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Diffuse II – A Hydrogen Isotope Diffusion and Trapping Simulation Program Upgrade

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M. F. Hardwick, S. L. Robinson

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Sandia National Laboratories

Albuquerque, New Mexico 87185 and Livermore, California 94550

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Diffuse II – A Hydrogen Isotope Diffusion and Trapping Simulation Program Upgrade

Michael F. Hardwick
Steven L. Robinson
GTS Engineering Department
Sandia National Laboratories
Livermore, CA 94551

Abstract

Diffuse is a finite difference computer program which may be used to calculate the one-dimensional diffusion and trapping of atoms in a host material under general initial, source, and boundary conditions.

Diffuse was originally written in Fortran prior to 1980, and rewritten in 1983 in order to run on the Sandia Cray computers in use through the early 1990's. When the mainframe computers were retired, the Gas Transfer System (GTS) Development Department ported the code to the PC platform, where it ran as a simple console application. All graphical output was lost during this port. GTS code developers have completed an upgrade that provides a Windows 95/NT Diffuse application and restores all of the original graphical output. This upgrade is called Diffuse II version 1.0. This report serves both as a users manual for Diffuse II v 1.0 and as a general software development reference.

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Executive Summary

Diffuse is a finite difference computer program which may be used to calculate the one-dimensional diffusion and trapping of atoms in a host material under general initial, source, and boundary conditions.

Diffuse was originally written in Fortran prior to 1980, and rewritten in 1983 in order to run on the Sandia Cray computers in use through the early 1990's. When the mainframe computers were retired, the Gas Transfer System (GTS) Development Department ported the code to the PC platform, where it ran as a simple console application. All graphical output was lost during this port. GTS code developers have completed an upgrade that provides a Windows 95/NT Diffuse application and restores all of the original graphical output. This upgrade is called Diffuse II version 1.0.

This report serves both as a user's manual for Diffuse II v 1.0 and as a general software development reference. The intent of the software description is to help other developers understand the development philosophy and software structure so that bugs may be more easily eliminated and future upgrades may be simplified.

User's Manual

Scope

This user's manual is not intended as a comprehensive guide to the physical models implemented in the Diffuse code. Model specific information can be found in the original DIFFUSE user's manual¹. This manual serves only to describe how to use the Windows 95/NT Diffuse II upgrade.

Overview

Diffuse is a finite difference computer program which calculates the one-dimensional diffusion and trapping of atoms in different materials under general initial, source, and boundary conditions. Diffuse enables the user to compute, singly or in combination:

- 1) bulk diffusion of one or two species in a multi-layer medium, including a temperature gradient, and
- 2) tritium decay resulting in trapped helium upon decay (i.e. no migration).

While the computational code supports trapping and detrapping, this version of the user interface, written specifically for gas transfer applications, does not support the introduction of trap distributions. The inclusion of trapping support would allow the code to be more broadly applicable and should be considered an important upgrade for the next release.

The diffusing species may arise from:

- 1) implantation
- 2) diatomic gas phase entry at surfaces, or
- 3) initial surface concentrations.

Simple geometries for which results may be computed are:

- 1) a semi-infinite slab,
- 2) an infinitely long solid or hollow cylinder, or
- 3) a solid or hollow sphere.

Code History

Diffuse was originally written in Fortran prior to 1980, and modified by M. Baskes in 1983 enabling it to run on the Sandia Cray computers in use then and through the early 1990's. The partial differential equations of Fickian diffusion were solved using a Sandia-written numerical solver. Diffuse ran initially on CDC computers, using cardfile inputs. Later, it ran on the Cray computers first under COS and then CTSS. The final configuration used the VAX computers for input/output to the Cray computers. In this configuration, terminal operation was available.

1. Baskes, M. I., DIFFUSE, Sandia National Laboratories, SAND83-8231, June 1983

In the mid-1990's the Cray computers on which the code ran were relocated to Sandia/NM and over the next few years became less and less accessible. Several responses were developed. Initially, Diffuse was incorporated into an integrated design-tool environment using a CORBA (Common Object Request Broker Architecture) wrapper. This activity was funded as a GTS pilot under the Product Realization program, but ended with no plans or funding to maintain the design tool environment. When the mainframe computers were finally retired, GTS Development Department ported the code to the PC platform, where it ran as a console application. Unfortunately, because the Diffuse plotting routines required a graphics library that was not available for the PC platform, all graphical output was lost. During this upgrade, the console application was converted to a Windows 95/NT application with a modern user-interface and all graphical output was restored.

Installation

Although Diffuse is intended to be installed on only a limited number of machines, an automated installation program was developed to automate installation onto a Windows 95/NT computer. The installation program, *DiffuseSetup.exe*, was created with *InstallShield Express 2*. The program copies the required files to the appropriate directories on the selected hard drive, makes required registry updates, and creates program groups and menu items.

Run Diffuse II by double-clicking the *Diffwin.exe* icon or an appropriate shortcut or by selecting the Diffwin menu item from the Start menu.

Diffuse Display

The Diffuse II display is shown in Figure 1. The Diffuse II main frame, which also displays the name of the currently selected document in its title bar, houses the system menu, toolbar, and main output window. The main output window contains a single graph that displays calculation results in plot form. The *Diffuse Input* tabbed dialog, also called a property sheet, provides the user with the means to enter the problem definition. Unlike the main output window, the tabbed dialog is not constrained to remain within the main frame boundaries. It can be moved to any desired location on the screen.

Diffuse II allows the user to manipulate multiple sessions (documents) at the same time, a capability that is useful when comparing several different problems. Selecting *New* from the *File* menu starts an additional session and presents an additional main output window and its contained graph. The number of concurrent sessions is limited only by the amount of available memory and the user's ability to maintain an understanding of the multiple windows. Although multiple main output windows may be displayed, only a single input tabbed dialog window is shown. The values in the tabbed dialog always correspond to the currently selected main output window.

Data from a Diffuse II session may be stored by selecting *Save* or *Save As* from the *File* menu. If the data has not yet been saved or if *Save As* is selected, the system presents the *Save As* dialog that allows the user to

Figure 1: The Diffuse display

select a file name and location for storage. Selecting *Open* from the *File* menu restores saved data. In this case the system presents the *Open* dialog that allows the user to browse for the desired file. Plot data in the main output window may be previewed or printed by selecting *Print Preview* or *Print* from the File menu. Only the problem definition data (*i.e.*, the data contained in the three pages of the input tabbed dialog -- see "Input Tabbed Dialog" on page 12) is saved. When reading data from an existing file, the user must click the *Calculate* button to recreate the problem solution data.

The next two manual sections describe the input tabbed dialog and the main output window in more detail.

Input Tabbed Dialog

The tabbed dialog is used to enter information that defines the problem to be analyzed and is initialized with default parameters appropriate for a single layer of stainless steel subjected to a tritium gas pressure on one side while the other is held at zero concentration. The input tabbed dialog contains three pages, each accessed by clicking the appropriate tab. The first page defines the material sample, the second page defines program control parameters, and the third page defines the environment and boundary conditions.

Sample Page

The *Sample* page, shown in Figure 2, allows the user define the material sample to be evaluated. In general, the sample is a composite of a maximum of five individual layers of different materials. The number of layers in the sample of interest is selected in the *No. of Samples* list box. General geometric data is entered in the second section of general sample data. A planar, cylindrical, or spherical sample geometry may be selected from the *Shape* list box. The value entered in the *Inside Radius* edit box applies, of course, only to cylindrical and spherical geometries. The individual layer thickness is entered in the *Thickness* edit box while the distance of interest into the overall composite sample is entered into the *Profile* edit box. The profile distance value determines the distance scale for plotting and allows the user to focus the concentration plot results on the near surface area of interest. For convenience, the profile value may be quickly set to the composite thickness by clicking the *max* button.

Material Properties	
Material	Stainless Steel
Ed	0.999
D0	0.0047
Es	0.0607
S0	0.00079
Density	8.5e+022
$\bar{Q}$	0.065

Geometry	
Shape	Spherical
Inside radius	2.54
Thickness	0.1
Profile	0.1

Diffusing Species	
No. species	2
Species 1	Tritium
Species 2	Deuterium

Boundary Conditions	
Front	Solvant's Law
Back	Solvant's Law

Calculate

Figure 2: The *Sample* page of the *Diffuse Input* tabbed dialog

The identity of the gas(es) to which the composite sample is subjected is defined in the *Diffusing Species* data section. The number of species, which is limited to a maximum of two, is selected in the *No. Species* list box while the individual gases are identified by the selections in the *Species 1* and *Species 2* list boxes.

The material properties and boundary conditions for the individual layers are defined in the right side of the Sample Page. The layer for which properties are to be defined is selected in the *Sample Number* list box, the upper limit of which is determined by the *No. of Samples* value. For convenience, entire data sets for the common materials shown in Table 1, may be entered by selecting the desired material in the *Mat'l Name* list box. Individual property values, described in Table 2, may be overridden by simply entering the desired value in the appropriate box. Because this version of Diffuse II does retrieve material information from a database, the new data set cannot be stored under the same or different material name. However, saving the problem data file, as later described, does save all user entered data.

The interface boundary conditions for each layer are defined in the *Boundary Conditions* section of the Sample Page. The available interface options are shown in Table 3. Note that all interior interfaces should use the *Interface* boundary condition

Clicking the *Calculate* button initiates a Diffuse II calculation and, if successful, updates the output in the main window.

Table 1: Available Materials

Material
Aluminum
Beryllium
Carbon
Copper
Inconel
Iron
Molybdenum
Nickel
Stainless Steel
Titanium
Tungsten
Vanadium
Zirconium

Table 2: Material Properties

Property	Units	Description
Ed	eV	Activation enthalpy for diffusion
D0	cm ² amu ^{1/2} / sec	Pre-exponential constant for diffusion
Es	eV	Activation energy for solubility
S0	afrac / atm ^{1/2}	Pre-exponential constant for solubility
Density	atoms / cm ³	Atomic packing density for the host matrix
Q-star	eV	Heat of transport for the diffusing species
Stick		Sticking coefficient for adsorption from gas (0 to 1)

Table 3: Boundary Conditions

Condition	Description
Reflection	The boundary reflects all diffusing species
Zero Conc.	Diffusing species concentration is zero at the boundary
Seivert's Law	Concentration is proportional to the square root of pressure
Recombination	Diffusing species must recombine at the boundary according to a rate equation with a rate constant determined by other the other user-defined parameters
Interface	Specifies an internal layer interface

Control Page

The *Control* page is shown in Figure 3. Here the user enters information that controls execution of the computational part of Diffuse II. During the computation, the composite sample is divided into a one-dimensional mesh with a number of nodes equal to the value entered in the *Number of mesh nodes* edit box.

Although this version of Diffuse II does not use the *Number of cycle repeats* value, the edit box is included to simplify its inclusion into the next release. The *Number of cycle repeats* defines the number of times that the sequence of steps defined in the Data page is repeated.

The remaining control parameters allow the user to determine the relative distribution of mesh points throughout the material layers so that large concentration gradients may be appropriately represented. The values in these edit boxes are evaluated in a relative, not absolute, manner. A layer with a larger value receives a proportionally greater number of mesh nodes. If all values are equal, the mesh nodes are uniformly distributed.

The screenshot shows a software dialog box titled "Diffuse Input". It has three tabs: "Sample", "Control", and "Data". The "Control" tab is currently selected. The dialog contains several input fields with labels to their left:

- Number of mesh nodes:** The input field contains the value "100".
- Number of cycle repeats:** The input field contains the value "0".
- Number of cycle edits:** The input field contains the value "1".
- Fraction of mesh points in near surface region:** The input field contains the value "0.25".
- Relative number of mesh points in material no.:** This is a list of five input fields, each preceded by a number from 1 to 5. All five input fields contain the value "1".

At the bottom right of the dialog, there is a button labeled "Calculate".

Figure 3: The *Control* page of the *Diffuse Input* tabbed dialog

Data Page

The *Data* page, shown in Figure 4, allows the user to enter information describing a series of pressure and temperature boundary conditions to which the composite sample is subjected. The value in the *Number of DATA cards* list box determines the number of steps in the boundary condition sequence and is limited to a maximum of five. The individual steps may be selected for data entry or review by selecting the appropriate card number from the *Card Number* list box. The *Time interval* edit box contains the time step for the selected card. The *Number of print edits* list box is not used by this version of Diffuse II.

The pressure boundary conditions for each of the gas species identified in the Sample page are defined in the *Pressures* section of the page. Here, values are entered for each species and for the front and back sides of the composite sample. Note that if only one species is selected in the sample page, the species 2 edit boxes are grayed and cannot be accessed. Each pressure boundary condition is specified by two values, an initial value and a ramp ($\Delta p/\text{time}$). By entering appropriate values in these edit boxes for each data card, the user may specify a piecewise linear approximation to a continuous time-varying pressure condition. Note that Diffuse II does not calculate the pressure increase due to tritium decay in a closed volume. To model such a case, the user must calculate the tritium partial pressure time history, decompose it to a piecewise linear approximation, and enter the appropriate initial and ramp values for each data card.

Temperatures may be specified for each side of the individual material layers that comprise the composite sample. Similar to the case with the pressure boundary conditions, only those edit boxes associated with defined material layers from the Sample page are enabled for user input. Also similar is the fact that each

Diffuse Input

Sample Control Data

No. of DATA cards 2

Card Number 2 New run

No. print edits 1

Time interval 1 yr

Pressures

Species	Init Value (atm)	Ramp (atm/yr)
1 Front	340.229	0
1 Back	340.229	0
2 Front	340.229	0
2 Back	340.229	0

Temperatures

Init Value (K)	Ramp (K/yr)
313	0
0	0
0	0
0	0
0	0
0	0

Calculate

Figure 4: The *Data* page of the *Diffuse Input* tabbed dialog

temperature is defined by two values, an initial value (K) and a ramp (K/sec). By entering appropriate values in these edit boxes for each data card, the user may specify a piecewise linear approximation to a continuous time-varying temperature condition. Note that Diffuse II interprets temperature values of zero as being equal to the value from the previous layer. Therefore, to enter a uniform time-invariant temperature condition, the user need only enter the desired temperature in the upper left edit box while ensuring that all other values are zero. Diffuse II does not calculate temperature increases due to tritium self-heating.

Main Output Window

The main output window, as shown in Figure 5, contains a graph window for each open document. The graph window provides access to plots that display species concentration profiles, species release rates, or species release integrals. In addition, each plot contains an individual curve for each data card that is defined. The curves are identified by the legend above the graph. When the user clicks anywhere in a graph pane it becomes active and therefore the target of all plot related toolbar and menu commands. The *View* menu, shown in Figure 6, allows the user to select the plot type for display. The available plots types are described in Table 4. Each plot type holds several different plots; the exact number is dependent

Figure 6: View menu

Figure 5: Diffuse main output window

Table 4: Available Plot Types

Type	Plot	Description
Concentration profile	Diffusing species 1 (DS1)	Species (or sum) concentration as a function of distance into the composite sample
	Decay product 1 (DP1)	
	Sum (DS1 + DP1)	
	Diffusing species 2 (DS2)	
	Decay product 2 (DP2)	
	Sum (DS2 + DP2)	
	Sum (DS1 + DS2)	
Release Rate	Diffusing species 1 (front)	Rate of release of species from either the front or back surface of the composite sample. Negative value is into the material.
	Diffusing species 1 (back)	
	Diffusing species 2 (front)	
	Diffusing species 2 (back)	
Release Integral	Diffusing species 1 (front)	Rate of release of species from either the front or back surface of the composite sample. Negative value is into the material.
	Diffusing species 1 (back)	
	Diffusing species 2 (front)	
	Diffusing species 2 (back)

Figure 7: Toolbar

upon the number of species defined. As an alternative to using the View menu for selecting plot type, the user may click one of the three plot type buttons on the toolbar, as shown in Figure 7. The plot scroll buttons allow the user to scroll forwards or backwards through the list of available plots. An additional toolbar button, the Tabbed Dialog Visibility button, allows the user to alternately show and hide the tabbed dialog.

Right-clicking on the graph reveals the Graph Control property pages, as shown in Figure 8, and allows the user to interactively change the graph's appearance. The large number of available pages provides access to almost all graph characteristics. Note, however, that changes made to one graph affect all others.

Figure 8: Graph Control property pages

Figure 9: Option menu

Miscellaneous Options

The *Option* menu, shown in Figure 9, allows the user to select numerical units for entered and displayed time and pressure quantities. This option permits the entry of understandable numerical values for the problem of interest. Available time units include seconds, days, months, and years while available pressure units include atmospheres and pound per square inch (psi).

Viewing the Input and Output Files

The files input to and written by the Diffuse II computational program can be viewed by selecting the desired item from the final two presented in the *View* menu. The user may select either the last generated (current) input file or currently selected plot data file. Because each calculation overwrites the files generated during the previous calculation, only the most recent file sets are available. This version of Diffuse II includes an integral file viewer that is aware of data changes made by the user. Once a calculation is performed, the new data is automatically displayed in the open viewer.

Input File

The input file, *indif.dat*, is a Fortran *namelist* formatted text file read by the Diffuse II computational program. It may be viewed by selecting *Last Input File* from the *View* menu. Diffuse II then starts the data viewer and loads the last input file generated. This simple viewer only allows the displayed contents to be written to a file or copied into a buffer for later pasting into another application. A sample display is shown in Figure 10. Reference 1 provides a detailed description of each of the namelist variables.

Plot Data File

The plot data files are formatted text files that contain the numerical data used to generate the plots in the graph display. The data used to generate the currently selected plot may be displayed by selecting *Last Plot Data* from the *View* menu. Diffuse II then starts the data viewer and loads the last plot file generated for the selected plot type. A sample display is shown in Figure 11. When more than one data card has been created during problem definition, selecting this menu option displays the data card selection dialog shown in Figure 12. Here the user selects the desired data card number from the list box. Clicking the OK button displays the requested data.

```
Diffuse Data Viewer - Namelist Input File
File Edit

$sample
    igeon=2.
    r0=2.54.
    profile=0.1,
    tritium=.T.,
    idiff=2.
    mass=3. 2.
    length=0.1.
    front=2.
    back=1.
    mat='aE '
    ED=0.559.
    D0=0.0047.
    ES=0.0607.
    S0=0.00079.
    DEN=8.5e+022.
    QSTAR=-0.065.
    STICK=0.

Send
$control
    nodes=100.
    ncycles=0.
    nprintc=1.
    fimp=0.25.
    fmat=1.

Send
$data
    nprint=1.
    cprint=.T..
    nplot=3.
    ptype='con','rate','int'.
    yaxis='all','all','all'.
    xaxis='profile','time','time'.
    newrun=.T..
    time=3.15576e+007.
    temp0=313. 0.
    ramp=0. 0.
    p0=340.229. 340.229. 340.229.
    pramp=0. 0. 0. 0.

Send
```

Figure 10: Sample input file

Diffuse Data Viewer - Plot Data (Card 1)						
con profi all						
nsets= 7						
Profile						
Concentration, C1, C2 (all)						
n	profile	c11	c12	c13	c21	c22
0	0.0000E+00	1.0415E-03	5.2441E-05	1.0939E-03	1.1016E-03	
1	1.0204E-03	9.6569E-04	5.2441E-05	1.0181E-03	1.0297E-03	
2	3.0612E-03	8.1725E-04	4.0868E-05	8.5812E-04	8.8840E-04	
3	5.1020E-03	6.7891E-04	3.1640E-05	7.1055E-04	7.5500E-04	
4	7.1429E-03	5.5479E-04	2.4355E-05	5.7914E-04	6.3295E-04	
5	9.1837E-03	4.4695E-04	1.8652E-05	4.6560E-04	5.2428E-04	
6	1.1224E-02	3.5571E-04	1.4222E-05	3.6993E-04	4.2974E-04	
7	1.3265E-02	2.8018E-04	1.0802E-05	2.9099E-04	3.4907E-04	
8	1.5306E-02	2.1876E-04	8.1774E-06	2.2694E-04	2.8133E-04	
9	1.7347E-02	1.6954E-04	6.1722E-06	1.7571E-04	2.2521E-04	
10	1.9388E-02	1.3056E-04	4.6469E-06	1.3520E-04	1.7924E-04	
11	2.1429E-02	9.9997E-05	3.4907E-06	1.0349E-04	1.4194E-04	
12	2.3469E-02	7.6237E-05	2.6171E-06	7.8854E-05	1.1191E-04	
13	2.5510E-02	5.7892E-05	1.9589E-06	5.9851E-05	8.7904E-05	
14	2.7551E-02	4.3812E-05	1.4640E-06	4.5276E-05	6.8820E-05	
15	2.9592E-02	3.3058E-05	1.0927E-06	3.4151E-05	5.3725E-05	
16	3.1633E-02	2.4881E-05	8.1466E-07	2.5695E-05	4.1836E-05	
17	3.3673E-02	1.8685E-05	6.0676E-07	1.9291E-05	3.2507E-05	
18	3.5714E-02	1.4005E-05	4.5152E-07	1.4456E-05	2.5210E-05	
19	3.7755E-02	1.0479E-05	3.3573E-07	1.0815E-05	1.9517E-05	
20	3.9796E-02	7.8298E-06	2.4947E-07	8.0793E-06	1.5088E-05	
21	4.1837E-02	5.8428E-06	1.8526E-07	6.0281E-06	1.1649E-05	
22	4.3878E-02	4.3552E-06	1.3751E-07	4.4927E-06	8.9826E-06	
23	4.5918E-02	3.2431E-06	1.0201E-07	3.3452E-06	6.9198E-06	
24	4.7959E-02	2.4130E-06	7.5651E-08	2.4886E-06	5.3258E-06	
25	5.0000E-02	1.7939E-06	5.6081E-08	1.8500E-06	4.0957E-06	
26	5.2041E-02	1.3328E-06	4.1560E-08	1.3744E-06	3.1475E-06	
27	5.4082E-02	9.8968E-07	3.0790E-08	1.0205E-06	2.4173E-06	
28	5.6122E-02	7.3449E-07	2.2806E-08	7.5730E-07	1.8554E-06	
29	5.8163E-02	5.4486E-07	1.6888E-08	5.6174E-07	1.4234E-06	
30	6.0204E-02	4.0402E-07	1.2503E-08	4.1652E-07	1.0915E-06	
31	6.2245E-02	2.9948E-07	9.2555E-09	3.0874E-07	8.3670E-07	
32	6.4286E-02	2.2192E-07	6.8503E-09	2.2877E-07	6.4113E-07	
33	6.6327E-02	1.6441E-07	5.0694E-09	1.6949E-07	4.9111E-07	

Figure 11: Example plot data file

Figure 12: The Data Card selection dialog

The plot data file concentration, release rate, and release integral columns are labeled with a subscripted alphabetic code, where c = concentration, yr = release rate, and yi = release integral. The first subscript refers to the species number while the second refers to the diffusing species itself (1), its decay product (2), or the sum of the two (3).

Miscellaneous

Code Limitations

Diffuse II currently performs only minimal input value checks. As a result, if the user errs when entering values, the Diffuse computational routines may receive data that is not completely appropriate. Depending upon the nature of the error, the computation may complete and provide erroneous output data that can generally be identified in the output plots. On the other hand, certain input errors may result in more dramatic responses. If the calculation does not complete in a short amount of time, the user can open the computational message output window by clicking on the DiffuseSG2 button on the taskbar. If the calculation is experiencing difficulty, a message may be displayed in this window. Note that the taskbar button is available only while the computational routines are executing. While future versions of Diffuse II may implement a more complete input-checking algorithm, the current version places the responsibility for ensuring consistent input primarily upon the user.

Software Description

This section briefly describes the Diffuse II software development philosophy and structure. The intent of recording this information is to provide future developers with the basis needed for code debugging or upgrading.

Development Environment

The Diffuse II upgrade was developed on a Windows NT PC using the Microsoft Visual Studio integrated development environment (IDE)¹. Visual Studio provides an environment that enables a developer to efficiently write, test, and debug code. All C and C++ code was compiled with Microsoft's Visual C++ 6.0 compiler while the Fortran was compiled with Digital Visual Fortran 5.0 compiler².

Code Structure

Diffuse II contains three executable files, *DiffWin.exe*, *Diffsub2SG.exe*, and *Sgw32.exe*. *DiffWin.exe* is the executable image created by compiling and linking the C++ user interface code while *Diffsub2SG.exe* is the image created by compiling and linking the Fortran computational code. *Sgw32.exe* is a local automation server that produces the plots in the graph pane of the main output window. The user runs Diffuse II by executing the interface image. When the *Calculate* button is clicked, the user interface runs the computational code by spawning a new synchronous process. Once the computational code terminates, the system destroys that process and returns control to the interface code. With this structure, the interface and computational codes run in separate process spaces and do not share memory.

The described structure was selected for one primary reason. The original Fortran Diffuse console application, from which the computational code was derived, used very little interactive user input. Rather, all important inputs were provided in a namelist formatted text file. Additionally, the code wrote all important output data to similar text files. This file I/O configuration of the original Diffuse provided a simple means of file-based communication between the interface and computational codes and required a minimum of Fortran source modification. *indif.dat* is the input file written by the interface while *diff.txt* and *dif.kg** (* = 1 to 15) are the summary report and plot data files written by the computational routines.

Computational Code

As previously mentioned, the finished computational code is a minimal modification of the original Fortran

1. Microsoft Corporation, One Microsoft Way, Redmond, Washington 98052-6399, <http://www.microsoft.com>

2. Digital Equipment Corporation, Maynard, Massachusetts, <http://www.dec.com>

Diffuse application and is itself an executable application. The modifications, which are documented in the source code, include minor syntactic changes to access the Visual Fortran QuickWin run-time library, which adds some windowing capabilities to the application. These statements prevent the application from displaying a window when it executes. Rather, the application window is minimized and is visible only as a taskbar button. While it is active, however, the user may click the button to expand the window. The computational segment was built as a *Standard Graphics* application using the Visual Studio 97 AppWizard. A Standard Graphics configuration was chosen because it supports the QuickWin library routines and allows the window to be minimized at execution.

When it executes, the code expects to find a namelist formatted text file called *indif.dat* in the same directory defined by the DIFFDIR registry variable. If the file is not present, the code will not execute successfully. During execution, the code writes several files: *diff.txt*, which contains text-based summary report, *dif.plt*, the summary plot file, and the individual plot files. The number of individual plot files is determined by the number of data cards identified in the problem definition. The generic individual plot file name is *dif.kg**, where * is an integer between 1 and 15. The file number is given by:

$$\text{file number} = 3(\text{card number} - 1) + \text{graph number} + 1$$

where *card number* = the data card number selected by the user (1 through 5) and *graph number* = 0 for concentration plots, 1 for release rate plots, and 2 for release integral plots.

User Interface Code

The user interface code, written in C++, was built using Visual Studio's MFC (Microsoft Foundation Class) AppWizard as a MDI (multiple document interface) application. The Microsoft Foundation Classes provide object-oriented wrappers around most of the Windows 95/NT API (application programming interface) routines while the MDI architecture allows a user to concurrently work on several Diffuse II documents. The finished interface code comprises many classes, some of which were generated by the AppWizard, most of which were developer-generated, and some of which were generated by the inclusion of software components. The classes are summarized in Table 5. Some of the more interesting classes are described in more detail below.

Property Sheet and Page Classes

The property sheet is the tabbed dialog that contains each of the three property pages. Although the user enters data in these pages, it is stored communally in the document object. The MFC *UpdateData()* statement transfers data to and from the property page edit and list boxes and the dialog class member variables. Two dialog class member functions, *SetMemberData()* and *SetDocumentData()*, transfer data between the corresponding dialog and document member variables.

Each page is responsible for maintaining its own display. Display maintenance includes routine tasks such as

Table 5: Important Classes

Class Name	Description
CAboutDialog	The About Diffuse dialog class. This dialog is displayed from the Help menu.
CChildFrame	The child frame window class.
CControlDlg	The Control dialog (property page) class
CDataDlg	The Data dialog (property page) class
CDiffMsgDlg	The calculation animation dialog class
CDiffWinApp	The application class
CDiffWinDoc	The document class
CDiffWinView	The view class
CGetDCDlg	A dialog class that allows the user to select a data card number when viewing plot data
CGraph	The graph class
CInputPropSheet	The input tabbed dialog (property sheet) class
CMainFrame	The applications main output frame window class.
CSampleDlg	The Sample dialog (property page) class
CSplashDlg	The splash screen dialog class
CSplashThread	A thread class used for the splash screen display

filling the edit boxes with appropriate values, enabling and disabling various controls, and storing edit box data to the member variables.

Document Class

The document object, represented by the *CDiffWinDoc* class, stores all of the data required for creating the computational routine input file, *indif.dat*. It writes this file once it is instructed to initiate a calculation. It then spawns the computational process, reads the resulting data from the appropriate disk files, and updates the graph. The document is also responsible for serializing all of its data and therefore implements all file input and output. A simple schema number written to the data file provides version control for future backward compatibility.

View Class

The view class, *CDiffWinView*, contains a single *CGraph* (provided by a purchased software component called Graph Control.¹) object that fills its client window. This graph is loaded with data and redrawn in response to user requests via the menu or toolbar items or in response to an updated calculation.

1. Graph Control, Pinnacle Publishing, Inc. PO Box 888, Kent, WA 98035-0888, (425) 251-1900, Fax (425) 252-5057, <http://www.pinpub.com>

Data Viewer Class

As previously mentioned, this version of Diffuse II uses an integral data viewer to display the contents of the input and output files. This functionality is implemented in the *CDataViewerDlg* class and is currently limited to data display, serialization to a file, and data copy to a buffer. Although no viewer printing support is yet provided, the copy ability allows the user to transfer the data to another application, such as NotePad, and then print. The viewer is able to receive an *UpdateInfo()* command, generally sent by the document after it has completed a calculation, and fill the viewer with the latest data. Adding direct print capability to the *CDataViewerDlg* class is a desirable upgrade.

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