

ADDENDUM

**USER'S GUIDE FOR THE  
INDUSTRIAL SOURCE COMPLEX (ISC3) DISPERSION MODELS**

**VOLUME I - USER INSTRUCTIONS**

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## **USER INSTRUCTIONS FOR THE REVISED ISCST3 MODEL (DATED 02035)**

This document provides user instructions for recent enhancements of the ISCST3 model, including the most recent version dated 02035 (February 4, 2002). The enhancements described in this Addendum include changes to the processing of multi-year averages for post-1997 PM<sub>10</sub> NAAQS analyses, enhancements to the model which were formerly available in draft form as ISCST390 (dated 97365), enhancements to the model for air toxics applications, and an option to specify variable emission rate factors that vary by season, hour-of-day, and day-of-week. The enhancements from the draft ISCST390 model include a conversion to Fortran 90 in order to make use of allocatable arrays for data storage, incorporation of the EVENT processing from the ISCEV3 model, an INCLUDED keyword option for the source, receptor and event pathways, and two new options for specifying area sources. The use of allocatable arrays provides much more flexibility for the end user of the ISCST3 model. The enhancements for air toxics applications include the Sampled Chronological Input Model (SCIM) option, optimizations for the area source and dry depletion algorithms, inclusion of the gas dry deposition algorithms based on the draft GDISCDFT model (dated 96248), and the option to output results by season and hour-of-day (SEASONHR). User instructions for these enhancements are provided below.

### **ENHANCEMENTS INTRODUCED WITH ISCST3 (DATED 98348)**

#### Post-1997 PM<sub>10</sub> Processing

A new NAAQS for modeling PM<sub>10</sub> was promulgated in July 1997. This guidance utilizes the expected second high value of the 24-hour NAAQS replaced by a 3-year average of the 99th percentile value of the frequency distribution and a 3-year average of the annual mean. Since the Guideline on Air Quality Modeling precludes the use of a 3-year data set, a policy was established that uses unbiased estimates of the 3-year averages, utilizing all meteorological data (both single and multiple years of data) available. An unbiased estimate of the 99th percentile is the fourth highest concentration, if one year of meteorological data are input to the model, or the multi-year average of the fourth highest concentrations, if more than one year of meteorological data are input to the model. Similarly, an unbiased estimate of the 3-year average annual mean is simply the annual mean, if only one year of meteorological data are input to the model, or the multi-year average annual mean if multiple years of meteorological data are used. Analogously to the original NAAQS situation, the entire area is in compliance when the highest fourth high (or highest average fourth high) and the highest annual mean (or the highest average annual mean) are less than or equal to the NAAQS.

The revised ISCST3 model will process the 24-hour and annual averages for PM<sub>10</sub> according to the new NAAQS if the pollutant ID specified on the CO POLLUTID card is

PM10 or PM-10, and the CO MULTYEAR card is not present. In this case, the model will compute an average of the fourth highest concentrations at each receptor across the number of years of meteorological data being processed. For a single year of data, the model will report the fourth highest concentration at each receptor. For a five year period of data, the model will report the average of the five fourth-highest values at each receptor. Also, for multiple year data files, the annual average will first be calculated for each individual year of data, and the average of these across the number of years will be calculated. This processing of the annual average across multiple years may give slightly different results than the PERIOD average across the same time period, due to differences in the number of calms from year to year. In order to accommodate this difference, the new PM<sub>10</sub> NAAQS makes use of the ANNUAL average keyword for specifying the long-term average.

Users should be aware of the following restrictions which are applied to the new PM<sub>10</sub> NAAQS processing.

1. The averaging periods are limited to the 24-hour and ANNUAL averages. Use of the PERIOD average or a short-term average other than 24-hour will result in a fatal error message being generated.
2. Only the FOURTH (or 4TH) highest value may be requested on the RECTABLE card for 24-hour averages. Specifying another high value on the RECTABLE card will result in a fatal error message being generated.
3. The model will only process complete years of meteorological data, although there is no restriction on the start date for the data. If less than one complete year of data is processed, a fatal error message will be generated. If additional meteorological data remains after the end of the last complete year of data, the remaining data will be ignored, and a non-fatal warning message will be generated specifying the number of hours ignored.
4. The MULTYEAR card cannot be used with the new PM<sub>10</sub> NAAQS. Multiple year analyses should be accomplished by including the multiple years of meteorology in a single data file.
5. Since the 24-hour average design values for post-1997 PM<sub>10</sub> analyses may consist of averages over a multi-year period, they are incompatible with the EVENT processor. If the MAXIFILE option is used to output 24-hour average threshold violations, these may be used with the EVENT processor. Therefore, if the EVENTFIL option is used without the MAXIFILE option for post-1997 PM<sub>10</sub> analyses, a non-fatal warning message will be generated, and the EVENTFIL option will be ignored.

The revised ISCST3 model may still be used to perform PM<sub>10</sub> analyses according to the pre-1997 NAAQS. This may be accomplished as before by use of the

MULTYEAR card on the CO pathway, except that the syntax for this keyword has been changed slightly. The syntax and type are now as follows:

<b>Syntax:</b>	CO MULTYEAR <u>H6H</u> Savfil (Inifil)
<b>Type:</b>	Optional, Non-repeatable

where H6H is a new secondary keyword that identifies this as a pre-1997 analysis, the Savfil parameter specifies the filename for saving the results arrays at the end of each year of processing, and the Inifil parameter specifies the filename to use for initializing the results arrays at the beginning of the current year. The Inifil parameter is optional, and should be left blank for the first year in the multi-year series of runs. Other than the additional secondary keyword of H6H, the MULTYEAR card works the same as in previous versions of ISCST3. A non-fatal warning message will be generated if the MULTYEAR card is used for pre-1997 NAAQS analyses.

### Memory Allocation

The revised ISCST3 model will allocate data storage as needed based on the number of sources, receptors, source groups, and other input requirements, up to the maximum amount of memory available on the computer being used. The minimum system requirements for this version of the model are a 386 or higher processor with a math coprocessor and at least 2 MB of extended memory.

The revised ISCST3 model uses allocatable arrays to allocate data storage at model runtime rather than at compile time, as done by the previous version of ISCST3. The ISCST3 model preprocesses the model runstream input file to determine the data storage requirements for a particular model run, and then allocates the input data arrays before processing the setup data. Once the setup processing is completed, the model allocates storage for the result arrays. When allocating data storage, the ISCST3 model traps for errors, e.g., not enough memory available to allocate. If the allocation is unsuccessful, then an error message is generated by the model and further processing is prevented. If the CO RUNORNOT NOT option is selected, the model will still go through all array allocations so that the user can determine if sufficient memory is available to complete the run. Also, an estimate of the total amount of memory needed for a particular run is printed out as part of the first page of printed output.

The parameters that are established at model runtime are as follows:

- NSRC           = Number of Sources
- NREC           = Number of Receptors
- NGRP           = Number of Source Groups
- NAVE           = Number of Short Term Averaging Periods
- NVAL           = Number of High Values by Receptor (RECTABLE Keyword)
- NTYP           = Number of Output Types (CONC, DEPOS, DDEP and WDEP)

NMAX	= Number of Overall Maximum Values (MAXTABLE Keyword)
NQF	= Number of Variable Emission Rate Factors Per Source
NPDMAX	= Number of Particle Diameter Categories Per Source
IXM	= Number of X-coord (Distance) Values Per Receptor Network
IYM	= Number of Y-coord (Direction) Values Per Receptor Network
NNET	= Number of Cartesian and/or Polar Receptor Networks
NEVE	= Number of Events for EVENT processing

In the case of NPDMAX, if no particle information is present in the input runstream, then NPDMAX is set to 1, otherwise it is set to 20. Other parameters are set to the actual numbers required for a particular model run.

A change has also been made that affects the length of filenames that may be specified in the ISCST3 model input file. A new PARAMETER called ILEN\_FLD has been added to MODULE MAIN1 in MODULES.FOR, which is initially assigned a value of 80. This PARAMETER is now used to specify the maximum length of individual fields on the input runstream image, and also to declare the length of all filename and format variables. This includes the input and output filenames specified on the command line.

### EVENT Processing

The revised ISCST3 model incorporates the EVENT processing from the ISCEV3 model. Currently, ISCST3 can be run in either the original ISCST3 mode or in the ISCEV3 mode for a particular model run. The input requirements of each mode are the same as for the original ISCST3 and ISCEV3 models, respectively. In other words, ISCST3 will accept input files that have been setup for either ISCST3 or ISCEV3.

### INCLUDED Option

The INCLUDED keyword option allows for the user to incorporate source, receptor, and/or event data from a separate file into an ISCST3 model runstream file. Multiple INCLUDED cards may be placed anywhere within the source, receptor and/or event pathway, after the STARTING card and before the FINISHED card (i.e., the STARTING and FINISHED cards cannot be included in the external file). The data in the included file will be processed as though it were part of the runstream file. The syntax and type of the INCLUDED keyword are summarized below:

<b>Syntax:</b>	SO INCLUDED Incfil RE INCLUDED Incfil EV INCLUDED Incfil
<b>Type:</b>	Optional, Repeatable

where the Incfil parameter is a character field of up to 80 characters (controlled by the ILEN\_FLD PARAMETER in MAIN1) that identifies the filename for the included file.

The contents of the included file must be valid runstream images for the applicable pathway. If an error is generated during processing of the included file, the error message will report the line number of the included file. If more than one INCLUDED file is specified for a particular pathway, the user will first need to determine which file the error occurred in.

### AREAPOLY and AREACIRC Source Type Options

The ISCST3 model includes two new options for specifying area sources. These are identified by the AREAPOLY and AREACIRC source types on the SO LOCATION keyword. The syntax, type and order of the LOCATION keyword are summarized below:

<b>Syntax:</b>	SO LOCATION Srcid Srctyp Xs Ys (Zs)
<b>Type:</b>	Mandatory, Repeatable
<b>Order:</b>	Must be first card for each source input

where the Srcid parameter is the alphanumeric source ID defined by the user (up to eight characters), Srctyp is the source type, which is identified by one of the secondary keywords - POINT, VOLUME, AREA, AREAPOLY, or AREACIRC - and Xs, Ys, and Zs are the x, y, and z coordinates of the source location in meters. All three of the area source types use the same numerical integration algorithm for estimating impacts from area sources, and are merely different options for specifying the shape of the area source. The AREA source keyword may be used to specify a rectangular-shaped area source with arbitrary orientation; the AREAPOLY source keyword may be used to specify an area source as an irregularly-shaped polygon of up to 20 sides; and the AREACIRC source keyword may be used to specify a circular-shaped area source (modeled as an equal-area polygon of up to 20 sides). Note that the source elevation, Zs, is an optional parameter. The x (east-west) and y (north-south) coordinates are for the center of the source for POINT, VOLUME, and AREACIRC sources, and are for one of the vertices of the source for AREA and AREAPOLY sources. The source coordinates may be input as Universal Transverse Mercator (UTM) coordinates, or may be referenced to a user-defined origin.

The main source parameters for the AREAPOLY and AREACIRC source types are input on the SRCPARAM card, which is a mandatory keyword for each source being modeled. These inputs are described below

### AREAPOLY Source Type

The AREAPOLY source type may be used to specify an area source as an arbitrarily-shaped polygon of between 3 and 20 sides (the number of sides allowed may be increased by modifying the NVMAX and NVMAX2 parameters in MODULES.FOR). This source type option provides the user with considerable flexibility for specifying the shape of an area source. The syntax, type and order for the SRCPARAM card for AREAPOLY sources are summarized below:

<b>Syntax:</b>	SO SRCPARAM Srcid Aremis Relhgt Nverts (Szinit)
<b>Type:</b>	Mandatory, Repeatable
<b>Order:</b>	Must follow the LOCATION card for each source input

where the Srcid parameter is the same source ID that was entered on the LOCATION card for a particular source, and the other parameters are as follows:

- Aremis - area emission rate in  $g/(s \cdot m^2)$ ,
- Relhgt - release height above ground in meters,
- Nverts - number of vertices (or sides) of the area source polygon,
- Szinit - initial vertical dimension of the area source plume in meters (optional).

As with AREA sources, the emission rate for the source is an emission rate per unit area, which is different from the point and volume source emission rates, which are total emission rates (g/s) for the source. The number of vertices (or sides) used to define the area source polygon may vary between 3 and 20. The locations of the vertices are specified by use of the AREAVERT keyword, which applies only to AREAPOLY sources. The syntax, type and order for the AREAVERT keyword used for AREAPOLY sources are summarized below:

<b>Syntax:</b>	SO AREAVERT Srcid Xv(1) Yv(1) Xv(2) Yv(2) ... Xv(I) Yv(I)
<b>Type:</b>	Mandatory for <u>AREAPOLY</u> sources, Repeatable
<b>Order:</b>	Must follow the LOCATION and SRCPARAM card for each source input

where the Xv(I) and Yv(I) are the x-coordinate and y-coordinate values of the vertices of the area source polygon. There must be Nverts pairs of coordinates for the area source, where Nverts is the number of vertices specified for that source on the SRCPARAM card. The first vertex, Xv(1) and Yv(1), must also match the coordinates given for the source location on the LOCATION card, Xs and Ys. The remaining vertices may be defined in either a clockwise or counter-clockwise order from the point used for defining the source location.

### AREACIRC Source Type

The AREACIRC source type may be used to specify an area source as a circular shape. The model will automatically generate a regular polygon of up to 20 sides to approximate the circular area source. The polygon will have the same area as that specified for the circle. The syntax, type and order for the SRCPARAM card for AREACIRC sources are summarized below:

<b>Syntax:</b>	SO SRCPARAM Srcid Aremis Relhgt Radius (Nverts) (Szinit)
<b>Type:</b>	Mandatory, Repeatable
<b>Order:</b>	Must follow the LOCATION card for each source input

where the Srcid parameter is the same source ID that was entered on the LOCATION card for a particular source, and the other parameters are as follows:

- Aremis - area emission rate in  $g/(s\cdot m^2)$ ,
- Relhgt - release height above ground in meters,
- Radius - radius of the circular area in meters,
- Nverts - number of vertices (or sides) of the area source polygon (optional, 20 sides will be used if omitted),
- Szinit - initial vertical dimension of the area source plume in meters (optional).

As with AREA sources, the emission rate for the source is an emission rate per unit area, which is different from the point and volume source emission rates, which are total emission rates (g/s) for the source.

## **ENHANCEMENTS INTRODUCED WITH ISCST3 (DATED 99155)**

### TOXICS Option

The revised ISCST3 model includes enhancements for air toxics applications. These enhancements include the Sampled Chronological Input Model (SCIM) option, optimizations for the area source and dry depletion algorithms, inclusion of the gas dry deposition algorithms based on the draft GDISCDFT model (dated 96248), and the option to output results by season and hour-of-day (SEASONHR). In order to utilize these enhancements, the user must include the TOXICS keyword on the CO MODELOPT card. Since the TOXICS option is a non-regulatory default option, the DFAULT keyword should not be included on the MODELOPT card. If the DFAULT keyword is present on the MODELOPT card, the DFAULT option will override the TOXICS option if it is present, and any other enhancements dependent on the TOXICS option. The enhancements associated with the TOXICS option are described below.

### Sampled Chronological Input Model (SCIM) Option

If the non-default TOXICS option is specified, the user may also use the SCIM option to reduce model runtime. The SCIM option can only be used with the ANNUAL average option, and is primarily applicable to multi-year model simulations. The

approach used by the SCIM option is to sample the meteorological data at a user-specified regular interval to approximate the long-term (i.e., ANNUAL) average impacts. Since wet deposition does not occur at regular intervals, the user can also specify a separate wet sampling interval to reduce the uncertainty introduced by sampling for wet deposition. The DEPOS option is ignored when SCIM is selected because, depending upon whether or not the user selected the separate wet hour sampling, the dry deposition and wet deposition rates can be based on different sets of sampled hours. Therefore, the annualized deposition rates for the two types of deposition are calculated separately. For this reason, the user is advised to calculate dry and wet deposition rates separately (using DDEP and WDEP, respectively) and add the two to obtain the total deposition rate when the SCIM option is used. Studies have shown that the uncertainty in modeled results introduced by use of the SCIM option is generally lower for area sources than for point sources.

When only the regular sampling is selected, all hourly impacts (concentration, dry deposition flux and the wet deposition flux) are calculated in the normal fashion for each sampled hour. The annual average concentration is then simply calculated by dividing the cumulative concentration for the sampled hours by the number of hours sampled (arithmetic average), and the annual dry and the wet deposition fluxes are calculated by scaling the respective cumulative fluxes for the sampled hours by the ratio of the total hours to the sampled hours. The following illustrates the calculation of the ANNUAL impacts when only the regular sampling is selected:

$$\begin{aligned}
 C &= \Sigma C_s / N_s \\
 D &= \Sigma D_s (N_t / N_s) \\
 W &= \Sigma W_s (N_t / N_s)
 \end{aligned}$$

where:

$C, D, W$  = Calculated conc, dry flux and wet flux, respectively  
 $\Sigma C_s, \Sigma D_s, \Sigma W_s$  = Cumulative impacts for the sampled hours  
 $N_s$  = Number of sampled hours  
 $N_t$  = Total number of hours in the data period

When the wet hour sampling is also selected along with regular sampling, the impacts are calculated slightly differently. The concentrations and the dry deposition fluxes are based on the weighted contributions from the regular samples, modeled as dry hours, and the wet hour samples. The regular samples consist of all the hours based on regular sampling interval, but the effects of precipitation are ignored so that their contribution represents only dry conditions, while the contribution from the wet hour samples represents only wet conditions. The wet deposition fluxes are only based on the wet hour samples. The following illustrates the calculation of the ANNUAL impacts when both the regular sampling as well as the wet hour sampling are selected:

$$C = \frac{\sum C_d (N_{td}/N_{sd}) + \sum C_w (N_{tw}/N_{sw})}{N_t}$$

$$D = \sum D_d (N_{td}/N_{sd}) + \sum D_w (N_{tw}/N_{sw})$$

$$W = \sum W_w (N_{tw}/N_{sw})$$

where:

$C, D, W$  = Calculated conc, dry flux and wet flux, respectively

$\sum C_d, \sum D_d$  = Cumulative impacts for regular (dry) sampled hours

$\sum C_w, \sum D_w, \sum W_w$  = Cumulative impacts for sampled wet hours

$N_{sd}$  = Number of regular sampled hours, modeled as dry

$N_{sw}$  = Number of sampled wet hours

$N_{td}$  = Total number of dry hours in the data period

$N_{tw}$  = Total number of wet hours in the data period

$N_t$  = Total number of hours in the data period ( $N_{td} + N_{tw}$ )

To use the SCIM option, the user must include the SCIM and TOXICS keywords on the CO MODELOPT card, and also specify the SCIM sampling parameters on the ME SCIMBYHR card. The SCIM parameters on the SCIMBYHR card specify the starting hour and sampling interval for the regular or dry sample, and also for the wet sample if used. The syntax and type of the SCIMBYHR keyword are summarized below:

<b>Syntax:</b>	ME SCIMBYHR NRegStart NRegInt NWetStart NWetInt (Filnam)
<b>Type:</b>	Optional, Non-repeatable

where the NRegStart and NRegInt parameters specify the first hour to be sampled and the sampling interval when performing the regular sampling, respectively, and NWetStart and NWetInt parameters specify the first wet hour to sample and the wet hour sampling interval, respectively. Optionally, the user can create an output file by specifying the Filnam parameter containing the meteorological data for the sampled hours (in the same format used in the summary of the first 24 hours of data included in the main output file).

Although the ME SCIMBYHR is an optional card, it is required when using the SCIM option. NRegStart is required to have a value from 1 through 24, i.e., the first sampled hour must be on the first day in the meteorological data file. There are no restrictions for NRegInt; however, NRegInt would generally be greater than 1. For example, NRegInt could be based on the formula  $(24n+1)$ , where "n" is the number of days to skip between samples, in order to ensure a regular diurnal cycle to the sampled hours (e.g., 25 or 49). NWetStart must be no greater than NWetInt. An input of 0 (zero) for NWetInt indicates that the user has not selected the wet hour sampling.

## Optimized Area Source and Dry Depletion Algorithms

When the TOXICS option is specified, the area source and dry depletion integration routines are optimized to reduce model runtime. This is accomplished by incorporation of a 2-point Gaussian Quadrature routine for numerical integration for some situations instead of the Romberg numerical integration utilized in the regulatory default mode. In addition, for area sources with dry depletion, another optimization option is available to reduce model runtime by specifying the AREADPLT keyword on the CO MODELOPT card. When the AREADPLT option is specified the model will apply a single “effective” depletion factor to the undepleted area source integral, rather than applying the numerical integration for depletion within the area source integral. If AREADPLT is selected, the DRYDPLT option for non-area sources is automatically selected.

### Gas Dry Deposition Algorithm

The revised ISCST3 model has the option to model the effects of dry deposition for gaseous pollutants. In order to utilize this algorithm, the non-default TOXICS option must be specified on the CO MODELOPT card. There are three new keywords on the CO pathway and one new keyword on the SO pathway that are used for specifying inputs for the gas dry deposition algorithm. The user has the option of specifying the deposition velocity to be used with the CO GASDEPVD card, or allowing the model to calculate the deposition velocities. If the user does not specify the deposition velocity with the GASDEPVD keyword, then the state of vegetation must be specified with the CO VEGSTATE card, and the source parameters for gas deposition must be specified with the SO GASDEPOS card. The user also has the option to override certain default reference parameters through use of the CO GASDEPRF card. The inputs for these keywords are described below. The use of the gas dry deposition algorithm in ISCST3 also requires additional meteorological parameters, which can be provided by the MPRM meteorological preprocessor. The formats for the meteorological data input file for gas dry deposition applications is also described below.

### Specifying the State of Vegetation

An optional keyword is available on the Control pathway to allow the user to specify the state of vegetation for use with the gaseous dry deposition algorithm of the ISCST3 model. Three options are available on this keyword, one for active and unstressed vegetation, one for active and stressed vegetation, and another for inactive vegetation.

The syntax and type of the VEGSTATE keyword are summarized below:

<b>Syntax:</b>	CO VEGSTATE <u>UNSTRESSED</u> or <u>STRESSED</u> or <u>INACTIVE</u>
<b>Type:</b>	Optional, Non-repeatable

where the secondary keyword options describe the three options for the state of vegetation. The state of vegetation is used in the model, along with ambient temperature and incoming short-wave radiation, to determine the resistance to transport through the

stomatal pores. For unirrigated vegetation, the user should select the appropriate option for vegetation state based on existing soil moisture conditions. For irrigated vegetation, the user should assume that the vegetation is active and unstressed.

#### Option for Overriding Default Reference Parameters for Gas Dry Deposition

An optional keyword is available on the Control pathway to allow the user to override the default reference parameters of cuticle resistance, ground resistance, and pollutant reactivity for use with the gas dry deposition algorithm.

The syntax and type of the GASDEPRF keyword are summarized below:

<b>Syntax:</b>	CO GASDEPRF Rcutr Rgr Reactr (Refpoll)
<b>Type:</b>	Optional, Non-repeatable

where the parameter Rcutr is the reference value for cuticle resistance, Rgr is the reference value for ground resistance, Reactr is the reference value for pollutant reactivity, and Refpoll is the optional name of the reference pollutant. If the GASDEPRF keyword is omitted, then the following default reference values for SO<sub>2</sub> are used by the model: Rcutr = 30 s/cm; Rgr = 10 s/cm; and Reactr = 8.

#### Option for Specifying the Deposition Velocity for Gas Dry Deposition

An optional keyword is available on the Control pathway to allow the user to specify the deposition velocity for use with the gaseous dry deposition algorithm of the ISCST3 model. A single deposition velocity can be input for a given model run, and is used for all sources of gaseous pollutants. Selection of this option will by-pass the algorithm for computing deposition velocities for gaseous pollutants, and should only be used when sufficient data to run the algorithm are not available. Results of the ISCST3 model based on a user-specified deposition velocity should be used with extra caution.

The syntax and type of the GASDEPVD keyword are summarized below:

<b>Syntax:</b>	CO GASDEPVD Uservd
<b>Type:</b>	Optional, Non-repeatable

where the parameter Uservd is the gaseous dry deposition velocity (m/s). A non-fatal warning message is generated by the model if a value of Uservd greater than 0.05 m/s (5 cm/s) is input by the user. When the GASDEPVD keyword is used, the VEGSTATE and GASDEPRF keywords for the CO pathway, and the GASDEPOS keyword for the SO pathway, are no longer applicable and cannot be used in the same model run.

### Specifying Source Parameters for Gas Dry Deposition

The input of source parameters for gas dry deposition is controlled by the GASDEPOS keyword on the SO pathway. The gas dry deposition variables may be input for a single source, or may be applied to a range of sources.

The syntax, type, and order for the GASDEPOS keyword are summarized below:

<b>Syntax:</b>	SO GASDEPOS Srcid (or Srcrng) Diff Alphas Reac Rsubm Henry
<b>Type:</b>	Optional, Repeatable
<b>Order:</b>	Must follow the LOCATION card for each source input

where the Srcid or Srcrng identify the source or sources for which the inputs apply, the parameter Diff is the molecular diffusivity for the pollutant being modeled ( $\text{cm}^2/\text{s}$ ), Alphas is the solubility enhancement factor ( $\alpha_*$ ) for the pollutant, Reac is the pollutant reactivity parameter, Rsubm is the mesophyll resistance term ( $r_m$ ) for the pollutant ( $\text{s}/\text{cm}$ ), and Henry is the Henry's Law coefficient for the parameter. Values of these physical parameters for several common pollutants may be found in chemical engineering handbooks and various publications, such as the Air/Superfund National Technical Guidance Study Series (EPA, 1993). The Alphas and Henry parameters are only used when applying the algorithm over a water surface. If no water surfaces are present in a particular application, then dummy (non-zero) values may be input for Alphas and Henry. The model converts the input units for Diff to  $\text{m}^2/\text{s}$  and Rsubm to  $\text{s}/\text{m}$  before being used in the computations.

### Meteorological Formats for Gas Dry Deposition

Since the deposition algorithms require additional meteorological variables, the exact format of ASCII meteorological data will depend on whether the dry and/or wet deposition algorithms are being used. If the deposition algorithms are being used, then the unformatted data file cannot be used. The order of the meteorological variables for the formatted ASCII files and the default ASCII format are as follows when the CARD option is used:

ASCII Meteorological Formats With the <u>CARD</u> Option		
Variable	Fortran Format	Columns
Year (last 2 digits)	I2	1-2
Month	I2	3-4
Day	I2	5-6
Hour	I2	7-8
Flow Vector (deg.)	F9.4	9-17
Wind Speed (m/s)	F9.4	18-26
Ambient Temperature (K)	F6.1	27-32
Stability Class (A=1, B=2, ... F=6)	I2	33-34
Rural Mixing Height (m)	F7.1	35-41
Urban Mixing Height (m)	F7.1	42-48
Wind Profile Exponent ( <u>CARD</u> only)	F8.4	49-56
Vertical Potential Temperature Gradient (K/m) ( <u>CARD</u> only)	F8.4	57-65
Friction Velocity (m/s) (Dry or Wet Deposition Only)	F9.4	66-74
Monin-Obukhov Length (m) (Dry or Wet Deposition Only)	F10.1	75-84
Surface Roughness Length (m) (Dry or Wet Deposition Only)	F8.4	85-92
Incoming Short-wave Radiation (W/m <sup>2</sup> ) (Gas Dry Deposition Only)	F8.1	93-100
Leaf Area Index (Gas Dry Deposition Only)	F8.3	101-108
Precipitation Code (00-45) (Wet Deposition Only)	I4	109-112 (93-96 without Gas Dry Deposition)
Precipitation Rate (mm/hr) (Wet Deposition Only)	F7.2	113-119 (97-103 without Gas Dry Deposition)

The order and default format of the meteorological variables for the formatted ASCII files without the CARD option are as follows:

ASCII Meteorological Formats Without the <u>CARD</u> Option		
Variable	Fortran Format	Columns
Year (last 2 digits)	I2	1-2
Month	I2	3-4
Day	I2	5-6
Hour	I2	7-8
Flow Vector (deg.)	F9.4	9-17
Wind Speed (m/s)	F9.4	18-26
Ambient Temperature (K)	F6.1	27-32
Stability Class (A=1, B=2, ... F=6)	I2	33-34
Rural Mixing Height (m)	F7.1	35-41
Urban Mixing Height (m)	F7.1	42-48
Friction Velocity (m/s) (Dry or Wet Deposition Only)	F9.4	49-57
Monin-Obukhov Length (m) (Dry or Wet Deposition Only)	F10.1	58-67
Surface Roughness Length (m) (Dry or Wet Deposition Only)	F8.4	68-75
Incoming Short-wave Radiation ( $W/m^2$ ) (Gas Dry Deposition Only)	F8.1	76-83
Leaf Area Index (Gas Dry Deposition Only)	F8.3	84-91
Precipitation Code (00-45) (Wet Deposition Only)	I4	92-95 (76-79 without Gas Dry Deposition)
Precipitation Rate (mm/hr) (Wet Deposition Only)	F7.2	96-102 (80-86 without Gas Dry Deposition)

## Season by Hour-of-Day Output Option (SEASONHR)

When the non-default TOXICS option is specified, the user may request an output file containing the average results (CONC, DEPOS, DDEP and/or WDEP) by season and hour-of-day. To select this option, the user must include the SEASONHR keyword on the OU pathway. The syntax, type, and order for the SEASONHR keyword are summarized below:

<b>Syntax:</b>	OU SEASONHR GroupID FileName (FileUnit)
<b>Type:</b>	Optional, Repeatable

where the GroupID parameter specifies the source group to be output, FileName specifies the name of the output file, and the optional FileUnit parameter specifies an optional file unit and must be greater than 20. If FileUnit is left blank, then the model will dynamically assign a file unit based on the formula  $302 + \text{IGRP} * 10$ , where IGRP is the group index number. A sample from a SEASONHR output file is shown below:

```

* ISCST3 (99155): Example of SEASONHR Output File Option
* MODELING OPTIONS USED:
* CONC          WDEP    RURAL  FLAT          TOXICS          WETDPL
*      FILE OF SEASON/HOUR VALUES FOR SOURCE GROUP: ALL
*      FOR A TOTAL OF 216 RECEPTORS.
*      FORMAT: (4(1X,F13.5),1X,F8.2,2X,A8,2X,I4,2X,I4,2X,I4,2X,A8)
*      X          Y          AVERAGE CONC          WET DEPO          ZELEV          GRP          NHRS  SEAS  HOUR  NET ID
*
8.68241      49.24039      0.00000      0.00603      0.00      ALL      87      1      1  POL1
17.36482     98.48077      0.00000      0.00177      0.00      ALL      87      1      1  POL1
86.82409     492.40387     0.18098      0.00008      0.00      ALL      87      1      1  POL1
173.64818    984.80774     2.52520      0.00001      0.00      ALL      87      1      1  POL1
868.24091   4924.03857    2.07470      0.00000      0.00      ALL      87      1      1  POL1
1736.48181  9848.07715    0.93252      0.00000      0.00      ALL      87      1      1  POL1
17.10101     46.98463     0.00000      0.00002      0.00      ALL      87      1      1  POL1
34.20201     93.96926     0.00000      0.00000      0.00      ALL      87      1      1  POL1
171.01007    469.84631     0.15772      0.00000      0.00      ALL      87      1      1  POL1
342.02014    939.69263     2.48554      0.00000      0.00      ALL      87      1      1  POL1
1710.10071   4698.46289    6.09119      0.00000      0.00      ALL      87      1      1  POL1
3420.20142   9396.92578    4.49830      0.00000      0.00      ALL      87      1      1  POL1
25.00000     43.30127     0.00000      0.00017      0.00      ALL      87      1      1  POL1
50.00000     86.60254     0.00000      0.00001      0.00      ALL      87      1      1  POL1
250.00000    433.01270     0.10114      0.00000      0.00      ALL      87      1      1  POL1
500.00000    866.02539     2.12970      0.00000      0.00      ALL      87      1      1  POL1
2500.00000   4330.12695    2.79993      0.00000      0.00      ALL      87      1      1  POL1
5000.00000   8660.25391    1.97200      0.00000      0.00      ALL      87      1      1  POL1

```

The NHRS column in the output file contains the number of non-calm and non-missing hours used to calculate the season-by-hour-of-day averages. The SEAS column is the season index, and is 1 for winter, 2 for spring, 3 for summer and 4 for fall. The records loop through hour-of-day first, and then through the seasons.

## ENHANCEMENTS INTRODUCED WITH ISCST3 (DATED 00101)

## Removal of UNIFORM Option for Meteorological Data

The unformatted meteorological data option (ME INPUTFIL UNIFORM) is no longer supported by the ISCST3 model. Unnecessary code has been removed, and proper error handling has been implemented. Users with unformatted meteorological data should first convert the data to an ASCII format using the BINTOASC utility program available on the SCRAM website. The unformatted data file option has been removed for several reasons, including the fact that unformatted files are not portable across different computer systems and compilers, and that unformatted files cannot be used with the deposition algorithms in ISCST3.

## Season by Hour-of-Day and Day-of-Week Emission Factors

The variable emission rate factor option controlled by the EMISFACT keyword on the SO pathway has been modified to include an option to specify variable emission rate factors that vary by season, hour-of-day, and day-of-week. The day-of-week variability allows for different emission factors to be specified for Weekdays (Monday-Friday), Saturdays, and Sundays.

The syntax, type and order of the EMISFACT keyword are summarized below:

<b>Syntax:</b>	SO EMISFACT Srcid (or Srcrng) Qflag Qfact(i),i=1,n
<b>Type:</b>	Optional, Repeatable
<b>Order:</b>	Must follow the LOCATION card for each source input

where the Srcid parameter is the same source ID that was entered on the LOCATION card for a particular source. The user also has the option of using the Srcrng parameter for specifying a range of sources for which the emission rate factors apply, instead of identifying a single source. This is accomplished by two source ID character strings separated by a dash, e.g., STACK1-STACK10.

The parameter Qflag is the variable emission rate flag, and is one of the following secondary keywords:

- SEASON    emission rates vary seasonally (n=4),
- MONTH     emission rates vary monthly (n=12),
- HROFDY    emission rates vary by hour-of-day (n=24),
- STAR       emission rates vary by speed and stability category (n=36),
- SEASHR    emission rates vary by season and hour-of-day (n=96), and

SHRDOW emission rates vary by season, hour-of-day, and day-of-week [M-F, Sat., Sun.] (n=288)

The Qfact array is the array of factors, where the number of factors is shown above for each Qflag option. The EMISFACT card may be repeated as many times as necessary to input all of the factors, and repeat values may be used for the numerical inputs. An example of each of these options is presented below, with column headers to indicate the order in which values are to be input.

**				WINTER	SPRING	SUMMER	FALL											
SO	EMISFACT	STACK1	SEASON	0.50	0.50	1.00	0.75											
**				JAN	FEB	MAR	APR	MAY	JUN	JUL	AUG	SEP	OCT	NOV	DEC			
SO	EMISFACT	STACK1	MONTH	0.1	0.2	0.3	0.4	0.5	0.5	0.5	0.6	0.7	1.0	1.0	1.0			
**				1	2	3	4	5	6	7	8	9	10	11	12			
SO	EMISFACT	STACK1	HROFDY	0.0	0.0	0.0	0.0	0.0	0.5	1.0	1.0	1.0	1.0	1.0	1.0			
**				13	14	15	16	17	18	19	20	21	22	23	24			
SO	EMISFACT	STACK1	HROFDY	1.0	1.0	1.0	1.0	1.0	0.5	0.0	0.0	0.0	0.0	0.0	0.0			
**	or, equivalently:			1-5	6	7-17	18	19-24										
SO	EMISFACT	STACK1	HROFDY	5*0.0	0.5	11*1.0	0.5	6*0.0										
**		Stab. Cat.:		A	B	C	D	E	F	(6 WS Cat.)								
SO	EMISFACT	STACK1	STAR	6*0.5	6*0.6	6*0.7	6*0.8	6*0.9	6*1.0									
SO	EMISFACT	STACK1	SEASHR	enter 24 hourly scalars for each of the four seasons (winter, spring, summer, fall), e.g.,														
**				Winter	Spring	Summer	Fall											
SO	EMISFACT	STACK1	SEASHR	24*0.50	24*0.50	24*1.00	24*0.75											
SO	EMISFACT	STACK1	SHRDOW	enter 24 hourly scalars for each of the four seasons (winter, spring, summer, fall), first for Weekdays (Monday-Friday), then for Saturdays, and finally for Sundays, e.g.,														
**	Weekdays:			Winter	Spring	Summer	Fall											
SO	EMISFACT	STACK1	SHRDOW	24.1.0	24*0.8	24*0.6	24*0.8											
**	Saturdays:																	
SO	EMISFACT	STACK1	SHRDOW	24*0.5	24*0.4	24*0.3	24*0.4											
**	Sundays:																	
SO	EMISFACT	STACK1	SHRDOW	24*0.25	24*0.2	24*0.15	24*0.2											

## ENHANCEMENTS INTRODUCED WITH ISCST3 (DATED 02035)

### HE>ZI Option for Receptors Below Stack Base

A non-default option called HE>ZI has been added to the CO MODELOPT keyword to address a potential problem that may occur for cases when the receptor elevation is below the stack base elevation. In these cases the mixing height (ZI), which is terrain-following, may drop below the plume centerline height (HE), which is horizontal, resulting in anomalously large concentrations due to the actual plume approaching the centerline of one of the image plumes in the Vertical Term. When the HE>ZI option is specified on the CO MODELOPT card, the model limits the plume centerline height (HE) to be less than or equal to the mixing height (ZI) when calculating the Vertical Term. The model

also generates informational messages that identify when this adjustment has been made. Since HE>ZI is a non-default option, it will be overridden if the DFAULT option is specified.

### References

Environmental Protection Agency, 1993: Air/Superfund National Technical Guidance Study Series, Models for Estimating Air Emission Rates from Superfund Remedial Actions. EPA-451/R-93-001, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina 27711.