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Sensitivity Analysis of AIRDOS-EPA Using ADGEN with Matrix Reduction Algorithms

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ABSTRACT

ADGEN was developed to automate the calculation of sensitivities of a few model results to all input data in existing FORTRAN 77 computer models. ADGEN is now included as one of two options available to users of the Gradient Enhanced Software System (GRESS). GRESS was initially developed to automate the calculation of sensitivities of all model results to a few input parameters by application of the calculus chain rule during the forward run of the computer model. The ADGEN option automates the application of adjoint sensitivity theory to calculate first derivatives of model results to input data by first creating, and then solving, an adjoint equation for the computer model. The purpose of this report is twofold: (1) to present the development of two algorithms that significantly improve the application of ADGEN; and, (2) to demonstrate the application of ADGEN to the AIRDOS-EPA computer model.

1. INTRODUCTION

GRESS is an efficient automated software system for calculating sensitivities of model results to input data in existing FORTRAN 77 computer models. The GRESS/ADGEN option calculates first derivatives of selected model results with respect to an almost unlimited amount of data by application of the adjoint method. However, data storage has been a major limiting factor. The ADGEN application to the PRESTO-II computer model required more than 322 megabytes of direct access storage. The purpose of this report is: (1) to describe two new algorithms that significantly reduce data storage and execution time for application of the ADGEN option; and, (2) to demonstrate the application of ADGEN to the AIRDOS computer model.

Section II is a review of the CHAIN and ADGEN options for calculating sensitivities as implemented in GRESS. Section III introduces two matrix reduction algorithms developed for ADGEN applications. Results achieved by applying matrix reduction to the PRESTO-II benchmark are discussed. Section IV presents results from a comprehensive sensitivity analysis of the AIRDOS computer model. Conclusions and recommendations are given in Section V.

2. A MATHEMATICAL FOUNDATION FOR THE GRESS AND ADGEN CODE SYSTEMS

A brief discussion of the mathematics implemented with the GRESS CHAIN and ADGEN options is provided as an aid to understanding the data storage problems encountered when applying ADGEN to large codes. This section provides the basic foundation for the matrix reduction algorithms presented in the next section.

2.1 A MATHEMATICAL MODEL OF A COMPUTER PROGRAM

In a FORTRAN program, calculated left-hand-side variables are a function of previously defined left-hand-side variables and data, either through mathematical operations or read statements. This relationship can be expressed as

$$\bar{y} := \bar{f}(\bar{y}) \tag{1}$$

where the symbol,:=, indicates a value assignment (i.e., store) operation, the components of the column vector, $\bar{y}$, are all the terms on the left-hand-side of real number replacement statements, and the column vector, $\bar{f}$, represents the right-hand-side mathematical operations. The vector, $\bar{y}$, includes both model calculated results and data. Read statements are treated the same as setting a variable equal to a constant.

In a FORTRAN program a symbol cannot explicitly depend on itself. When a FORTRAN variable is redefined, mathematically, it is not the same variable. In the statement, $X := X+5.0$, the X on the left and the X on the right represent two different locations in the solution vector, $\bar{y}$. Mathematically, the equation can be thought of as, $X_2 = X_1 + 5.0$

Therefore to represent Eq. (1) mathematically the dependence of a variable on itself must be considered explicitly. If we define

$$\frac{dy_i}{dy_i} = 1, \text{ for all i} \quad . \tag{2}$$

Then Eq. (1) can be rewritten as

$$\bar{y} = \bar{f}(\bar{y}) \quad . \tag{3}$$

Consider the following four lines of FORTRAN:

$$
\begin{aligned}
&READ\ (5,*)\ A, B, D \\
&X = A**2 + B**2 \\
&W = A*X + D**2 \\
&Z = X**2 + W + A**3 + D**3
\end{aligned}
$$

The components in Eq. (3) are

$$
\bar{y} = \begin{bmatrix} A \\ B \\ D \\ X \\ W \\ Z \end{bmatrix} \qquad \bar{f} = \begin{bmatrix} \text{input parameter} \\ \text{input parameter} \\ \text{input parameter} \\ A**2 + B**2 \\ A*X + D**2 \\ X**2 + W + A**3 + D**3 \end{bmatrix}
$$

2.2 DIFFERENTIATING THE MATHEMATICAL MODEL

Differentiating Eq. (3), with respect to $\bar{y}$, yields

$$
\frac{d\bar{y}}{d\bar{y}} = \frac{\partial \bar{f}}{\partial \bar{y}} \cdot \frac{d\bar{y}}{d\bar{y}} + I \tag{4}
$$

where the identity matrix, I, provides the explicit dependence of a variable on itself necessary to make Eq. (4) meaningful. Eq. (4) can be rearranged, such that

$$
\left[I - \frac{\partial \bar{f}}{\partial \bar{y}} \right] \bullet \frac{d\bar{y}}{d\bar{y}} = I \quad . \tag{5}
$$

Eq. (5) can be represented in a more compact form as,

$$
AY' = I \tag{6}
$$

where

$$
A = \left[I - \frac{\partial \bar{f}}{\partial \bar{y}} \right]
$$

and

$$Y' = \frac{d\bar{y}}{d\bar{y}} \quad .$$

Since FORTRAN equations are solved in a sequential fashion, FORTRAN variables are dependent on previously defined variables. Therefore,

$$\frac{\partial f_i}{\partial y_j} = 0 \ , \ \text{for j} \geq \text{i}$$

so that the matrix, $\frac{\partial \bar{f}}{\partial \bar{y}}$, is a lower triangular matrix with zeros on and above the diagonal. Therefore, the matrix, A, is nonsingular and invertible.

Solving Eq. (6) for Y' yields

$$Y' = A^{-1} \tag{7}$$

Since A is a lower triangular matrix, derivatives in the solution matrix Y', can easily be resolved using forward substitution. Also, since the transpose of A is upper triangular, components of Y' can be calculated using back substitution as represented by Eq. (8).

$$[Y']^{tr} = [A^{-1}]^{tr} = [A^{tr}]^{-1} \quad . \tag{8}$$

The *tr* superscript is used to represent the transpose of the matrix.

2.3 THE GRESS CHAIN OPTION

The GRESS CHAIN option is utilized to calculate and report sensitivities of model results with respect to a subset of the input data. The method used is to resolve Eq. (7) for selected columns in the matrix, Y', by forward substitution in memory. A fully resolved column in Y' represents the derivatives of every real variable with respect to the user selected variable or parameter associated with that column. Since selected columns in Y' are resolved by forward substitution in memory, the A matrix is never saved. At any given point during execution, the user can retrieve the total first derivatives of a calculated variable with respect to all the declared parameters. Since GRESS does not know *a priori* which results are of interest, it is necessary to propagate the derivatives for the user selected parameters through every row in the matrix. The amount of execution time and memory required for the CHAIN option increases rapidly with the number of declared parameters. Therefore, when applying the CHAIN option to large codes, the user may be limited to a few declared parameters.

2.4 THE GRESS ADGEN OPTION

The GRESS ADGEN option is used to calculate the derivatives of a selected model result with respect to all the input data to the model. Resolving a row of Y' yields the derivatives of a single result with respect to all the real variables in the model. For a FORTRAN program, solving for a selected row in Y' yields the same result that is achieved by solving the adjoint equation for the numerical model defined by the computer code as discussed in Refs. (1-12). The GRESS ADGEN option is used to create an A matrix on a direct access storage device. The GRESS Version 0.0 ADGEN utility programs, TMAT and YSOLVE, are used to calculate and report derivatives of interest. TMAT is used to transpose the A matrix. The YSOLVE program calculates and reports the derivatives for a selected column of $[Y']^{tr}$.

2.5 ESTIMATING DATA STORAGE REQUIREMENTS FOR ADGEN

The A matrix created by GRESS Version 0.0 can be excessively large. For a moderately sized program, it is not uncommon for the A matrix to have on the order of 10^7 rows. If only the non-zero terms are stored, the data set can require as much as 200 megabytes of storage.

There are three pieces of information stored with each row:

(1) Np = number of non-zero derivatives;

(2) C's = column numbers for non-zero derivatives;

(3) D's = values of derivatives.

Items 2 and 3 are repeated Np times. The row number of the left-hand-side term is not stored, since it can be determined during processing. The present version uses four byte words for Np, D, and C. Therefore, eight bytes are required for each non-zero derivative in the row, and an additional four bytes for each row to store the derivative count, Np. The amount of storage required for either A or A-transpose can be estimated as follows.

$$\text{Storage} = (\#\text{ of rows}) * [4 + (\text{average Np}) * 8] \text{ bytes} \qquad (9)$$

For a matrix with 10^7 rows and an average of two non-zero terms off the diagonal per row, the amount of storage would be 200 megabytes. Using Eq. (9):

$$\text{Storage} = (10^7) * [4 + (2*8)] \text{ bytes} = 200 \text{ megabytes.}$$

In application, this amount of storage has been required for codes that used 1 minute of execution time on a VAX 8600 prior to enhancement. The ADGEN application to the PRESTO-II model required a total of 322 megabytes to store both the A and A-transpose matrices.

3. MATRIX REDUCTION ALGORITHMS FOR ADGEN

Presented in this chapter are two matrix reduction algorithms that were implemented in the present GRESS system to reduce the data storage required by an ADGEN application.[13] Results achieved by applying matrix reduction to the PRESTO-II computer model are discussed.

3.1 FORWARD AND BACK REDUCTION

Mathematically, the matrix reduction techniques are based on the fact that the rows in the A matrix are linearly independent and the matrix is non-singular. It can easily be proven that any submatrix from a linearly independent, nonsingular matrix, is also linearly independent and nonsingular.[14] This means that if a row and corresponding column (i.e., row i, column i) are removed from the matrix, the remaining matrix is still linearly independent and nonsingular. Therefore, Eqs. (1–8) are still valid for any submatrix extracted from the A matrix. Since parameters and results of interest are declared by the user, and are "known" during execution of the enhanced model, information is available that can be used to extract a problem dependent submatrix, thus reducing the data stored, and the number of calculations required to solve for selected derivatives.

The example shown in Fig. 1 is used to illustrate the storage of unnecessary information in the A matrix.

```
          .
          .
          .
      PI=3.141593
      DO 20 I=1,1000
           DO 10 J=1,10000
              RES(I,J)=PI*D(I,J)
10         CONTINUE
20    CONTINUE
          .
          .
          .
```

Fig. 1. Example program used to demonstrate forward and back reduction algorithms.

In this example, the FORTRAN equation

$$RES(I,J) = PI*D(I,J)$$

would be executed ten million times. Each time the equation is executed, a new row in the A matrix is created with two non-zero derivatives. The derivative of RES(I,J) with respect to PI and the derivative of RES(I,J) with respect to D(I,J) are both stored. The total amount of storage required for just this equation can be estimated using Eq. (9).

$$\text{storage} = (\text{ten million rows}) * [\ 4 + 2*(8)] = 200 \text{ megabytes}$$

The variable PI in this example accounts for 80 megabytes of the 200 megabytes of storage. If PI were treated as a constant, rather than a variable, the size of this data set could be reduced to 120 megabytes (a 40 per cent reduction).

Forward Reduction utilizes parameter dependency to identify and eliminate constants while generating the A matrix. When creating the A matrix, partial derivatives are calculated and stored for every equation solved. However, only derivatives of rows that are dependent on user specified parameters (or input data) are actually needed. If any term on the right-hand side of an equation is dependent on a declared parameter, then the term being calculated is also dependent; and therefore, the derivative is needed. If there is no dependency on the right, then the row is not needed. The application of Forward Reduction to the example in Fig. 1 would result in PI not being included in the A matrix as an independent variable, thus achieving the 80 megabyte reduction in storage.

Once the A matrix exists, the results of interest for derivative calculation are available. Back Reduction uses this information to extract the submatrix that contains only results of interest, declared parameters, and other rows on which the chosen results of interest depend. If both Forward and Back Reduction algorithms are used, the remaining submatrix will contain only the independent parameters, the dependent results of interest, and the intermediate variables required to map the parameters into the results.

The example in Fig. 1 will be used to illustrate Back Reduction. Assume that we are only interested in the result RES(I,J) when J is equal to 10000. Since I ranges from 1 to 1000, there will be only 1000 rows in the submatrix extracted by Back Reduction. The 120 megabyte data set representing the A matrix after Forward Reduction is the starting point. Since all but 1000 rows can be removed, the size of the data set after Back Reduction for those values for RES when J equals 10000 would be

$$\text{storage} = (1000 \text{ rows}) * [\ 4 + 1*(8)] = 1200 \text{ bytes.}$$

In performing Forward and Back Reduction as described no data or results of interest are removed from the A matrix. There is no loss in the generality of the ADGEN option as implemented in GRESS.

3.2 MATRIX REDUCTION APPLIED TO PRESTO-II

The PRESTO-II computer model[15] was used as a benchmark for the GRESS Version 0.0 adjoint matrix generation option, ADGEN. A more complete discussion of the benchmark is included in Ref. 12. First, the computational and storage requirements for ADGEN without matrix reduction are provided. The results achieved using matrix reduction are then presented.

PRESTO-II was developed as a non site-specific screening model for evaluating the possible health effects due to shallowland disposal of radioactive waste. The model has approximately 6,900 lines of coding. The PRESTO-II computer resource requirements are for the Barnwell sample problem included in Ref. 15. This problem calculates a time-dependent radiation dose to a man from transport of 42 radionuclides over a one thousand year time span.

PRESTO-II was enhanced with the EXAP precompiler, GRESS Version 0.0. Derivatives for two results with respect to 2800 parameters were calculated. The resource requirements for creating and solving the $[A]$ matrix are shown in Table 1. The PRESTO-II $[A]$ matrix had more than eight million rows and 322 megabytes of direct access storage were required to create the $[A]^{tr}$ matrix. The $[A]$ matrix is considered a scratch data set, and may be deleted once $[A]^{tr}$ is created.† However, the $[A]^{tr}$ matrix (144 megabytes) must remain active for the YSOLVE step. YSOLVE reads $[A]^{tr}$ and calculates the derivatives for one result with respect to all the declared parameters (i.e., a column of $[Y]^{tr}$). The YSOLVE step can be re-executed for additional results of interest that were specified during the execution of the enhanced model.

Table 1. Resource Requirements for Creating and Solving the *A* Matrix Created by PRESTO-II

Job Step	Run Time (Min:Sec)	Data Set created	Storage (megabytes)
Enhanced Presto-II	24:51	[A]	178
TMAT*	8:09	$[A]^{tr}$	144
YSOLVE (1 result)*	4:59		
			322 (total)

*TMAT and YSOLVE are described in Ref. 8.

Simple modifications to the GRESS/ADGEN run-time library routines were made to implement the Forward Reduction algorithm. Results, summarized in Table 2, show a decrease in the size of $[A]^{tr}$ from 144 megabytes to 86 megabytes due to the Forward Reduction algorithm, alone. Because of the nature of the algorithm changes, the intermediate step of creating a separate forward matrix, then transposing it, was also eliminated. This removed the TMAT utility from the calculational sequence.

† A GRESS utility, TMAT, is used to convert the $[A]$ matrix into the $[A]^{tr}$ matrix.

Table 2. Resource Requirements for Creating and Solving the *A* Matrix Created by PRESTO-II with Forward and Back Reduction

Job Step	Run Time (Min:Sec)	Data Set created	Storage (megabytes)
Enhanced model	24:01	$[A]^{tr}$	86
BREDUCE[a]	3:32	$[A]^{tr}$	11
YSOLVE	:34		
			97(total)

[a]BREDUCE is test program for implementing the Back Reduction algorithm that creates a subset of $[A]^{tr}$.

The Back Reduction algorithm was implemented in a utility program, BREDUCE, to be executed after the creation of the A matrix. BREDUCE was used to create the sub-set of $[A]^{tr}$ that contains only those terms on which the results of interest (as specified by the user in the run step) depend. The results after execution of the Back Reduction algorithm show the amount of data storage to be reduced to 11 megabytes. The execution time to reduce the matrix and solve for derivatives for one response with respect to 2800 parameters is less than the time it takes to solve for one response with the entire matrix. The time to solve for a second result would be 34 seconds, as opposed to the nearly 5 minutes required to solve the unreduced matrix.

4. SENSITIVITY ANALYSIS OF AIRDOS-EPA

This chapter provides the results from a preliminary sensitivity analysis of AIRDOS-EPA. The sample problem description and steps in applying the GRESS ADGEN option are reviewed. A report of the sensitivities for two responses are presented and verified by both the GRESS CHAIN option and by direct parameter perturbations. Finally the results from the application of matrix reduction are discussed.

4.1 SAMPLE PROBLEM DESCRIPTION

AIRDOS-EPA is a computer model[16] that is used to estimate: radionuclide concentrations in air; rates of deposition on ground surfaces; ground surface concentrations; intake rates via inhalation of air and ingestion of meat, milk and fresh vegetables; and radiation doses to man from airborne releases of radionuclides. Both point sources and uniform area sources of atmospheric releases of radionuclides can be evaluated. Time-averaged meteorological data for a given locality is part of the input to the code which then estimates air and ground concentrations and intake rates by man at various distances and directions from the release point. Meteorological data are usually supplied as a function of 16 directions, 6 wind speeds and 6 or 7 stability classes.

Two additional programs are ordinarily used in connection with AIRDOS-EPA, PREPAR[17] and DARTAB[18]. PREPAR is a user-friendly code that prepares a data set for input to AIRDOS-EPA. DARTAB takes the output from AIRDOS-EPA and combines it with other data to produce the radiation doses to man. We considered only AIRDOS-EPA and used a sample data set furnished by the Radiation Shielding Information Center. We modified that data set further to consider only one radioisotope, U-238. The data set contains only one source, a stack 185 meters high. There is a 20 by 20 grid of 400 small areas of 10,000 square meters each containing 4 meat animals, 2 milk cattle and a population of 1. The complete input data set is provided in Appendix A. The output produced (Appendix B) lists the ground level air concentrations, the amount deposited on the ground, and the intake by man by ingestion and inhalation at ten distances along each of the standard 16 wind directions. Direction 1 is north, direction 2 is north-northwest, etc., around to direction 16 which is north-northeast. The sample problem took 2.66 seconds CPU time on a VAX 8600.

4.2 PROCESSING AIRDOS WITH GRESS/ADGEN

There are four steps in applying ADGEN with matrix reduction to an existing FORTRAN 77 program.

1. Precompilation with EXAP.

2. Creation of the adjoint matrix with Forward Reduction.

3. Application of Back Reduction to reduce storage.

4. Solving the adjoint matrix for selected results.

EXAP will accept a majority of ANSI-X3.9 FORTRAN 77. Specific limitations are discussed in Ref. 8. Precompilation with EXAP did not require any changes to the AIRDOS-EPA source code for the selected sample problem. However, two minor modifications were made because of potential impact to future sample problems. First, a statement function was replaced by a function subprogram. EXAP does not support statement functions. Removal of the statement function did not impact the results for the sample problem used in the study. Second, an AMOD function reference was replaced by AAAMOD; and, a function subprogram AAAMOD was added to the AIRDOS source code. EXAP Version 0.0 did not include AMOD as an acceptable function because of potential discontinuities in the calculated derivatives. The procedure employed with AIRDOS was to write a FORTRAN 77 function subprogram, AAAMOD, that performed the function of AMOD. AAAMOD was included with the AIRDOS source code prior to processing with EXAP. With this method, any discontinuities are handled the same as with any other sequence of FORTRAN code.

To perform the ADGEN application, three subroutine calls were added to the enhanced AIRDOS source code. The first executed line in the enhanced code is a call to subroutine SETRXX with the character string 'ADJOINT' as the argument. This "switches" the run-time library into ADGEN mode. To identify potential results for sensitivity calculation a call to subroutine POTRXX is required. For this application the first and last calculated values of FIOP (ingestion intake) were selected. Finally, a call to subroutine CLEARXX is inserted as the last executed line in the code to complete the creation of the adjoint matrix, the parameter dictionary, and the list of potential responses.

When the enhanced code is executed five datasets are created as shown in Table 3. These represent the parameter dictionary, the response dictionary, and the adjoint matrix (actually three datasets). Once the adjoint matrix exists the Back Reduction algorithm is applied by executing a program named BREDUCE. The output from BREDUCE is simply a reduced form of the adjoint matrix as represented in Table 3. The resource requirements and savings due to matrix reduction are discussed later in this chapter.

Table 3. Data Sets Created During an ADGEN Application

Name	Description
Parameter Dictionary	List of parameter names
Response Dictionary	List of response names
Adjoint Matrix:	(3 data sets)
– Number of Pairs	Non-zero derivative count for a row
– Column Numbers	for right-hand-side real variables
– Derivative Values	single precision partial derivative

The final step is to calculate and report sensitivities using the ADGEN utility YSOLVE. YSOLVE was upgraded to calculate derivatives from the reduced adjoint matrix.

4.3 REPORT OF SENSITIVITIES

The first and last values of output variable FIOP (ingestion intake) were selected as results of interest for sensitivity calculations. These two values of FIOP correspond to the ingestion intake at the first distance in direction 1 (north) and at the last distance in direction 16 (north-northeast), respectively. All REAL variables input via FORTRAN READ statements were automatically included in the parameter dictionary as parameters of interest. A total of 1271 input parameters were included. Tables 4 and 5 list the parameters with sensitivities greater than 0.1 for the two output variables.

Table 4. ADGEN Sensitivities Greater Than 0.1 for Ingestion Intake (FIOP) at 500 Meters N

Parameter	Derivative	Sensitivity
UDCAT(4,01)	−1.58 E+00	−5.80 E−01
UDCAT(5,01)	−5.91 E−01	−1.46 E−01
UDCAT(6,01)	−1.39 E+00	−1.55 E−01
FRAW(4)	1.11 E+01	5.81 E−01
FRAW(5)	1.66 E+01	1.46 E−01
FRAW(6)	3.65 E+01	1.56 E−01
SC(1)	1.36 E+06	9.98 E−01
REL(1,1)	1.37 E+02	1.00 E+00
RVEG	1.12 E+01	8.23 E−01
F3VEGM	−1.80 E+02	−1.22 E+01
DD1	2.36 E+01	8.65 E−01
LAMW	−3.81 E+03	−8.09 E−01
YSUBV2	−1.65 E+01	−8.65 E−01
UV	7.04 E−02	9.07 E−01
FSUBG	1.24 E+01	9.07 E−01
P	−8.57 E−03	−1.35 E−01
R2	5.91 E+01	8.65 E−01
BSUBV2	4.39 E+02	1.35 E−01

Table 5. ADGEN Sensitivities Greater Than 0.1 for Ingestion Intake (FIOP) at 10,000 Meters NNE

Parameter	Derivative	Sensitivity
UDCAT(4,16)	−3.69 E−02	4.98 E−01
UDCAT(5,16)	−1.70 E−02	−1.74 E−01
UDCAT(6,16)	−4.34 E−02	−2.07 E−01
FRAW(109)	2.79 E−01	5.10 E−01
FRAW(110)	3.04 E−01	1.80 E−01
FRAW(111)	6.18 E−01	2.20 E−01
PH(1)	−4.59 E−04	−2.56 E−01
SC(1)	2.81 E+04	8.48 E−01
VD(1)	2.15 E+01	1.16 E−01
REL(1,1)	3.32 E+00	1.00 E+00
RVEG	−2.08 E+00	−6.26 E+00
F3VEGM	−4.37 E+00	−1.22 E+01
DD1	5.75 E−01	8.65 E−01
LAMW	−9.26 E+01	−8.09 E−01
YSUBV2	−4.01 E−01	−8.65 E−01
UV	1.71 E−03	9.07 E−01
FSUBG	3.01 E−01	9.07 E−01
P	−2.08 E−04	−1.35 E−01
R2	1.44 E+00	8.65 E−01
BSUBV2	1.07 E+01	1.35 E−01

The only parameters with sensitivities greater than 1.0 are RVEG and F3VEGM, the latter having a sensitivity of −12.2. This means that a 1 per cent increase in F3VEGM will cause a 12.2 percent decrease in FIOP. F3VEGM is defined as the minimum fraction of vegetables ingested from outside the area. Further investigation showed that AIRDOS was actually using the difference between 1.0 and F3VEGM (0.924). A 1.0 percent change in F3VEGM causes approximately a 10 percent change in the difference leading to the large sensitivity. Though it was not tested, the sensitivity would be expected to decrease as the value for F3VEGM moved closer to 0.5. It is important to note that even though the derivatives behave normally, the way a parameter is used can lead to a misinterpretation of the values for the sensitivities.

The wind input data for a given direction affects only the output in that same direction and no others; therefore, parameters such as UDCAT(1,01), UDAV(1,01) and FRAW(1,01) have non-zero derivatives for the first value of FIOP and zero derivatives for the last value of FIOP. For the parameter PH, the physical height of the source stack, there is a hundred-fold difference in the sensitivities, primarily due to the distances involved (see Appendix C). The parameter REL, the release rate from the stack, has a sensitivity of 1.00, as expected. Most of the parameters listed after REL are radionuclide-independent variables and have the same sensitivity at each location. One exception is RVEG. The sensitivity of RVEG, the vegetable ingestion ratio, changes from +0.82 to −6.25 as the direction changes from N to NNE and distance increases from 500 meters to 10,000 meters.

As an aid to further investigation Appendix C lists the derivatives and sensitivities for all input parameters having non-zero derivatives for the two values of FIOP. In a few cases, e.g., parameter ANLAM, the sensitivity is zero although the derivative is not zero. This occurs when a parameter has a value of zero; however, for a different sample problem ANLAM may not have a value of zero.

4.4 VERIFICATION OF SENSITIVITIES

The capability of the enhanced version of AIRDOS-EPA to correctly calculate analytic first derivatives and sensitivities using computer calculus was tested by comparison of the ADGEN results with derivatives calculated by both the GRESS CHAIN option and direct parameter perturbations. All sensitivities calculated with the CHAIN option agreed with those calculated by ADGEN to seven significant digits. This close agreement is due to the fact that both CHAIN and ADGEN are calculating analytic derivatives. Sensitivities that were verified using the CHAIN option are flagged with an asterisk (*) in Tables 6 and 7.

Results from direct perturbations as shown in Table 6 and 7 verify that the ADGEN derivatives are correctly calculated. All parameter perturbations were on the order of 1 per cent. Since AIRDOS-EPA is a single precision code, it is not feasible to calculate sensitivities that are less than 10^{-5} by direct parameter perturbations.

Table 6. Perturbation Analysis for Response FIOP at 500 Meters, North

	Normalized Sensitivities	
Parameter	ADGEN	Direct (~1% Perturbation)
RVEG	8.23 E−01	8.22 E−01
F3VEGM	−1.22 E+01	−1.22 E+01
F3BEFM	−1.70 E−03	−1.70 E−03
DD1	8.65 E−01	8.65 E−01
LAMW*	−8.09 E−01	−8.02 E−01
TSUBE2*	5.64 E−01	5.52 E−01
YSUBV1*	−1.29 E−05	−1.39 E−05
YSUBV2*	−8.65 E−01	−8.65 E−01
QSUBF*	1.37 E−05	1.36 E−05
UV*	9.07 E−01	9.07 E−01
UF*	1.37 E−05	1.36 E−05
UL*	9.28 E−02	9.28 E−02
FSUBG*	9.07 E−01	9.07 E−01
FSUBL*	9.28 E−02	9.28 E−02
TSUBB*	4.22 E−02	4.18 E−02
R2	8.65 E−01	8.65 E−01
FSUBFI*	1.37 E−05	1.39 E−05
BSUBV2*	1.35 E−01	1.35 E−01

*Indicates parameters that were also verified by GRESS CHAIN option.

Table 7. Perturbation Analysis for Response FIOP at 10,000 Meters, North–Northwest

	Normalized Sensitivities	
Parameter	**ADGEN**	**Direct (~1% Perturbation)**
RVEG	−6.25 E+00	−6.25 E+00
F3VEGM	−1.22 E+01	−1.22 E+01
F3BEFM	−1.70 E−03	−1.70 E−03
DD1	8.65 E−01	8.65 E−01
LAMW*	−8.09 E−01	−8.02 E−01
TSUBE2*	5.64 E−01	5.52 E−01
YSUBV1*	−1.29 E−05	−1.39 E−05
YSUBV2*	−8.65 E−01	−8.65 E−01
QSUBF*	1.37 E−05	1.36 E−05
UV*	9.07 E−01	9.07 E−01
UF*	1.37 E−05	1.36 E−05
UL*	9.28 E−02	9.28 E−02
FSUBG*	9.07 E−01	9.07 E−01
FSUBL*	9.28 E−02	9.28 E−02
TSUBB*	4.22 E−02	4.18 E−02
R2	8.65 E−01	8.65 E−01
FSUBFI*	1.37 E−05	1.39 E−05
BSUBV2*	1.35 E−01	1.35 E−01

*Indicates parameters that were also verified by GRESS CHAIN option.

4.5 RESULTS FROM MATRIX REDUCTION

Resource requirements for creating and solving the AIRDOS-EPA adjoint matrix with and without matrix reduction are summarized in Table 8. Forward Reduction achieved a 22 percent decrease in storage; however, due to the elimination of TMAT, an additional 8 megabytes of disk storage were also eliminated from the procedure.

Table 8. Resource Requirements for Creating and Solving the AIRDOS-EPA Adjoint Matrix with Reduction

Job Step	Execution Time (cpu seconds)	Storage (megabytes)
ADGEN without reduction:		
Creating the matrix	90	6.3*
Solving for 1 response	17	
ADGEN with reduction:		
Creating the matrix (Forward Reduction)	60	4.9
Back Reduction	13	0.011
Solving for 1 response	2	

*This does not include an additional 8 megabytes of disk storage required to create the A matrix under GRESS Version 0.0.

The savings due to Back Reduction were quite dramatic for the sample problem selected. Back Reduction reduced data storage from 4.9 megabytes to 0.011 megabytes. This clearly indicates that the AIRDOS-EPA code is calculating many results through independent calculational paths. Though these results are all potentially important, they are also strongly correlated as indicated in Tables 4 and 5. Many of the most significant sensitivities are identical.

5. CONCLUSIONS AND RECOMMENDATIONS

Forward and Back Reduction algorithms significantly increase the size of codes (measured in CPU time) to which the ADGEN option can be applied. The GRESS Version 0.0 ADGEN option can require an excessive amount of data storage limiting the user to codes that execute in less than 1 to 2 minutes of CPU time. The adjoint matrix generated by GRESS Version 0.0 for a code that executes in 1 minute can exceed 200 megabytes. With the implementation of Forward and Back Reduction it should be possible to apply the ADGEN option to codes with 4 to 6 minutes of execution time. However, as was shown with the AIRDOS-EPA computer program, the numerical algorithms implemented in the model and the responses selected for sensitivity calculations can greatly impact data storage requirements.

Probably the most significant result from the sensitivity analysis of AIRDOS-EPA was that no modifications were required to make AIRDOS compatible with the GRESS software. GRESS is most successful with codes that adhere closely to the ANSI X3.9-1978 FORTRAN 77 standard. As little as two years ago, most codes required 1 to 3 man months just to make them compatible with the GRESS precompiler.

Techniques and algorithms to further reduce CPU time and data storage with ADGEN applications are being investigated. In the future it should be possible to completely eliminate data storage as a limiting factor. For the present, when performing a sensitivity analysis on large codes with ADGEN it can be very cost effective to limit the number of responses included in the study. Also, storage can be reduced by limiting the number of declared parameters in a single run, and then making multiple runs to screen all the input data.

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APPENDIX A
AIRDOS SAMPLE PROBLEM INPUT

APPENDIX A

SAMPLE INPUT DATA SET FOR AIRDOS-EPA

```
OPTIONS 01020 0011
        1        16         1        10
 5.000E+01 5.000E+01 5.000E+01 5.000E+01 5.000E+01 5.000E+01 5.000E+01
AREA
 1.000E+03
 7.000E-01
      500       800      1000      1500      2000      3000      4000      5000
     8000     10000         0         0         0         0         0         0
        0         0         0         0
AIR
     1000
 1.020E+02 2.853E+02 7.280E-02 1.090E-01 1.455E-01
.1207.0245.0195.0145.0398.0790.0761.0471.0705.0702.0852.0930.0799.0630.0722.0448
0.7722.5720.0000.7721.3091.6652.5721.1872.3872.3441.1872.5720.0001.4110.0002.572
2.5752.8822.2321.9342.2022.3692.5182.0951.5652.2661.7802.0881.8202.2092.1561.496
4.4514.5842.8212.6522.9603.7483.5952.7623.4823.5603.4323.9514.0264.1143.9274.160
5.0254.2183.9033.7243.5764.5214.8244.3475.3435.6996.3636.1796.1115.1764.7844.487
3.3603.3303.0312.9323.0862.9583.3943.6673.8673.9783.9553.8803.7643.7903.7323.399
1.5281.5841.4051.1331.4691.6431.5671.6471.6651.4591.6141.7021.4411.4061.7501.580
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0.7722.5720.0000.7721.8272.1522.5721.6722.5122.4971.6722.5720.0001.9370.0002.572
3.3423.0423.0032.5292.9753.1343.2992.8312.4343.0002.7083.0072.7723.1113.0482.758
5.3374.9533.8283.5563.4494.1044.0763.6604.0594.2344.0834.4374.4514.5964.5974.933
5.6835.0074.6504.6934.5805.6145.7465.3806.1846.5967.1456.9816.7625.8945.4425.326
3.5973.5683.2343.1093.3003.1433.6313.8784.0374.1184.1014.0463.9573.9773.9313.636
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0.0000.0000.0000.0000.0000.0000.0000.0000.0000.0000.0000.0000.0000.0000.0000.000
    0.0010    0.0182    0.0904    0.7125    0.1196    0.0582    0.0000
    0.0024    0.0094    0.0816    0.7012    0.1351    0.0702    0.0000
    0.0000    0.0236    0.0652    0.7089    0.1201    0.0821    0.0000
    0.0041    0.0290    0.0552    0.7164    0.1180    0.0773    0.0000
    0.0073    0.0483    0.0633    0.6566    0.1207    0.1038    0.0000
    0.0038    0.0511    0.1443    0.6704    0.0751    0.0553    0.0000
    0.0014    0.0524    0.1438    0.6385    0.0894    0.0745    0.0000
    0.0025    0.0369    0.0828    0.5869    0.1806    0.1102    0.0000
    0.0043    0.0405    0.1038    0.6184    0.1602    0.0729    0.0000
    0.0034    0.0611    0.1002    0.6674    0.1317    0.0362    0.0000
    0.0014    0.0375    0.0909    0.7152    0.1066    0.0485    0.0000
    0.0012    0.0312    0.0817    0.6978    0.1387    0.0495    0.0000
    0.0000    0.0225    0.0860    0.7281    0.1236    0.0398    0.0000
    0.0027    0.0202    0.1118    0.6490    0.1488    0.0675    0.0000
    0.0000    0.0168    0.1093    0.6148    0.1938    0.0654    0.0000
    0.0013    0.0129    0.0638    0.6073    0.1963    0.1184    0.0000
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NUCLIDES
        1
U-238
 0.000E+00 1.000E-05 1.800E-03 0.000E+00
 1.000E-01
        0
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1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04
1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04
1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04
1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04
1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04
1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04
1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04
1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04
1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04
1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04
1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04
1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04
1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04
1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04
1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04
1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04
1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04
1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04
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1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04
1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04	1.000E+04
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 1.000E+00 9.240E-01 1.000E+00 9.920E-01 0.000E+00 1.000E+00
 9.167E+05 1.000E+00 0.000E+00 3.652E+04 5.000E-01
 0.000E+00 2.160E+03 3.360E+02 3.360E+02
 2.900E-03
 7.200E+02 1.440E+03
 2.800E-01 7.160E-01
 4.000E-01
 4.300E-01
 1.560E+01
 2.000E+00
 1.760E+02 1.120E+02 8.500E+01 1.818E+01
 2.000E+01
 1.000E+00 1.000E+00
 1.000E+02
 2.150E+02
  0.0038200.0000 11.0000
  0.5700  0.2000
W BODY  R MAR   ENDOST  THYROID BREAST  *PUL*   S WALL  INT WALLLIVER   PANCREAS
KIDNEYS
U-238    11 4.247E-13 1.038E+00 2.654E-03 1.260E-03          0 0.000E+00 0.000E+00
0.0420.0160.0500.0410.1700.0280.0220.0200.0230.0160.024
 1.400E-04 1.600E-06 2.100E-02 4.200E-03
 5.480E-05 0.000E+000  0.0000  0.0000  0.0000  0.0000
    0   0    0    0    0 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
         Y     1.000E+00    2.000E-03
W BODY     1.729E+02
R MAR      3.099E-01
ENDOST     3.800E+00
THYROID    1.072E-02
BREAST     1.158E-02
*PUL*      8.327E+02
S WALL     1.866E-02
INT WALL   1.716E-01
LIVER      1.300E-02
PANCREAS   1.232E-02
KIDNEYS    1.515E+00
            2.000E-03
            7.905E-03
            1.147E-02
            1.486E-01
            3.461E-04
            3.537E-04
            3.473E-04
            3.984E-03
            9.141E-02
            2.980E-04
            3.521E-04
            5.915E-02
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APPENDIX B
AIRDOS SAMPLE PROBLEM OUTPUT

CONCENTRATIONS AND INTAKE RATES FOR U-238

DIR	DIST (M)	AIR CONC (CI/M**3)	GRND CONC (CI/M**2)	INGES INTAKE (PCI/YEAR)	INHAL INTAKE (PCI/YEAR)
1	500	1.31E-18	6.40E-09	1.37E+01	1.05E-02
1	800	6.20E-18	4.01E-09	8.56E+00	4.97E-02
1	1000	1.02E-17	3.22E-09	6.87E+00	8.18E-02
1	1500	1.68E-17	2.17E-09	4.63E+00	1.35E-01
1	2000	1.93E-17	1.64E-09	3.50E+00	1.55E-01
1	3000	1.96E-17	1.11E-09	2.36E+00	1.57E-01
1	4000	1.95E-17	8.39E-10	1.79E+00	1.57E-01
1	5000	2.03E-17	6.81E-10	1.45E+00	1.63E-01
1	8000	2.17E-17	4.44E-10	9.48E-01	1.74E-01
1	10000	2.14E-17	3.63E-10	7.75E-01	1.72E-01
2	500	1.88E-19	1.45E-09	3.10E+00	1.51E-03
2	800	7.29E-19	9.09E-10	1.94E+00	5.86E-03
2	1000	1.18E-18	7.28E-10	1.55E+00	9.50E-03
2	1500	2.23E-18	4.88E-10	1.04E+00	1.79E-02
2	2000	2.82E-18	3.68E-10	7.87E-01	2.27E-02
2	3000	3.30E-18	2.48E-10	5.30E-01	2.65E-02
2	4000	3.67E-18	1.89E-10	4.03E-01	2.95E-02
2	5000	4.11E-18	1.53E-10	3.27E-01	3.30E-02
2	8000	4.80E-18	1.00E-10	2.14E-01	3.86E-02
2	10000	4.80E-18	8.22E-11	1.75E-01	3.85E-02
3	500	1.98E-20	1.33E-09	2.83E+00	1.59E-04
3	800	8.62E-19	8.30E-10	1.77E+00	6.92E-03
3	1000	1.80E-18	6.66E-10	1.42E+00	1.45E-02
3	1500	3.28E-18	4.48E-10	9.58E-01	2.64E-02
3	2000	3.75E-18	3.39E-10	7.24E-01	3.01E-02
3	3000	3.79E-18	2.28E-10	4.87E-01	3.04E-02
3	4000	3.82E-18	1.73E-10	3.69E-01	3.07E-02
3	5000	4.01E-18	1.40E-10	2.99E-01	3.22E-02
3	8000	4.36E-18	9.12E-11	1.95E-01	3.50E-02
3	10000	4.31E-18	7.45E-11	1.59E-01	3.46E-02
4	500	6.25E-19	1.08E-09	2.30E+00	5.02E-03
4	800	2.18E-18	6.77E-10	1.45E+00	1.75E-02
4	1000	3.02E-18	5.44E-10	1.16E+00	2.43E-02
4	1500	3.77E-18	3.66E-10	7.82E-01	3.03E-02
4	2000	3.66E-18	2.76E-10	5.90E-01	2.94E-02
4	3000	3.22E-18	1.85E-10	3.95E-01	2.58E-02
4	4000	3.09E-18	1.40E-10	2.99E-01	2.48E-02
4	5000	3.21E-18	1.13E-10	2.42E-01	2.58E-02
4	8000	3.45E-18	7.34E-11	1.57E-01	2.77E-02
4	10000	3.42E-18	5.99E-11	1.28E-01	2.75E-02
5	500	1.83E-18	2.96E-09	6.32E+00	1.47E-02
5	800	7.31E-18	1.86E-09	3.98E+00	5.87E-02
5	1000	1.06E-17	1.50E-09	3.21E+00	8.54E-02
5	1500	1.33E-17	1.01E-09	2.17E+00	1.07E-01
5	2000	1.25E-17	7.65E-10	1.63E+00	1.00E-01
5	3000	1.02E-17	5.13E-10	1.10E+00	8.22E-02
5	4000	9.26E-18	3.87E-10	8.26E-01	7.44E-02
5	5000	9.22E-18	3.13E-10	6.68E-01	7.41E-02
5	8000	9.40E-18	2.02E-10	4.32E-01	7.55E-02
5	10000	9.29E-18	1.65E-10	3.52E-01	7.46E-02
6	500	1.58E-18	4.63E-09	9.88E+00	1.27E-02
6	800	1.01E-17	2.91E-09	6.22E+00	8.12E-02
6	1000	1.74E-17	2.35E-09	5.02E+00	1.40E-01
6	1500	2.71E-17	1.60E-09	3.42E+00	2.18E-01
6	2000	2.90E-17	1.22E-09	2.61E+00	2.33E-01
6	3000	2.56E-17	8.27E-10	1.77E+00	2.06E-01
6	4000	2.22E-17	6.26E-10	1.34E+00	1.78E-01
6	5000	2.04E-17	5.06E-10	1.08E+00	1.64E-01
6	8000	1.79E-17	3.26E-10	6.96E-01	1.44E-01
6	10000	1.69E-17	2.66E-10	5.67E-01	1.36E-01
7	500	4.78E-19	4.42E-09	9.44E+00	3.84E-03
7	800	7.30E-18	2.78E-09	5.93E+00	5.86E-02

7	1000	1.43E-17	2.24E-09	4.79E+00	1.15E-01
7	1500	2.45E-17	1.53E-09	3.26E+00	1.97E-01
7	2000	2.71E-17	1.17E-09	2.49E+00	2.18E-01
7	3000	2.44E-17	7.90E-10	1.69E+00	1.96E-01
7	4000	2.10E-17	5.97E-10	1.28E+00	1.68E-01
7	5000	1.90E-17	4.82E-10	1.03E+00	1.53E-01
7	8000	1.61E-17	3.09E-10	6.59E-01	1.29E-01
7	10000	1.51E-17	2.51E-10	5.36E-01	1.21E-01
8	500	8.59E-19	3.08E-09	6.57E+00	6.90E-03
8	800	5.11E-18	1.93E-09	4.13E+00	4.10E-02
8	1000	8.62E-18	1.56E-09	3.32E+00	6.92E-02
8	1500	1.31E-17	1.05E-09	2.25E+00	1.05E-01
8	2000	1.39E-17	7.99E-10	1.71E+00	1.11E-01
8	3000	1.22E-17	5.38E-10	1.15E+00	9.84E-02
8	4000	1.08E-17	4.06E-10	8.67E-01	8.67E-02
8	5000	1.01E-17	3.27E-10	6.99E-01	8.14E-02
8	8000	9.30E-18	2.10E-10	4.48E-01	7.47E-02
8	10000	8.94E-18	1.70E-10	3.64E-01	7.18E-02
9	500	1.18E-18	3.96E-09	8.45E+00	9.44E-03
9	800	9.66E-18	2.49E-09	5.32E+00	7.76E-02
9	1000	1.70E-17	2.02E-09	4.31E+00	1.37E-01
9	1500	2.52E-17	1.38E-09	2.94E+00	2.02E-01
9	2000	2.52E-17	1.05E-09	2.23E+00	2.03E-01
9	3000	2.07E-17	7.04E-10	1.50E+00	1.66E-01
9	4000	1.72E-17	5.31E-10	1.13E+00	1.38E-01
9	5000	1.54E-17	4.27E-10	9.12E-01	1.24E-01
9	8000	1.30E-17	2.73E-10	5.83E-01	1.05E-01
9	10000	1.24E-17	2.22E-10	4.74E-01	9.98E-02
10	500	9.84E-19	3.53E-09	7.54E+00	7.90E-03
10	800	9.52E-18	2.23E-09	4.76E+00	7.65E-02
10	1000	1.71E-17	1.80E-09	3.85E+00	1.38E-01
10	1500	2.53E-17	1.24E-09	2.64E+00	2.03E-01
10	2000	2.51E-17	9.40E-10	2.01E+00	2.02E-01
10	3000	2.04E-17	6.34E-10	1.35E+00	1.64E-01
10	4000	1.69E-17	4.78E-10	1.02E+00	1.36E-01
10	5000	1.52E-17	3.85E-10	8.23E-01	1.22E-01
10	8000	1.29E-17	2.47E-10	5.28E-01	1.04E-01
10	10000	1.24E-17	2.02E-10	4.31E-01	9.93E-02
11	500	9.62E-19	4.04E-09	8.62E+00	7.73E-03
11	800	9.10E-18	2.54E-09	5.43E+00	7.31E-02
11	1000	1.65E-17	2.05E-09	4.39E+00	1.32E-01
11	1500	2.50E-17	1.40E-09	3.00E+00	2.01E-01
11	2000	2.55E-17	1.07E-09	2.28E+00	2.05E-01
11	3000	2.15E-17	7.20E-10	1.54E+00	1.73E-01
11	4000	1.83E-17	5.44E-10	1.16E+00	1.47E-01
11	5000	1.67E-17	4.39E-10	9.37E-01	1.34E-01
11	8000	1.46E-17	2.82E-10	6.03E-01	1.17E-01
11	10000	1.40E-17	2.30E-10	4.92E-01	1.12E-01
12	500	4.75E-19	4.32E-09	9.22E+00	3.82E-03
12	800	6.49E-18	2.71E-09	5.79E+00	5.21E-02
12	1000	1.23E-17	2.19E-09	4.67E+00	9.87E-02
12	1500	1.95E-17	1.48E-09	3.17E+00	1.57E-01
12	2000	2.04E-17	1.13E-09	2.40E+00	1.64E-01
12	3000	1.80E-17	7.59E-10	1.62E+00	1.44E-01
12	4000	1.61E-17	5.74E-10	1.23E+00	1.29E-01
12	5000	1.54E-17	4.64E-10	9.92E-01	1.24E-01
12	8000	1.47E-17	3.00E-10	6.42E-01	1.18E-01
12	10000	1.43E-17	2.45E-10	5.24E-01	1.15E-01
13	500	9.47E-20	3.70E-09	7.90E+00	7.60E-04
13	800	4.11E-18	2.32E-09	4.96E+00	3.30E-02
13	1000	8.41E-18	1.87E-09	3.99E+00	6.75E-02
13	1500	1.45E-17	1.27E-09	2.70E+00	1.16E-01
13	2000	1.59E-17	9.60E-10	2.05E+00	1.27E-01
13	3000	1.47E-17	6.48E-10	1.38E+00	1.18E-01
13	4000	1.36E-17	4.91E-10	1.05E+00	1.09E-01
13	5000	1.32E-17	3.98E-10	8.50E-01	1.06E-01
13	8000	1.30E-17	2.58E-10	5.51E-01	1.04E-01

13	10000	1.27E-17	2.11E-10	4.51E-01	1.02E-01
14	500	1.00E-18	3.43E-09	7.33E+00	8.06E-03
14	800	4.44E-18	2.15E-09	4.60E+00	3.57E-02
14	1000	7.15E-18	1.73E-09	3.69E+00	5.74E-02
14	1500	1.17E-17	1.17E-09	2.50E+00	9.36E-02
14	2000	1.33E-17	8.86E-10	1.89E+00	1.07E-01
14	3000	1.29E-17	5.99E-10	1.28E+00	1.04E-01
14	4000	1.20E-17	4.53E-10	9.68E-01	9.62E-02
14	5000	1.16E-17	3.66E-10	7.83E-01	9.35E-02
14	8000	1.12E-17	2.36E-10	5.05E-01	8.97E-02
14	10000	1.07E-17	1.92E-10	4.11E-01	8.63E-02
15	500	5.39E-20	3.97E-09	8.48E+00	4.33E-04
15	800	2.39E-18	2.49E-09	5.31E+00	1.92E-02
15	1000	5.28E-18	2.00E-09	4.26E+00	4.24E-02
15	1500	1.11E-17	1.35E-09	2.88E+00	8.91E-02
15	2000	1.38E-17	1.02E-09	2.18E+00	1.11E-01
15	3000	1.42E-17	6.92E-10	1.48E+00	1.14E-01
15	4000	1.35E-17	5.24E-10	1.12E+00	1.08E-01
15	5000	1.32E-17	4.24E-10	9.06E-01	1.06E-01
15	8000	1.29E-17	2.74E-10	5.86E-01	1.04E-01
15	10000	1.25E-17	2.24E-10	4.77E-01	1.00E-01
16	500	2.15E-19	2.84E-09	6.07E+00	1.73E-03
16	800	1.98E-18	1.78E-09	3.80E+00	1.59E-02
16	1000	3.65E-18	1.43E-09	3.05E+00	2.93E-02
16	1500	5.94E-18	9.59E-10	2.05E+00	4.77E-02
16	2000	6.45E-18	7.23E-10	1.54E+00	5.18E-02
16	3000	6.30E-18	4.85E-10	1.04E+00	5.06E-02
16	4000	6.35E-18	3.67E-10	7.83E-01	5.10E-02
16	5000	6.73E-18	2.96E-10	6.33E-01	5.40E-02
16	8000	7.47E-18	1.91E-10	4.08E-01	6.00E-02
16	10000	7.49E-18	1.56E-10	3.32E-01	6.01E-02

APPENDIX C
DERIVATIVES AND SENSITIVITIES OF SELECTED RESPONSES

ADGEN DERIVATIVES AND SENSITIVITIES

PARAMETER NAME	FIOP (N at 500 meters) Derivative	Sensitivity	FIOP (NNE at 10,000 m) Derivative	Sensitivity	Direct Derivative (~1% Perturbation)
PR(1)	-1.52092E-04	-5.56876E-04	7.15682E-09	1.07747E-06	
PR(2)	-2.80296E-05	-2.02592E-04	3.36528E-07	5.06632E-05	
PR(3)	-2.38364E-09	-7.98794E-09	-3.42220E-06	-5.35236E-04	
PR(4)	0.00000E+00	0.00000E+00	-4.06344E-04	-6.44756E-02	
PR(5)	0.00000E+00	0.00000E+00	-5.00645E-05	-7.53725E-03	
PR(6)	0.00000E+00	0.00000E+00	-6.63420E-09	-6.70756E-07	
PERD(01)	1.13139E+02	1.00000E+00	0.00000E+00	0.00000E+00	
PERD(16)	0.00000E+00	0.00000E+00	7.41323E+00	1.00000E+00	
UDCAT(1,01)	-1.01613E-01	-5.74445E-03	0.00000E+00	0.00000E+00	
UDCAT(2,01)	-1.53249E-01	-2.88971E-02	0.00000E+00	0.00000E+00	
UDCAT(3,01)	-2.54903E-01	-8.30831E-02	0.00000E+00	0.00000E+00	
UDCAT(4,01)	-1.57669E+00	-5.80181E-01	0.00000E+00	0.00000E+00	
UDCAT(5,01)	-5.91365E-01	-1.45504E-01	0.00000E+00	0.00000E+00	
UDCAT(6,01)	-1.38653E+00	-1.55143E-01	0.00000E+00	0.00000E+00	
UDCAT(1,16)	0.00000E+00	0.00000E+00	-2.19621E-04	-1.70083E-03	
UDCAT(2,16)	0.00000E+00	0.00000E+00	-5.99928E-03	-2.70237E-02	
UDCAT(3,16)	0.00000E+00	0.00000E+00	-4.55246E-03	-5.70235E-02	
UDCAT(4,16)	0.00000E+00	0.00000E+00	-3.68968E-02	-4.98494E-01	
UDCAT(5,16)	0.00000E+00	0.00000E+00	-1.70491E-02	-1.74489E-01	
UDCAT(6,16)	0.00000E+00	0.00000E+00	-4.34078E-02	-2.06509E-01	
UDAV(1,01)	6.58256E-04	3.72129E-05	0.00000E+00	0.00000E+00	
UDAV(2,01)	5.98244E-07	1.46408E-07	0.00000E+00	0.00000E+00	
UDAV(3,01)	2.28197E-06	8.91844E-07	0.00000E+00	0.00000E+00	
UDAV(4,01)	3.45400E-05	1.43741E-05	0.00000E+00	0.00000E+00	
UDAV(5,01)	2.64059E-06	6.95541E-07	0.00000E+00	0.00000E+00	
UDAV(6,01)	5.42961E-06	8.13098E-07	0.00000E+00	0.00000E+00	
UDAV(1,16)	0.00000E+00	0.00000E+00	3.49535E-07	2.70692E-06	
UDAV(2,16)	0.00000E+00	0.00000E+00	3.39535E-06	2.81964E-05	
UDAV(3,16)	0.00000E+00	0.00000E+00	3.95771E-06	5.87854E-05	
UDAV(4,16)	0.00000E+00	0.00000E+00	3.26004E-05	5.22803E-04	
UDAV(5,16)	0.00000E+00	0.00000E+00	1.98077E-05	2.16857E-04	
UDAV(6,16)	0.00000E+00	0.00000E+00	4.63428E-05	2.91219E-04	
FRAW(1)	7.84620E+01	5.74567E-03	0.00000E+00	0.00000E+00	
FRAW(2)	2.17242E+01	2.89532E-02	0.00000E+00	0.00000E+00	
FRAW(3)	1.25646E+01	8.31760E-02	0.00000E+00	0.00000E+00	
FRAW(4)	1.11308E+01	5.80753E-01	0.00000E+00	0.00000E+00	
FRAW(5)	1.66383E+01	1.45720E-01	0.00000E+00	0.00000E+00	
FRAW(6)	3.65216E+01	1.55652E-01	0.00000E+00	0.00000E+00	
FRAW(106)	0.00000E+00	0.00000E+00	4.55010E-01	1.78106E-03	
FRAW(107)	0.00000E+00	0.00000E+00	7.56414E-01	2.93808E-02	
FRAW(108)	0.00000E+00	0.00000E+00	3.05814E-01	5.87480E-02	
FRAW(109)	0.00000E+00	0.00000E+00	2.79094E-01	5.10351E-01	
FRAW(110)	0.00000E+00	0.00000E+00	3.03822E-01	1.79578E-01	
FRAW(111)	0.00000E+00	0.00000E+00	6.17553E-01	2.20161E-01	
PH(1)	-1.80114E-04	-2.44006E-03	-4.59488E-04	-2.55953E-01	
ANLAM(1)	-2.35530E-02	0.00000E+00	-1.30790E-02	0.00000E+00	

PARAMETER NAME	FIOP (N at 500 meters) Derivative	Sensitivity	FIOP (NNE at 10,000 m) Derivative	Sensitivity	Direct Derivative (~1% Perturbation)
SC(1)	1.36287E+06	9.98009E-01	2.81734E+04	8.48308E-01	
VD(1)	3.79668E+00	5.00446E-04	2.14463E+01	1.16236E-01	
VG(1)	1.03989E-01	0.00000E+00	1.08157E+00	0.00000E+00	
REL(1,1)	1.36559E+02	1.00000E+00	3.32113E+00	1.00000E+00	
RVEG	1.12452E+01	8.23473E-01	-2.07833E+00	-6.25791E+00	
F3VEGM	-1.79680E+02	-1.21577E+01	-4.36985E+00	-1.21577E+01	-1.22E+01
RBEF	1.53958E-04	1.12742E-05	-2.84544E-05	-8.56770E-05	
F3BEFM	-2.33699E-02	-1.69766E-03	-5.68360E-04	-1.69766E-03	-1.70E-03
F3MLKM	-4.75606E-01	-3.48280E-02	-4.75606E-01	-1.43206E+00	
DD1	2.36256E+01	8.65037E-01	5.74580E-01	8.65037E-01	8.65E-01
TSUBH1*	-5.69046E-19	0.00000E+00	-1.38393E-20	0.00000E+00	
TSUBH2*	-2.73936E-18	-4.33295E-16	-6.66217E-20	-4.33295E-16	
TSUBH3*	-2.24210E-14	-5.51665E-13	-5.45282E-16	-5.51665E-13	
TSUBH4*	-2.19227E-13	-5.39405E-12	-5.33165E-15	-5.39405E-12	
LAMW*	-3.80808E+03	-8.08695E-01	-9.26130E+01	-8.08694E-01	-8.02E-01
TSUBE1*	7.23496E-08	3.81461E-06	1.75955E-09	3.81461E-06	
TSUBE2*	5.34392E-04	5.63513E-02	1.29965E-05	5.63513E-02	5.52E-02
YSUBV1*	-6.29830E-04	-1.29140E-05	-1.53176E-05	-1.29140E-05	-1.39E-05
YSUBV2*	-1.64984E+01	-8.65037E-01	-4.01243E-01	-8.65037E-01	-8.65E-01
QSUBF*	1.19846E-05	1.36908E-05	2.91467E-07	1.36908E-05	1.36E-05
UV*	7.03901E-02	9.07204E-01	1.71190E-03	9.07204E-01	9.07E-01
UF*	2.19952E-06	1.36908E-05	5.34928E-08	1.36908E-05	1.36E-05
UL*	7.03901E-02	9.27822E-02	1.71190E-03	9.27822E-02	9.28E-02
TSUBS*	-7.94018E-17	-1.16290E-16	-1.93106E-18	-1.16290E-16	
FSUBG*	1.23886E+01	9.07204E-01	3.01294E-01	9.07204E-01	9.07E-01
FSUBL*	1.26702E+00	9.27822E-02	3.08142E-02	9.27822E-02	9.28E-02
TSUBB*	5.76805E-03	4.22386E-02	1.40280E-04	4.22386E-02	4.18E-02
P	-8.57145E-03	-1.34950E-01	-2.08459E-04	-1.34950E-01	
R1	3.09390E-04	1.29140E-05	7.52443E-06	1.29140E-05	
R2	5.90641E+01	8.65037E-01	1.43645E+00	8.65037E-01	8.65E-01
LAMRR*	-2.34531E+04	-7.29396E-10	-5.70383E+02	-7.29395E-10	
FSUBFI*	1.16850E+02	1.36908E-05	2.84181E+00	1.36908E-05	1.39E-05
BSUBV1*	5.05103E-04	7.76748E-07	1.22842E-05	7.76748E-07	
BSUBV2*	4.38774E+02	1.34949E-01	1.06711E+01	1.34949E-01	1.35E-01
LAMSUR	-2.31032E+04	-9.27116E-02	-5.61874E+02	-9.27116E-02	

* indicates parameters also checked with the CHAIN option

APPENDIX D
DEFINITION OF AIRDOS-EPA PARAMETERS WITH NON-ZERO DERIVATIVES

APPENDIX D

DESCRIPTION OF INPUT PARAMETERS WITH NON-ZERO DERIVATIVES WITH ADGEN

PR	SPECIFIC PLUME RISE FOR EACH PASQUILL CATEGORY
PERD	WIND DIRECTION FREQUENCY (16 DIRECTIONS)
UDCAT	RECIPROCAL-AVERAGED WIND SPEEDS (7 PAS. CAT., 16 DIR.)
UDAV	TRUE-AVERAGE WIND SPEEDS (7 PAS. CAT., 16 DIR.)
FRAW	FREQUENCIES FOR PASQUILL STABILITITY CATEGORIES (112)
PH	PHYSICAL HEIGHT OF STACK (M)
ANLAM	EFFECTIVE RADIOLOGICAL DECAY CONSTANT IN THE PLUME (PER DAY)
SC	SCAVENGING COEFFICIENT (PER SEC)
VD	DRY DEPOSITION VELOCITY (M/SEC)
VG	GRAVITATIONAL (OR SETTLING) VELOCITY (M/SEC)
REL	RELEASE RATE OF RADIONUCLIDE FROM STACK (CI/YEAR)
RVEG	VEGETABLE INGESTION RATIO-IMMEDIATE SURROUNDING AREA/TOTAL WITHIN AREA
F3VEGM	MINIMUM FRACTION VEGETABLES INGESTED FROM OUTSIDE AREA
RBEF	MEAT INGESTION RATIO-IMMEDIATE SURROUNDING AREA/TOTAL WITHIN AREA
F3BEFM	MINIMUM FRACTION MEAT INGESTED FROM OUTSIDE AREA
F3MLKM	MINIMUM FRACTION MILK INGESTED FROM OUTSIDE AREA
DD1	FRACTION OF RADIOACTIVITY RETAINED ON PRODUCE AFTER WASHING
TSUBH1	TIME DELAY--INGESTION OF PASTURE GRASS BY ANIMALS (HR)
TSUBH2	TIME DELAY--INGESTION OF STORED FEED BY ANIMALS (HR)
TSUBH3	TIME DELAY--INGESTION OF LEAFY VEGETABLES BY MAN (HR)
TSUBH4	TIME DELAY--INGESTION OF PRODUCE BY MAN (HR)
LAMW	REMOVAL RATE CONSTANT FOR PHYSICAL LOSS BY WEATHERING (PER HOUR)
TSUBE1	PERIOD OF EXPOSURE DURING GROWING SEASON--PASTURE GRASS (HR)
TSUBE2	PERIOD OF EXPOSURE DURING GROWING SEASON--CROPS OR LEAFY VEGETABLES (HR)
YSUBV1	AGRICULTURAL PRODUCTIVITY BY UNIT AREA (GRASS-COW-MILK-MAN PATHWAY (KG/M**2))
YSUBV2	AGRICULTURAL PRODUCTIVITY BY UNIT AREA (PRODUCE OR LEAFY VEG INGESTED BY MAN (KG/M**2))
QSUBF	CONSUMPTION RATE OF CONTAMINATED FEED OR FORAGE BY AN ANIMAL IN KG/DAY (DRY WEIGHT)
UV	RATE OF INGESTION OF PRODUCE BY MAN (KG/YR)
UF	RATE OF INGESTION OF MEAT BY MAN (KG/YR)
UL	RATE OF INGESTION OF LEAFY VEGETABLES BY MAN (KG/YR)
TSUBS	AVERAGE TIME FROM SLAUGHTER OF MEAT ANIMAL TO CONSUMPTION (DAY)
FSUBG	FRACTION OF PRODUCE INGESTED GROWN IN GARDEN OF INTEREST
FSUBL	FRACTION OF LEAFY VEGETABLES GROWN IN GARDEN OF INTEREST
TSUBB	PERIOD OF LONG-TERM BUILDUP FOR ACTIVITY IN SOIL (YEARS)
P	EFFECTIVE SURFACE DENSITY OF SOIL (KG/SQ. M, DRY WEIGHT) (ASSUMES 15 CM PLOW LAYER)
R1	FALLOUT INTERCEPTION FRACTION FOR PASTURE
R2	FALLOUT INTERCEPTION FRACTION FOR VEGATABLE CROPS
LAMRR	RADIOACTIVE DECAY CONSTANT FOR THE RADIONUCLIDE (PER DAY)
FSUBFI	FRACTION OF ANIMAL'S DAILY INTAKE OF NUCLIDE WHICH APPEARS IN FLESH (DAYS/KG)
BSUBV1	CONC. FACTOR FOR UPTAKE OF NUCLIDE FROM SOIL FOR PASTURE AND FORAGE
BSUBV2	CONC. FACTOR FOR UPTAKE OF NUCLIDE FROM SOIL BY EDIBLE PARTS OF CROPS
LAMSUR	ENVIRONMENTAL DECAY CONSTANT FOR SURFACE FOR THE RADIONUCLIDE (PER DAY)

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