# **MODIFICATIONS TO THE**

# **CTDMPLUS AND CTSCREEN MODELS**

March 1993

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Since the release of CTDMPLUS/CTSCREEN (dated 91107), a number of problems have been discovered with the application of these This document is intended to inform model users of the models. nature of these problems and the manner in which they have been resolved. The new codes for CTDMPLUS/CTSCREEN (dated 93076) which incorporate the solutions to these problems are being made CTDMPLUS/CTSCREEN (dated 93076) available with this report. successfully passed through two months of beta-testing by a number The revised models have been reevaluated and of model users. comparisons with previous evaluation results are also presented here. It is important to note that some code changes are common to both CTDMPLUS and CTSCREEN and some are for CTSCREEN only. For further explanation of the terminology used in this report, readers are referred to the user's manuals for the models (Perry et al., 1989 and Perry et al., 1990).

### 1. MODIFICATIONS COMMON TO BOTH CTDMPLUS AND CTSCREEN

With one minor exception, the changes that are common to both models affect concentration calculations for stable/neutral conditions only. Changes that are unique to CTSCREEN affect calculations in both stable/neutral and convective conditions. A description of each problem encountered and a discussion of the change made to correct that problem are included here with a listing of the subroutines that required coding changes (the specific lines of code are not listed since they were often extensive).

1.1 WRAP CALCULATIONS IN THE BETA COORDINATE SYSTEM

CTDMPLUS	modules	modified:	DAYCALC.F	OR,	WRAPIN.	FOR,
			SEQMOD.FOR,	PASW	.CMN.	
CTSCREEN	modules	modified:	NITCALC.F	OR,	SEQSCR.	FOR,
			DAYSCR.FOR	ζ,	WRAPIN	.FOR,
			PASW.CMN			

Two problems have been identified that are related to the modeling of flow around the "elliptical terrain" in the stable WRAP calculations. These calculations are performed in a  $\beta$ -coordinate system which is illustrated in Figure 1. The  $\beta$ -axis is defined to be parallel to the stagnation streamline at the point where the streamline meets the ellipse (impingement or stagnation point). The origin of the  $\beta$ -axis is at the center of the WRAP ellipse (the ellipse representing the terrain for the level of interest). Travel time in the WRAP calculation is referenced along the  $x_{\beta}$  direction.

### 1.1.1a Problem

The first problem with the WRAP calculations concerns sources on the terrain that are located inside the WRAP ellipse. In CTDMPLUS/CTSCREEN (dated 91107), if the distance from the source to the hill-center is less than the length of the major axis of the ellipse, the major axis is set equal to just less than the sourceto-hill-center distance. This was intended to guarantee that the source is outside of the ellipse used to calculate horizontal flow distortions. This check was designed to avoid mathematical errors. Also, if this check results in the modified major axis being shorter than the minor axis, the minor axis is set equal to the major axis. Although some adjustment is necessary, the existing (91107) models' correction can result in considerably different flow characteristics than would be experienced about the original In addition, there are cases when a source is located ellipse. outside of the WRAP ellipse yet the source-to-hill-center distance is still less than the length of the major axis. The adjustment of the axes lengths for this situation is completely unnecessary. A better way of handling these sources close to or inside of the ellipse was needed.

# 1.1.2a Solution

In CTDMPLUS/CTSCREEN (dated 93076), the elliptical coordinates of the source are checked to see if the source is inside the WRAP ellipse. If so, the source is moved just outside of the ellipse by adjusting the value of  $x_{s\beta}$ , the source location in the  $\beta$ -coordinate system (Figure 1); this adjusted source location is then used only for the purpose of travel time calculations. If a source is outside of the ellipse, no modifications are necessary. In either case (source inside or outside of ellipse), no modifications are made to the size or shape of the ellipse in CTDMPLUS/CTSCREEN (dated 93076).

#### 1.1.3a Likely Impact

For sources that are located on or near (less than the major axis length from the hill center) the fitted terrain feature, there may be simulations where the WRAP ellipse would be modified in CTDMPLUS/CTSCREEN (dated 91107) (thus modifying the streamline patterns and stagnation point); no modification to the ellipse occurs in CTDMPLUS/CTSCREEN (dated 93076). Concentrations could be quite different for these situations.

#### 1.1.1b Problem

The second problem using the  $\beta$ -coordinate system involves the calculation of travel time from the source to receptor. In the stable/neutral WRAP portion of the code, the travel time is calculated using the actual position of the receptor  $(\mathbf{x}_{r\beta})$  in  $\beta$ -coordinates. A receptor that is laterally displaced from the stagnation streamline (off to the side of the hill), but having a short downwind distance in the  $\beta$ -coordinate system, will be associated with a short travel time. In some cases, this can result in an unrealistically large concentration at that receptor.

This situation is illustrated in Figure 2. This problem is particularly pronounced when the laterally displaced receptor is located on a section of the actual terrain contour that protrudes in the upwind direction (thus reducing the travel time along the  $x_{\beta}$ axis). Since the streamlines are determined for flow around the fitted ellipse (for a given simulation), the model does not specifically account for the contour protrusion upon which the receptor lies. This results in an inappropriate travel time estimate.

# 1.1.2b Solution

The CTDMPLUS and CTSCREEN codes have been modified so that receptors that are outside of the WRAP ellipse (for a given simulation) are moved onto the ellipse for the purpose of travel time calculations only. This approach is appropriate since the fitted ellipse parameters (and not the actual terrain contours) are used in determining the flow characteristics in the WRAP calculations. Receptors that are within the WRAP ellipse have there locations unchanged.

#### 1.1.3b Likely Impact

Because of the importance of travel time to the dispersion calculations, this modification will likely result in different concentrations than those obtained from CTDMPLUS/CTSCREEN (dated 91107); some concentrations may increase and others may decrease. Concentrations will be most affected in situations where the adjusted travel time is large compared to the total travel time to the receptors. In contrast, situations with sources that are many times the hillbase dimension from the terrain feature will result in relatively little difference in impacts due to this modification.

1.2 CONVERGENCE PROBLEM IN LOCATING SOURCE STREAMLINE

CTDMPLUS	modules	modified:	PATH.FOR	
CTSCREEN	modules	modified:	PATH.FOR,	NITCALC.FOR

# 1.2.1 Problem

In CTDMPLUS/CTSCREEN (dated 91107), the algorithm for computing the position of the streamline that passes through the source occasionally has problems converging on a solution. This results in the error message "ENDLESS LOOP IN PATH". This occurs only during stable/neutral situations. When this error is encountered, concentrations at all receptors are set equal to -999.0 for that simulation (hour) and processing continues with the next simulation.

# 1.2.2 Solution

An improved convergence routine has been included in CTDMPLUS/CTSCREEN (dated 93076) which greatly decreases the likelihood of nonconvergence. All of the previous situations in which convergence problems were found (or were reported by users) were tested with the new code and none failed to converge. However, if this error is found with CTDMPLUS/CTSCREEN (dated 93076), the action by the models is the same (e.g. -999.0 for all receptors and go on to the next simulation).

#### 1.2.3 Likely Impact

The impact of this change is two-fold. All of the previous simulations where the error was encountered will now yield concentrations. Also, with a new convergence routine, the location of the source streamline may be slightly different (although still within the convergence criteria) and thus may yield different concentrations at any receptor for any simulation than were previously found with CTDMPLUS/CTSCREEN (dated 91107).

1.3 METEOROLOGICAL PROFILE INFORMATION OUT OF ORDER CTDMPLUS modules modified: SEQMOD.FOR. CTSCREEN modules modified: SEQSCR.FOR.

CTDMPLUS requires that the meteorological tower information in the file PROFILE be input in order of increasing height. If the levels are not in order, a message ("PROFILE HEIGHT VALUE INCORRECT ....") is written to the CTDM.OUT file and processing is stopped.

#### 1.3.1 Problem

In CTDMPLUS/CTSCREEN (dated 91107) this check is performed incorrectly. When two measurement levels are compared in this check, one is referenced to tower base elevation and one is not. In some cases this may result in the error message even when data is entered properly.

# 1.3.2 Solution

CTDMPLUS/CTSCREEN (dated 93076) is corrected and both measurement levels are referenced to the tower base.

#### 1.3.3 Likely Impact

If users of CTDMPLUS/CTSCREEN (dated 91107) have encountered this error, the program was stopped. If the error message was not encountered, then there was no effect on subsequent computations. The coding error was ONLY in the check itself.

# 1.4 LIMIT ON THE CONVECTIVE SCALING VELOCITY

CTDMPLUS modules modified:	DAYCALC.FOR, RDSFC.FOR,
	SEQMOD.FOR, SFCMET.CMN.
CTSCREEN modules modified:	CONCALC.FOR, RDSFC.FOR,
	DAYSCR.FOR, SFCMET.CMN

In CTDMPLUS/CTSCREEN (91107), the value of  $w_*$  is set equal to the maximum of the current value of  $w_*$  and 0.167 times the wind speed at a height half-way between the stack and the plume height.

#### 1.4.1 Problem

In the case where multiple stacks are being modeled, this calculation may be in error for certain situations. The original value of  $w_*$  is calculated from surface parameters and the mixing height. The model then looks at the wind speed at the half-way height for stack one. If necessary,  $w_*$  will be changed. When the check is made on stack two which has a different plume height and possibly different half-way wind speed, the comparison is incorrectly made against the stack-one corrected value. The comparison should be made (for each stack) against the original value of  $w_*$  (calculated from the surface parameters and the mixing height).

# 1.4.2 Solution

To correct this problem, a new variable was created to keep the original value of  $w_*$  for later comparisons.

#### 1.4.3 Likely Impact

This correction to the code may result in different concentrations for CTDMPLUS calculations only and during unstable conditions only. The convective scaling velocity,  $w_*$ , is such an important parameter for the unstable calculation that the impact of this change on concentrations is hard to predict. There are many cases where this change has no effect. Since the wind speed profile is uniform in CTSCREEN, this change has NO EFFECT on CTSCREEN calculations.

#### 1.5 NEGATIVE EMISSION RATES

CTDMPLUS modules modified: INPSOR.FOR, SEQMOD.FOR,

#### 1.5.1 Problem

CTDMPLUS/CTSCREEN (dated 91107) do not allow the emission rate for any source to be less than or equal to zero. If this occurs, the model prints a warning to the user that an input error has been encountered and that source is not considered in further computations.

# 1.5.2 Solution

Since there are occasions when a user may wish to model a retiring source with a negative emission rate, the models have been modified to allow this with a message printed to the output file when negative emissions are encountered. Sources with zero emissions still trigger the "emission input error" message.

#### 1.6 SOURCE CONTRIBUTION TABLE OUTPUT FILE

CTDMPLUS modules modified:	CTDMPLUS.FOR, SEQMOD.FOR,
	SOURCES.FOR, INPAR.FOR
CTSCREEN modules modified:	CTSCREEN.FOR, SEQSCR.FOR,
	SOURCES.FOR, INPAR.FOR

### 1.6.1 Problem

CTDMPLUS/CTSCREEN (dated 91107) allowed the user to output a source contribution table (through the ISOR switch in the CTDM.IN file) in a text format in the CTDM.OUT file. This text information can be quite voluminous. In addition, CTSCREEN previously allowed no source contribution table.

### 1.6.2 Solution

The ISOR switch in the CTDM.IN file is now used by both models for obtaining source contribution information. First of all, source contribution (if chosen) is written to a separate file named

SOURCES (or \*.SRC with the menu driver). With both models the user now has a choice of text or binary as the format of that output file.

1.7 SPECIAL HANDLING OF RECEPTORS BELOW STACK TOP
CTDMPLUS modules modified: INPAR.FOR, DAYCALC.FOR,
SEQMOD.FOR, PARAMS.CMN
CTSCREEN modules modified: INPAR.FOR, DAYSCR.FOR,
NITCALC.FOR, PARAMS.CMN

#### 1.7.1 Problem

Often times in regulatory applications of CTDMPLUS and CTSCREEN with multiple sources having different stack heights, it is difficult to sort out which receptors have gotten the proper impact from a given source. CTDMPLUS and CTSCREEN, as complex terrain models, are only appropriate for receptors ABOVE stack top (for any given stack).

#### 1.7.2 Solution

An additional user option has been added to CTDMPLUS/CTSCREEN (dated 93076) (the ISTKTP switch in CTDM.IN) which, when set, will check the relationship between the receptor and stacks in order that any receptor below a given stack top will receive no contribution from that stack's emissions. The default setting is that all receptors will receive impact from all sources regardless of their elevations.

1.8 NOTE ON USING READ62 WITH CURRENT UPPER AIR DATA (CTDMPLUS ONLY)

It has been recently discovered by several users of CTDMPLUS that there may be a problem when processing the NCDC upper air (TD6201) files with the READ62 program (for producing the RAWIN

file for METPRO and CTDMPLUS). As with other preprocessors, READ62 expects the time field for the 00Z and 12Z soundings to be **EXACTLY** 0 and 12, respectively. In very recent years, NCDC appears to be reporting these soundings at more exact times (eg. 11:50). The program will not properly find the data in these cases and will assume missing data. User's need to check the TD6201 files (and edit them as needed) before running READ62. This has no bearing on CTSCREEN applications.

### 2.0 ADDITIONAL MODIFICATIONS TO CTSCREEN ONLY

Beyond the problems discussed in Section 1.0, there were a number of additional problems discovered which were applicable to CTSCREEN only. These are described in this section along with the CTSCREEN (dated 93076) solutions.

# 2.1 CALCULATION OF THE CONVECTIVE SCALING VELOCITY CTSCREEN modules modified: CONCALC.FOR

#### 2.1.1 Problem

In CTSCREEN (dated 91107), a value for  $w_*$  is calculated in the subroutine RDSFC (which reads the SURFACE file and sets some of the surface parameters). The call to this subroutine (from SEQSCR) is very early in the program and the input "default" mixing height (50m) is used in the calculation. Later in CTSCREEN, the mixing height is determined, for unstable conditions, as a function of hill height, but  $w_*$  (which is a function of mixing height) is never recalculated;  $w_*$  remains the original value calculated in RDSFC.

# 2.1.2 Solution

In CTSCREEN (dated 93076),  $w_*$  is recalculated at the beginning of the subroutine CONCALC (unstable conditions only) using the appropriate values for the mixing height,  $u_*$ , and L. This assures that the correct value for  $w_*$  is used in the plume rise equations and in the calculations in the DAYSCR subroutine.

#### 2.1.3 Likely Impact

Since w, is such an important parameter in the convective calculations, it is likely that this modification will affect most daytime concentrations from CTSCREEN. The importance of this change on the results of any simulation depends directly on the contrast between the actual mixing height and the default value of Tests have shown that "daytime" concentrations will 50m. generally decrease compared to CTSCREEN (dated 91107) as a result of this correction by as much as about 30%. In a few cases, the concentrations increased slightly. Maximum concentrations are still found to be safely conservative relative to observations and to CTDMPLUS estimates. This modification will have NO EFFECT on stable/neutral calculations.

# 2.2 DETERMINATION OF MIXING HEIGHT Modules modified: SEQSCR.FOR, DAYSCR.FOR

In CTSCREEN (dated 91107), the mixing height is determined as a function of hill height. If IAUTO=1, the mixing height is based upon the height of the hill (h) used in determining the wind direction. Three mixing heights, 0.5h, 1.0h, 1.5h, are calculated for each wind direction. All sources, hills, and receptors are modeled with each mixing height. For all other methods of wind direction determination, each wind direction is modeled with each of the 3 mixing heights determined for each hill. Therefore, in the case of 3 hills, all sources, hills, and receptors are modeled using all 9 mixing heights.

2.2.1 Problem

There are really two problems with the CTSCREEN (dated 91107) and the way in which mixing heights are calculated. First, in multiple hill situations, CTSCREEN is modeling receptors on one hill with mixing heights determined for that hill as well as the other hills. Receptors should only be modeled with the mixing height determined from the hill on which they reside. Secondly, there are situations when the 0.5h, 1.0h, and 1.5h selections of mixing height are inadequate. When a highly buoyant source with a stack top that is near the top of the hill, the buoyancy of the plume allows it to penetrate all three selected mixed layers; the result is no concentrations on the hill surface (not very good for a screening model).

#### 2.2.2 Solution

The CTSCREEN (dated 93076) method for selecting mixing heights is a bit more complicated but should reduce the runtime for multiple source and hill situations and will remove the problem of total plume penetration. The steps for calculating the mixing height are as follows:

 Loop over the primary stacks, calculating a mixing height for each that is associated with very little penetration (P = 0.1) in typical high plume rise situations. The CTSCREEN plume penetration equation is used.

$$P = \frac{3.9 - z_b (F_b/US)^{-1/3}}{2.6}$$

where

$$\begin{split} P &= \text{penetration factor (0.1),} \\ U &= \text{wind speed (2 m/s),} \\ z_i &= \text{mixing height (m),} \\ S &= (g/\theta) (d\theta/dz) = \text{the stability parameter } (\theta = 293 \text{ K}), \end{split}$$

 $d\theta/dz$  = the potential temperature gradient above  $z_i$  (0.03 K/m)  $z_b$  =  $z_i$  - stack height (m), and  $F_b$  = plume buoyancy flux  $(m^4s^3)$ .

The maximum of all these "small penetration" mixing heights is set equal to ZIMAX. Therefore ZIMAX represents the height of a mixed layer that will, for most conditions, contain a majority the pollutant material of all the plume being modeled. This is not necessarily a worst case mixing height, but approximately represents a maximum value important to the sources and the hill being considered.

2) Loop over the hills, calculating three mixing heights (0.5h, 1.0h, 1.5h) for each hill as a function of hill height (h) and store in an array dimensioned (maxhills,3). If ZIMAX is less than 0.9\*h, replace the 0.5\*h value of  $z_i$  with ZIMAX in the array. If ZIMAX is greater than 1.1\*h, replace the 1.5\*h value of mixing height in the array.

3) Loop over the  $z_i$  values and sources, calculating the P factor for each source using the penetration equation and parameters in step 1. If the P factors for all sources are greater than 0.9 for a particular  $z_i$ , omit that  $z_i$ . This is intended to screen out mixing heights which will have no effect on the maximum concentrations, thus speeding up the model run. As an example, consider a terrain feature with a height of 340 meters. Suppose ZIMAX is calculated to be 385 meters. Three  $z_i$  values, calculated from the hill height (0.5h, 1.0h, 1.5h), are: 170, 340, and 510 meters . Since ZIMAX is greater than 1.1\*h, it replaces the 510 meter  $z_i$ . Upon checking the plume penetration values for the three

mixing heights (step 3), assume the lowest mixing height is eliminated. So, only two mixing heights are ultimately used for further calculations: 170.0 and 386.7 meters.

4) Finally, in modeling the concentrations, each mixing height value selected will be labeled with the hill from which it was calculated. In DAYSCR, if the hill number we are modeling does not equal the one that corresponds to the  $z_i$ value being used, skip that hill and its receptors. So, in contrast to CTSCREEN (dated 91107) which modeled all receptors with all mixing heights, CTSCREEN (dated 93076) will only model receptors on a given hill with mixing heights associated with that hill. This has potential runtime savings.

### 2.2.3 Likely Impact

As with  $w_*$ , mixing height is a very important parameter for convective calculations. For situations using CTSCREEN (dated 91107) where very buoyant plumes were penetrating all selected mixing heights, users will find more reasonable concentrations with CTSCREEN (dated 93076). Concentrations for many situations will likely change with these modifications since the mixing heights may be different and only mixing heights associated with a particular hill will now be used for receptors on that hill. This modification has NO EFFECT on stable/neutral calculations.

# 2.2.4 Note

In CTSCREEN the simulation counter is incremented each time concentrations are written to the output file. In CTSCREEN (dated 91107), a simulation was associated with a selected set of the meteorology. Because of the new way mixing height is calculated and used, a simulation now means a selected set of meteorology on a given hill (-999.0 is written to receptors on other hills for a given simulation). Therefore the total number of simulations has increased in CTSCREEN (dated 93076); however, <u>overall runtime</u>

should decrease for multiple hill cases as a result of these modifications and overall runtime for single hill situations should remain about the same. The expected total number of simulations to be modeled is now written to the screen at the beginning of the run and the percent completion is reported every tenth simulation.

# 2.3 OTHER MODIFICATIONS TO CTSCREEN OUTPUT Modules modified: CTSCREEN.FOR, SEQSCR.FOR, CONCALC.FOR, NITCALC.FOR, DAYSCR.FOR, WRITSCR.FOR, IO.CMN, SCREN.CMN

#### 2.3.1 Problem

As a result of the past year's experience using CTSCREEN and as a result of user's comments, it was felt that the output information from CTSCREEN (dated 91107) could be improved. The changes to CTSCREEN output discussed in this section are in addition to those already discussed in Section 1.6 an 1.7.

### 2.3.2 Solution

In CTSCREEN (dated 93076) numerous changes were made to the output files and a new file was created. In CTSCREEN (dated 91107), the meteorology associated with a particular simulation was written to the concentration file (STCONC or UNCONC) along with the concentrations for that simulation. With CTSCREEN (dated 93076), the meteorology is written to a separate file, METDAT, instead. This allows easier postprocessing of the concentration file and creates a better summary of the meteorological conditions modeled. Also, the SUMRE and METDAT files contain new information. For stable/neutral simulations, wind direction, wind speed,  $\sigma_{\rm v}$ ,  $\sigma_{\rm w}$ , d@/dz, H<sub>c</sub>, plume height, and source contribution information are written to the files. For convertive simulations, wind direction, plume height,

and plume penetration fraction are written to the files. Examples of the SUMRE and METDAT files are shown in Figure 3 and 4, respectively. The user also now has several options concerning the output concentration files, STCONC and UNCONC. The user has the option (using the ICONC switch in CTDM.IN) to print no concentration files, print them in binary form, or print them in text form. The SUMRE and METDAT files will always be created, however the STCONC and UNCONC files can be eliminated to save disk space if desired. Users should note that the ICONC switch had been disabled in CTSCREEN (dated 93076). Additionally, CTSCREEN now computes, at the beginning of the program, the approximate number of simulations expected for the run and reports that to the screen. During execution, the percent run completion is periodically reported to the screen.

#### 2.3.3 Likely Impact

This modification has no impact on the CTSCREEN concentration estimates. It only improves the usefulness of the output information.

# 2.4 REPORTING OF SIMULATION NUMBER IN ERROR MESSAGES CTSCREEN modules modified: NITCALC.FOR

#### 2.4.1 Problem

With CTSCREEN (dated 91107) many of the diagnostic messages indicated the wrong simulation number because they were written before the simulation number was incremented. In fact, the number written is exactly one smaller than the correct number.

# 2.4.2 Solution

Code has been modified to output the correct simulation number in the diagnostic messages.

#### 2.4.3 Likely Impact

Some previous confusion; no impact on concentrations.

#### 3.0 TESTING AND REEVALUATION OF CTDMPLUS

CTDMPLUS was tested and reevaluated using the Lovett, Westvaco, and Widows Creek data sets from previous evaluations (Paumier et al, 1992; Burns et al, 1990; Strimaitis et al, 1987). Readers are referred to these previous evaluations for details on these data bases. The one small change in CTDMPLUS that could affect concentrations in convective conditions (Section 1.4) was found to have no effect on the top 25 concentration estimates with these three data bases. Therefore, our attention is drawn to the comparison of CTSCREEN (dated 91107) with CTSCREEN (dated 93076) for stable/neutral conditions. Figures 5 through 7 show the top 25 concentrations predicted by the new model compared against the top 91107) evaluations concentrations from CTSCREEN (dated 25 (quantile-quantile plots). While some individual concentration values changed, the conclusions of original evaluation studies remain valid.

Looking first at the Lovett data base comparison (Figure 5) we see that there were NO changes in the top 25 concentrations. At Lovett, the source to hill center distance is greater than the major axis length of either of the two terrain features modeled, so no modification of the axes lengths would have occurred using Also, the highest impacts were CTSCREEN (dated 91107). at receptors that were generally inside the WRAP ellipse. These receptors would not have been moved onto the WRAP ellipse in CTSCREEN (dated 93076), so their positions (and the travel time to them) would not have been modified from previous evaluations. Therefore, the consistency between CTSCREEN (dated 91107) and CTSCREEN (dated 93076) is not unexpected with this source-terrain geometry. In addition, this suggests that the modifications to the

code are not inappropriately affecting concentration estimates in situations and at receptors where the changes do not apply.

At the other two evaluation sites, the sources are closer to the important terrain. Therefore, in stable/neutral conditions, axes lengths were likely modified and receptors may have been moved onto the WRAP ellipse in some cases. This is shown in the results. For the Westvaco site (Figure 6), 14 of the top 25 concentrations changed, however these concentrations differed by less than 1% in all cases. At Widows Creek, 23 of 25 concentrations changed with differences ranging up to about 5%. Note that some concentrations increased and others decreased. Most importantly with all three reevaluations, any previous conclusions about the performance of CTSCREEN remain valid for CTSCREEN (dated 93076).

# 4.0 TESTING AND REEVALUATION OF CTSCREEN

The CTSCREEN model is designed to estimate the maximum 1-h impacts for stable/neutral and the maximum 1-h impacts for convective conditions. It then scales the greater of these two values for estimating the maximum 3-h, 24-h, and annual impacts. Before evaluating CTSCREEN (dated 93076), the impact of the changes on the analyses used to determine the scaling factor should be examined.

The test cases used in determining the factors for converting CTSCREEN 1-h estimates to 3-h, 24-h and annual averages are described in Perry et al (1990). These cases include twenty-two different source-terrain geometries with full а year of meteorology. Figures 8-10 show the comparison of the results for CTSCREEN (dated 91107) and CTSCREEN (dated 93076). Note that the ratios CTDMPLUS to CTSCREEN were calculated using CTDMPLUS (dated 91107). With only a few exceptions, the ratios (for all three averaging periods) remained about the same as those for CTSCREEN

(dated 91107). In two cases where the sources were close to the terrain, there were noticeable increases in the CTDMPLUS to CTSCREEN ratios. However, for all averaging times, these ratio increases (decreases in CTSCREEN estimates) gave no reason to change the conclusions of the previous analyses. Thus, the scaling factors will not change as a result of the modifications to the code.

CTSCREEN (dated 93076) was also reevaluated using the Westvaco, Lovett, and Widows Creek databases in the same manner as CTSCREEN (dated 91107) was originally evaluated by Burns et al (1991). A summary of the results of the comparison between "old" CTSCREEN (dated 91107) and "new" CTSCREEN (dated 93076) are shown in Figures 11-14.

In comparing the 1-hr averages (Figure 11), the overall maximum concentration for the Lovett case decreased by 8.7% with However, as Figure 11 indicates, the maximum is the new code. still well above the observed maximum at Lovett. Because of the way CTSCREEN scales from 1-h to the other averaging times, the maximum at Lovett for other periods also decreased by the same percentage (Figures 12-14) (Note that in the figures, maximum concentrations have been normalized by the maximum observed concentration for the appropriate averaging period; therefore, the percent change in normalized concentration may be different for the various averaging periods). The maximum concentration for stable conditions decreased and a different combination of meteorological conditions caused the highest concentration. It is interesting to note that for the meteorological conditions that were associated with the highest concentration in stable conditions with CTSCREEN (dated 91107), CTSCREEN (dated 93076) predicted a 33.4% lower concentration. This difference is caused by the receptors being moved onto the ellipse. For unstable conditions, the maximum concentration increased by 13% and occurred during different

meteorological conditions than that associated with the unstable maximum for CTSCREEN (dated 91107). The mixing height that caused the highest concentration in the earlier evaluation was not used in CTSCREEN (dated 93076) because it was replaced by *ZIMAX*.

For the Westvaco and Widows Creek data sets, the maximum concentration for stable conditions was unchanged. Since stable conditions were controlling at Westvaco, there are no changes in the CTSCREEN predicted "design" concentrations due to the modifications. For unstable conditions at these two sites, the maximum concentrations occurred for different meteorological conditions than in previous evaluations. In both cases this occurred because of the change in the calculation of the mixing height and the convective scaling velocity,  $w_*$ . At Widows Creek, convective conditions were found to be controlling. The model changes to mixing height and  $w_{\star},\ \text{resulted}$  in a decrease in the CTSCREEN predicted design concentration (unnormalized) of 14.1%. Again, the maximum is still safely above the observed maximum at that site for all averaging periods.

#### 5.0 CONCLUSIONS

The modifications made to CTDMPLUS primarily affect the for stable While calculations conditions. individual concentrations changed, the conclusions of previous evaluations regarding model performance did not. For CTSCREEN, changes were made to the code that affect both the calculations for stable conditions and the calculations for unstable conditions. Aqain, while individual concentrations changed, the conclusions from previous evaluations remain valid. In addition to the reevaluations, both models were exposed to two months of beta testing by eight modelers with prior experience with CTDMPLUS and CTSCREEN. Their very minor comments have been addressed and are included here as problems solved.

#### 6.0 REFERENCES

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Figure 1. Definition of the  $\beta$ -coordinate system used in the WRAP calculations in the two-dimensional flow around an ellipse. The  $x_\beta$  axis is aligned with the tangent to the stagnation streamline at the impingement point. The coordinates of the impingement (stagnation) point, source, and receptor along the  $x_\beta$  axis are denoted as  $x_{\alpha\beta}$ ,  $x_{s\beta}$ , and  $x_{r\beta}$ , respectively. The stagnation streamline  $(\psi_{\alpha})$  and the source streamline  $(\psi_s)$  are also shown.



**Figure 2**. Example case where a receptor far to the side of the plume centerline received maximum concentration. Dashed line indicates the WRAP ellipse.

Sensitivity Analysis of CTDMPLUS: CCB; Low-level Low-buoy; Close-in 101 SUMMARY FOR ALL STABLE HOURS <--- PEAK SOURCE --> CONC WD WS SIGV SIGW DTHDZ HCRIT NS SRC CTRB REC HPL US/M\*\*3 DEG M/S M/S M/S K/M М US/M\*\*3 # М 1.0 0.30 0.15 0.035 70.7 1 102 10.18 0.7 10.18 103.3 SUMMARY FOR ALL UNSTABLE HOURS <---- PEAK SOURCE - - - - > REC CONC WD WS ΖI W\* L NS SRC CTRB HPL PEN DEG # US/M\*\*3 M/S М M/S М US/M\*\*3 М 115.8 0.17 -90.0 23.87 1.0 1 23.87 104.3 11 0.6 0.39 SUMMARY FOR ALL HOURS REC CONC 24HR ANNUAL ЗHR US/M\*\*3 US/M\*\*3 US/M\*\*3 US/M\*\*3 # 11 23.87 16.71 3.58 0.72 RECEPTOR SUMMARY FOR STABLE HOURS <--- PEAK SOURCE --> WD WS SIGV SIGW DTHDZ HCRIT NS SRC CTRB REC CONC HPL US/M\*\*3 DEG M/S K/M US/M\*\*3 # M/S M/S М М 3.37 2.0 0.30 0.30 0.020 22.7 1 0.8 1 3.37 100.1 2 3.27 0.8 2.0 0.30 0.30 0.020 22.7 1 3.27 100.1 . 8.92 1.0 0.30 0.15 0.035 8.92 139 0.7 70.7 1 103.3 8.95 0.7 1.0 0.30 0.15 0.035 70.7 8.95 140 1 103.3 RECEPTOR SUMMARY FOR UNSTABLE HOURS

Figure 3 Excerpt from a sample SUMRE file.

Sensitivity Analysis of CTDMPLUS: CCB; Low-level Low-buoy; Close-in 101 SUMMARY FOR ALL STABLE HOURS <- PEAK REC -> <-- PEAK SOURCE ---> HCRIT NS SRC WD WS SIGV SIGW DTHDZ NR CONC SIM CTRB HPL M/S K/M US/M\*\*3 DEG M/S M/S Μ # US/M\*\*3 M 1 0.8 1.0 0.30 0.04 0.010 41 0.43 45.4 1 0.43 141.1 0.8 1.0 0.30 0.04 0.020 2 82 2.77 61.3 1 2.77 118.3 . . 95 0.6 5.0 0.75 0.75 0.010 11 2.21 1 1.6 2.21 79.7 5.0 0.75 0.75 0.020 122 0.6 2.13 3.5 1 96 2.13 79.7 SUMMARY FOR ALL UNSTABLE HOURS <- PEAK REC -> <---- PEAK SOURCE ----> SIM WD WS ΖI Μ\* L NR CONC NS SRC CTRB HPL PEN US/M\*\*3 DEG M/S М M/S US/M\*\*3 # М Μ 97 0.6 1.0 100.0 0.29 -10.0 136 6.70 1 6.70 90.0 0.59 115.8 0.31 -10.0 116 8.22 98 0.6 1.0 1 8.22 104.3 0.39 • . 167 0.6 6.0 100.0 1.00 -90.0 11 13.71 1 13.71 64.6 0.00 168 0.6 6.0 115.8 1.00 -90.0 11 12.08 12.08 1 64.6 0.00

Figure 4. Excerpt from a sample METDAT file.



**Figure 5**. Top 25 concentrations at Lovett predicted by CTDMPLUS (dated 91107) and CTDMPLUS (dated 93076).



**Figure 6**. Top 25 concentrations at Westvaco predicted by CTDMPLUS (dated 91107) and CTDMPLUS (dated 93076).



**Figure 7**. Top 25 concentrations at Widows Creek predicted by CTDMPLUS (dated 91107) and CTDMPLUS (dated 93076).



**Figure 8**. CTDMPLUS(3-h HSH)/CTSCREEN(1-h) concentrations for CTSCREEN (dated 91107) and CTSCREEN (dated 93076).



**Figure 9.** CTDMPLUS(24-h HSH)/CTSCREEN(1-h) concentrations from CTSCREEN (dated 91107) and CTSCREEN (dated 93076).



**Figure 10**. CTDMPLUS(Annual)/CTSCREEN(1-h) concentrations for CTSCREEN (dated 91107) and CTSCREEN (dated 93076).



**Figure 11**. Maximum predicted  $SO_2$  concentrations normalized by the maximum observed  $SO_2$  concentration for the 1-hour averaging period.



Figure 12. Maximum predicted  $SO_2$  concentrations normalized by the maximum observed  $SO_2$  concentration for the 3-hr averaging period.



**Figure 13**. Maximum predicted  $SO_2$  concentrations normalized by the maximum observed  $SO_2$  concentration for the 24-hour averaging period.



**Figure 14**. Maximum predicted  $SO_2$  concentrations normalized by the maximum observed  $SO_2$  concentration for the annual averaging period.