.1774	0.478	298.	0.000E+00	121.	197.
1.018E+04	1.094E-05	2.549E-05	1.1774	0.478	298.	0.000E+00	122.	199.
1.026E+04	1.078E-05	2.513E-05	1.1774	0.477	298.	0.000E+00	123.	200.
1.033E+04	1.063E-05	2.478E-05	1.1774	0.477	298.	0.000E+00	123.	201.
1.041E+04	1.048E-05	2.443E-05	1.1774	0.477	298.	0.000E+00	124.	202.
1.049E+04	1.033E-05	2.409E-05	1.1774	0.477	298.	0.000E+00	125.	204.
1.056E+04	1.019E-05	2.376E-05	1.1774	0.476	298.	0.000E+00	125.	205.
1.064E+04	1.005E-05	2.344E-05	1.1774	0.476	298.	0.000E+00	126.	206.
1.068E+04	9.984E-06	2.328E-05	1.1774	0.476	298.	0.000E+00	126.	207.

For the UFL of 3.00000E-03 mole percent, and the LFL of 2.00000E-03 mole percent:

The mass of contaminant between the UFL and LFL is: 1213.3   kg.

The mass of contaminant above the LFL is: 6662.1   kg.

TECHNICAL REPORT DATA
(Please read Instructions on the reverse before completing)

1. REPORT NO. EPA 450/4-88-006b	2.	3. RECIPIENT'S ACCESSION NO.
4. TITLE AND SUBTITLE A Dispersion Model for Elevated Dense Gas Jet Chemical Releases--Volume II, User's Guide		5. REPORT DATE April 1988
		6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S) Dr. Jerry Havens		8. PERFORMING ORGANIZATION REPORT NO.
9. PERFORMING ORGANIZATION NAME AND ADDRESS		10. PROGRAM ELEMENT NO.
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12. SPONSORING AGENCY NAME AND ADDRESS U.S. Environmental Protection Agency Office of Air Quality Planning and Standards Source Receptor Analysis Branch Research Triangle Park, N.C. 27711		13. TYPE OF REPORT AND PERIOD COVERED
		14. SPONSORING AGENCY CODE

15. SUPPLEMENTARY NOTES

EPA Project Officer: Dave Guinnup

16. ABSTRACT

   This document is the second of two volumes describing the development and use of a computer program designed to model the dispersion of heavier-than-air gases which are emitted into the atmosphere with significant velocity through elevated ports. Volume II addresses the user aspects of the program, discussing model inputs and outputs and describing the installation of the code onto the user's VAX computer. An example simulation is carried out to provide the user with a benchmark for the model's operation.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
Air pollution Dense gas Mathematical model Computer model	Dispersion Elevated sources	

18. DISTRIBUTION STATEMENT Release unlimited	19. SECURITY CLASS *(This Report)*	21. NO. OF PAGES 394
	20. SECURITY CLASS *(This page)*	22. PRICE

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