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A User's Guide for INPAGF_Launcher.DLL

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Abstract

Sandia National Laboratories (Sandia), a U.S. Department of Energy National Laboratory, has over 30 years experience in the assessment of radioactive waste disposal and at the time of this publication is providing assistance internationally in a number of areas relevant to the safety assessment of radioactive waste disposal systems. In cooperation with the Republic of Taiwan's Institute of Nuclear Engineering and Research (INER), Sandia National Laboratories (SNL) has developed software that provides an interface between a deterministic far field mass transport code and GoldSim™ (a commercial software used to conduct Monte Carlo analyses). The SNL developed software enables INER to perform probabilistic simulations for safety analysis and performance assessment of geologic disposal of commercial spent nuclear fuel. The following report details the software design, the steps necessary to use the software, and presents an example application of the paradigm of coupling deterministic codes to a contemporary probabilistic software application.

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A number of people at Sandia National Laboratories including, Donald Kalinich (Org. 6762), Hong-Nian Jow (Org. 6773) (Project Lead), F. Joseph Schelling (Org. 6772), and Cedric Sallaberry (Org. 6784) have made significant contributions to the technology transfer program which either directly or indirectly supported the development of the software documented in this report. In addition, Jerry McNeish (Org. 6784) provided an internal technical review of this report.

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CONTENTS

1. Introduction.....	9
1.1. Purpose.....	9
1.2. Software Identification.....	9
2. User Information.....	11
2.1. Introduction.....	11
2.2. How to Use this Software	11
2.3. Input Specification.....	12
2.3.1. INPAGF_Launcher Input Array: in()	13
2.3.2. INPAGF_Launcher RN.DAT Input File.....	15
2.3.3. Version of INPAG-F compatible with INPAGF_Launcher	17
2.3.4. INPAGF_Launcher Input Subroutines	17
2.4. Output Specification	17
2.4.1. INPAGF_Launcher Output Array: out().....	18
2.4.2. Output Files Read by INPAGF_Launcher DLL	19
2.4.3. INPAGF_Launcher Output Subroutines.....	19
2.5. Data Files	20
2.6. Defaults.....	20
2.7. Errors.....	20
2.8. Hardware/Software Environments.....	21
3. Installation and Test Cases.....	23
3.1. Installation.....	23
3.2. Test Cases	23
4. Summary	25
5. References.....	27
Appendix A: Source Code and Test Cases	29
A.0 Test Cases	29
A.1 INPAGF_Launcher_v3.DLL and Source Code.....	29
A.2 RN.DAT.....	29
A.3 INPAG-F Test Case Results	29
Distribution	30

FIGURES

Figure 1: Flow Chart for INPAGF_Launcher.....	12
Figure 2 : External DLL Element in GoldSim™ linking in() array to INPAGF_Launcher DLL	13
Figure 3 : Example GoldSim™ model file with 13 Input Blocks needed for INPAG-F input. ...	14
Figure 4: Example RN.DAT input file with 40 radionuclides and 6 stable isotope species.....	16
Figure 5: External DLL Element in GoldSim™ linking out() array to INPAGF_Launcher DLL	18

TABLES

Table 1 : INPAGF_Launcher.DLL Input Array	15
Table 2: Versions of INPAG-F that can be run with INPAGF_Launcher.....	17
Table 3: INPAGF_Launcher DLL Output Array.....	19
Table 4: Versions of INPAG-F output files that can be read by INPAGF_Launcher	19
Table 5: Common DLL Error Messages.....	20
Table 6: Steps for Installation and Testing	23

NOMENCLATURE

DOE	Department of Energy
INER	Institute of Nuclear Energy Research
INPAG-F	INER Performance Assessment Model for the Geologic Repository of Spent Fuel – Far Field Transport
INPAG-FL	INER Performance Assessment Model for the Geologic Repository of Spent Fuel – Far Field Transport (Laplace Transform Solution)
INPAG-N	INER Performance Assessment Model for the Geologic Repository of Spent Fuel – Near Field Transport
INPAG-NV2	INER Performance Assessment Model for the Geologic Repository of Spent Fuel – Near Field Transport Version 2
INPAG-NH	INER Performance Assessment Model for the Geologic Repository of Spent Fuel – Near Field Transport - Horizontal Emplacement
LHS	Latin Hypercube Sampling
SNF	Spent Nuclear Fuel
SNL	Sandia National Laboratories

1. INTRODUCTION

1.1. Purpose

The objective of the INPAGF_Launcher.DLL User's Guide is to provide documentation of the capabilities of the dynamically linked library (DLL) software as well as document the code used to create the application. The features of the DLL as well as required input and output information will be presented. An example model is included in Appendix A and should be used as an aide to using the INPAGF_Launcher DLL.

1.2. Software Identification

This user's guide documents the dynamically linked library software INPAGF_Launcher_v3.DLL. INPAGF_Launcher_v3.DLL discussed in this manual has been designated as open-source and is freely available. It can be accessed on a Sandia National Laboratories website at the following URL: <http://www.sandia.gov/icp/>. Copyright (2006) Sandia Corporation. Under the terms of Contract DE-AC04-94AL85000, Sandia Corporation and the United States Government retains certain rights in this software.

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2. USER INFORMATION

2.1. Introduction

INPAGF_Launcher software has been designed to interface between the commercial software GoldSim.exe (GoldSim Technology Group LLC, 2006) and INER's near field radionuclide mass transport code INPAG-F (Zhou, 2001). The INPAG-F code simulates the far field radionuclide mass transport of radionuclides containing commercial spent nuclear fuel (SNF). The INPAG-F code was coupled with GoldSim™ to create the framework for a probabilistic model capable of evaluating uncertainties in a potential SNF repository system. This document is intended as a user's guide for the INPAGF_Launcher software and the model file GoldSim™ is needed to execute a probabilistic simulation.

The INPAGF_Launcher software is called in the form of a direct link library (DLL) by GoldSim.exe during an execution of a GoldSim™ model file specifically designed for the purpose of running INPAG-F for a probabilistic simulation. All related libraries needed by the DLL are linked with it.

The INPAGF_Launcher is programmed in the FORTRAN 90 language, and developed with Compaq Visual FORTRAN Professional Edition 6.6a (Digital Equipment Corporation, 1998) and is implemented on the Windows XP operating system.

2.2. How to Use this Software

This software is called from a GoldSim™ model file. It is simply placed in a directory accessible to the GoldSim™ model file. Execution control of the DLL is provided by the GoldSim™ software (GoldSim Technology Group LLC, 2006, Appendix C). It is assumed the user has a basic proficiency with GoldSim™ and the necessary understanding of the features of the GoldSim™ code to operate this DLL. The GoldSim™ model file itself should be considered as part of the model documentation. In addition, a user must understand the features of the INPAG-F software (Zhou, 2001).

Since this software is a DLL, there is little direct interaction required between the user and the software. The GoldSim™ model file supplies the 11 data input blocks necessary for creating an INPAG-F input file to the INPAGF_Launcher DLL and receives the INPAG-N.EXE calculation results from the DLL. The user has access to the INPAGF_Launcher inputs and INPAG-F flux outputs through the GoldSim™ model. An example GoldSim™ model discussed in this manual has been designated as open-source and is freely available. The example model file is included with the report and can also be accessed on a Sandia National Laboratories website at the following URL: <http://www.sandia.gov/icp/>.

Figure 1 shows a flow chart of the operations carried out by the INPAGF_Launcher DLL. The INPAGF_Launcher requires that an array of input parameter values are passed from a GoldSim™ model file to the INPAGF_Launcher DLL. The input array should be defined using a GoldSim™ model as specified in the Table 1, and discussed in Section 2.3 Input Specification. When a GoldSim™ model is executed, the input array will be passed to the INPAGF_Launcher

DLL. The INPAGF_Launcher DLL will execute subroutines to parse the input array and write an INPAG-F input file to the local directory. The DLL will call the selected version of INPAG-F and execute the code using the generated input file. After the INPAG-F code has completed its simulation, the DLL will read selected output files and pass the output back to the GoldSim™ model file where it is loaded in a table element. These steps are repeated sequentially for each realization for a probabilistic simulation.

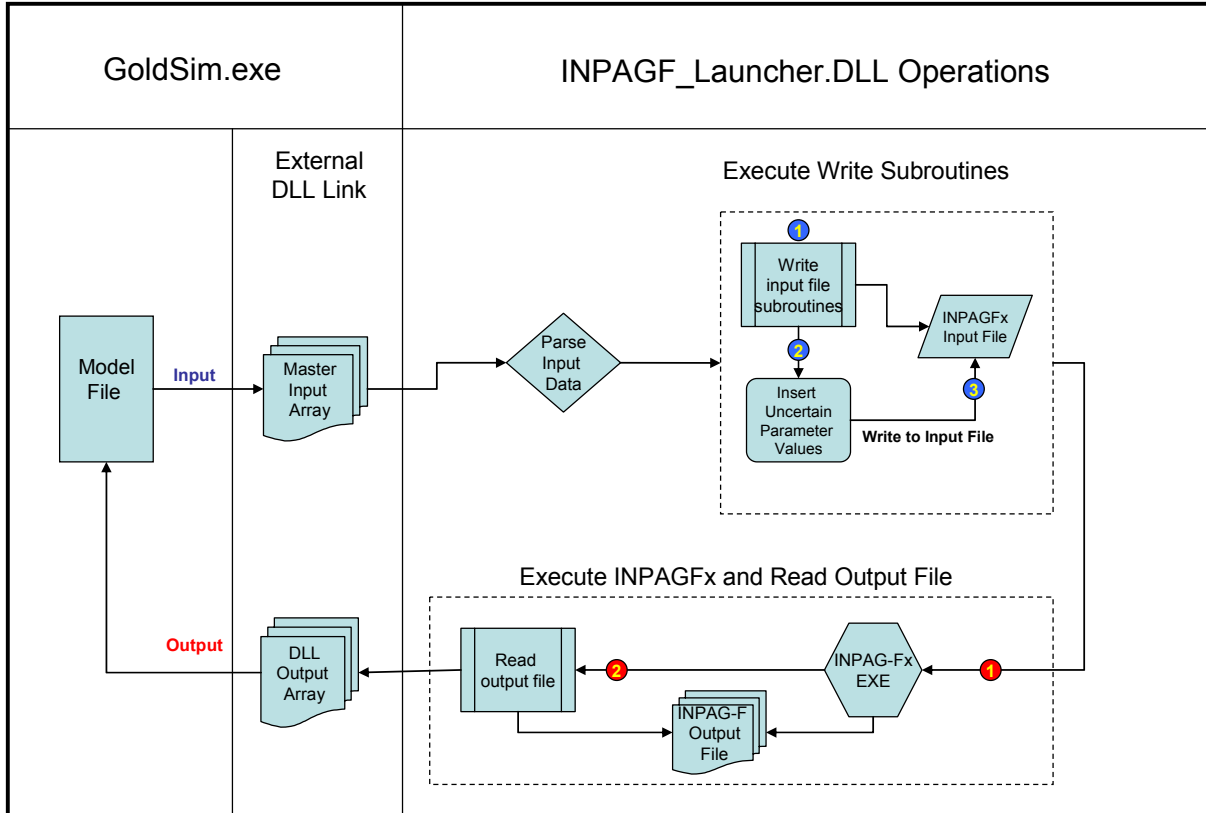


Figure 1: Flow Chart for INPAGF_Launcher

2.3. Input Specification

The inputs to the INPAGF_Launcher DLL come either from the “RN.DAT” file or from the in() array passed by a GoldSim™ model. The values passed to the DLL via the in() array can be single values or arrays of data. Table 1 lists the input array in() expected by the DLL.

The input values may be constants or stochastics that will be sampled once per realization during a probabilistic simulation.

2.3.1. INPAGF_Launcher Input Array: in()

An in() array needs to be defined in the GoldSim™ model file and passed to the INPAGF_Launcher DLL during execution of the code. Figure 2 shows an example DLL External Element (GoldSim User's Guide, GoldSim Technology Group LLC, 2006), which is used in the GoldSim™ model file to define a link between the GoldSim.exe and a DLL. The external DLL element requires the following inputs: 1) name of the DLL to be called [INPAGF_Launcher_v3.DLL], 2) the function being called [launch_inpagf], and 3) the input array [in()]. In addition, three outputs have been defined and are discussed in Section 2.4, Output Specification.

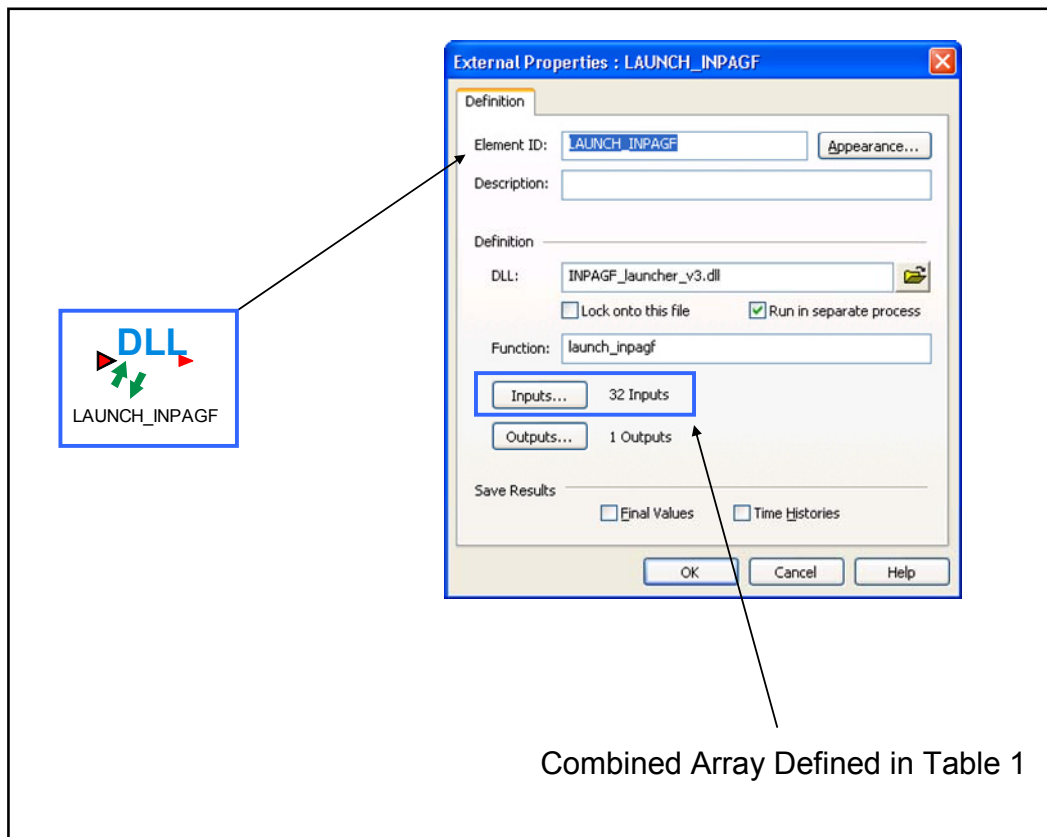


Figure 2 : External DLL Element in GoldSim™ linking in() array to INPAGF_Launcher DLL

The input array [in()] is defined in GoldSim™ and must contain all of the elements listed in the “in () Array” defined in Table 1. The array includes all of the input parameters required for both versions of INPAG-F. The first three elements in the array include a parameter that identifies the version of INPAG-F which is to be run, the realization number, and the number of radionuclides in the simulation. The remaining elements in the array make up the input parameter values for

each of the 10 input blocks required for INPAG-F input file. Figure 3 illustrates the eleven INPAG-F input blocks as defined in the example GoldSim™ input file. Each container in the example GoldSim™ file (shown in Figure 3), contains the input parameters listed in Table 1.

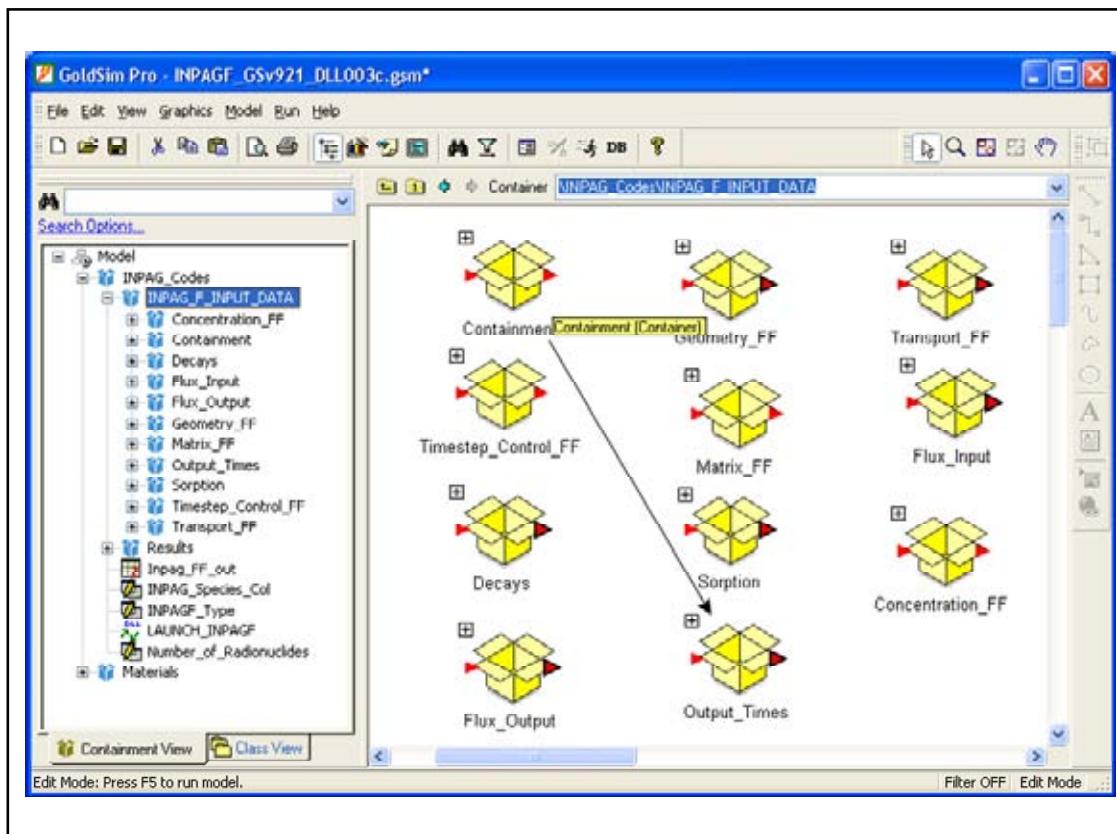


Figure 3 : Example GoldSim™ model file with 11 Input Blocks needed for INPAG-F input.

The input blocks and parameters are listed in Table 1 in the order that the DLL expects to receive them. The DLL accepts a value between 0 and 1 for the version of INPAG-F (0=INPAGF.EXE, 1=INPAGFL.EXE). It is important to note that two of the input parameters shown in Table 1 are vectors and include a number of elements equal to the number of radionuclide species. Thus, the total size of the input array will change with the number of radionuclides defined in the simulation.

Table 1 : INPAGF_Launcher.DLL Input Array

BLOCK	in() Array	Notes	in() Index	Type
N/A	INPAG_F_Type	Selects version of INPAG F to run	1	Value
	Realization	Realization number for probabilistic simulations.	2	Value
	Number_of_RN	Number_of_RN	3	Value
TIMESTEP-CONTROL	TOLERANCE		4	Value
	MIN-TIMESTEP		5	Value
DECAYS	DECAY RATES		6	Vector Species
FLUX-OUTPUT	UNITS MOLPYR	Value of 1 = Mol/yr, 0 = Bq/yr.	10	Value
GEOMETRY	GEOSPHERE-LENGTH		11	Value
	BOREHOLE-PITCH		12	Value
	SORPTION-DEPTH		13	Value
	CANISTER-LENGTH		14	Value
	FRACTURE-SPACING		15	Value
	FRACTURE-APERTURE		16	Value
	FRACTURE-GRIDS		17	Value
MATRIX	MATRIX-GRIDS		18	Value
	DENSITY		19	Value
MATRIX	POROSITY		20	Value
SORPTION	FF ROCK		21	Vector Species
OUTPUT-TIMES	START-TIME		25	Value
	END-TIME		26	Value
	# INTERVAL		27	Value
	NO-PER-DECADE		28	Value
TRANSPORT	DARCY-VELOCITY		29	Value
	FRACTURE-DIFFUSION		30	Value
	MATRIX-DIFFUSION		31	Value
	DISPERSIVITY		32	Value
FLUX-INPUT	FILENAME	Value of 1 to 5 corresponding the the five different input flux file names used for INPAGN versions.	33	Value
	UNITS	Value of 1 = Mol/yr, 0 = Bq/yr.	34	Value
CONCENTRATION	NO-OF-TIMES		35	Value
	CONC-TIMES		36	Value
	CONC-TIMES		37	Value
	CONC-TIMES		38	Value

Note: The in() array index number is scaled for four radionuclides for the example presented in Table 1.

2.3.2. INPAGF_Launcher RN.DAT Input File

The INPAGF_Launcher DLL needs to read a file called “RN.DAT”. The RN.DAT file is a simple text file that contains a list of the radionuclides included in the simulation. GoldSim™ cannot pass text STRINGS and therefore the radionuclide labels are needed for the DLL to write the INPAG-F input file. Figure 4 shows an example of a RN.DAT file that contains 40 radionuclide species and 6 stable isotope species. The RN.DAT file should list the radionuclides in the same order and format (excluding the half life) as the DECAYS input block required by INPAG-F. The RN.DAT input file must be defined in the order shown in Figure 4. The first value is the total number of radionuclides. The DLL uses this value to check that the in() array passed by GoldSim™ is the correct size. The second number lists the number of stable isotope

species included in an INPAG-N input file. This feature is only available in the INER versions for INPAGNV2.exe and INPAGNH.exe (INER, 2007). This value should be 0 for simulations without any stable isotopes defined.

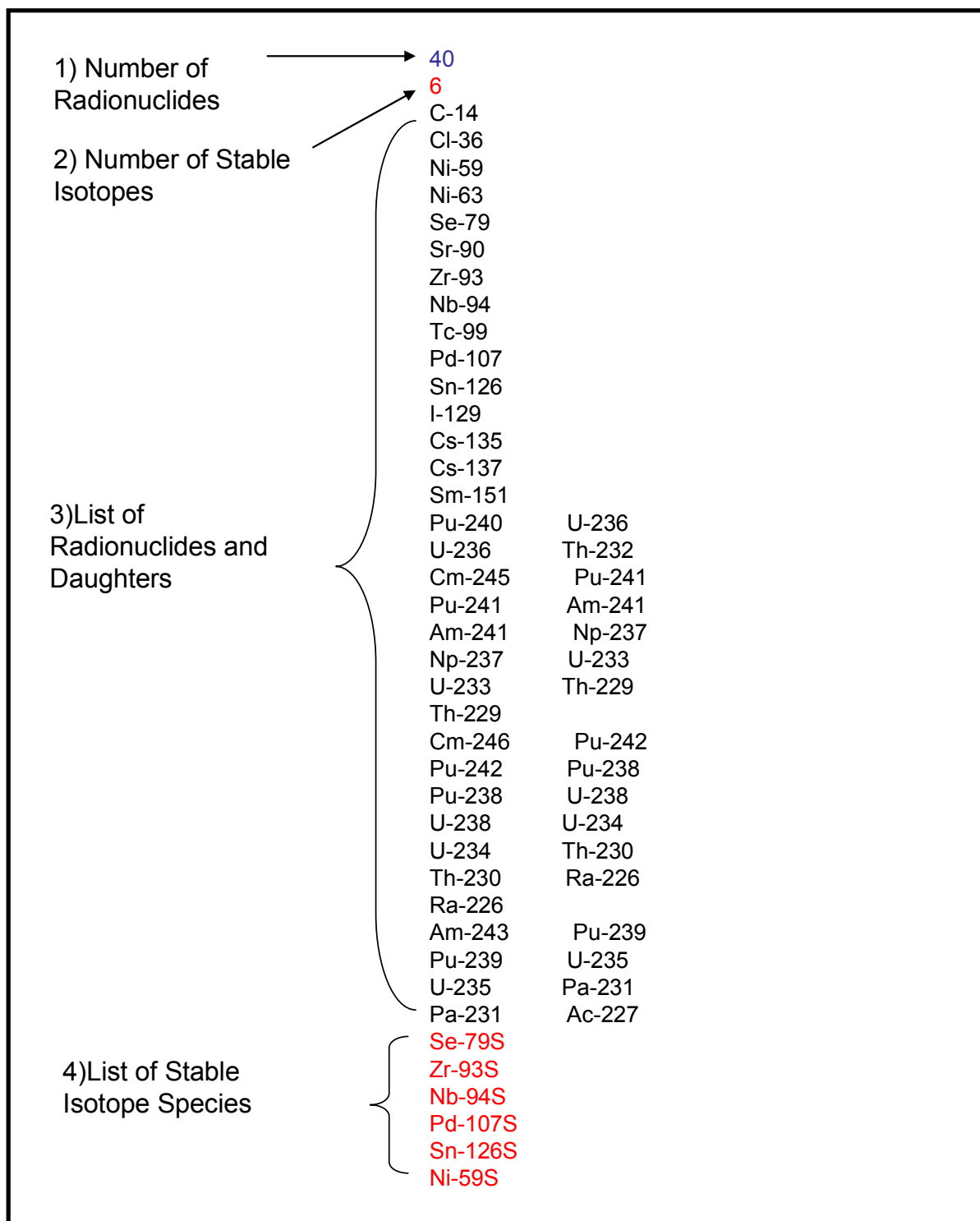


Figure 4: Example RN.DAT input file with 40 radionuclides and 6 stable isotope species.

2.3.3. Version of INPAG-F compatible with INPAGF_Launcher

The INPAGF_Launcher DLL is capable of executing with two versions of INPAG-F. The two versions are listed in Table 2.

Table 2: Versions of INPAG-F that can be run with INPAGF_Launcher

INPAG-N Version	Date	Description	Reference
INPAGF.EXE	04/19/2002	INPAG-F is developed for calculating far field radionuclide transport for the total system performance assessment of Taiwanese geological repository of spent nuclear fuel.	(Zhou, 2001)
INPAGFL.EXE	06/09/2004	Version of INPAG-F which uses a La Place Transform solution.	(Zhou & Kozak, 2004)

2.3.4. INPAGF_Launcher Input Subroutines

The INPAGF_Launcher DLL is executed using a series of calls to subroutines. The order of subroutine calls are listed below:

1. Title
2. Timestep_Control
3. Decays
4. Flux-Output
5. Geometry
6. Matrix
7. Sorption
8. Output_Times
9. Transport
10. Flux-Input
11. Concentration

The subroutines read the input values contained in the in() array passed by GoldSim™. Each subroutine writes the data to the INPAG-F input file. The source code is included in the attached CD ROM, as listed in Appendix A.

2.4. Output Specification

The outputs from the INPAGF_Launcher DLL come from the output flux file created after INPAG-F has successfully completed. The DLL reads the values from the INPAG-F output file and loads them into the out() array which comprises a single array of values that is passed to GoldSim.exe at the end of each INPAG-F model run. Table 3 lists the output array out() passed by the DLL to the GoldSim.exe. The output values will be passed to GoldSim.exe once per realization during a probabilistic simulation.

2.4.1. INPAGF_Launcher Output Array: out()

An out() array needs to be defined in the GoldSim™ model file to accept the out() array passed to the INPAGF_Launcher DLL during execution of the code. Figure 5 shows an example DLL External Element (GoldSim User's Guide, GoldSim, 2006), which is used in the GoldSim™ model file to define a link between the GoldSim.exe and a DLL. The external DLL element requires a 2-D table element to be defined. The INPAGF_Launcher DLL passes the total radionuclide flux from INPAG-F.

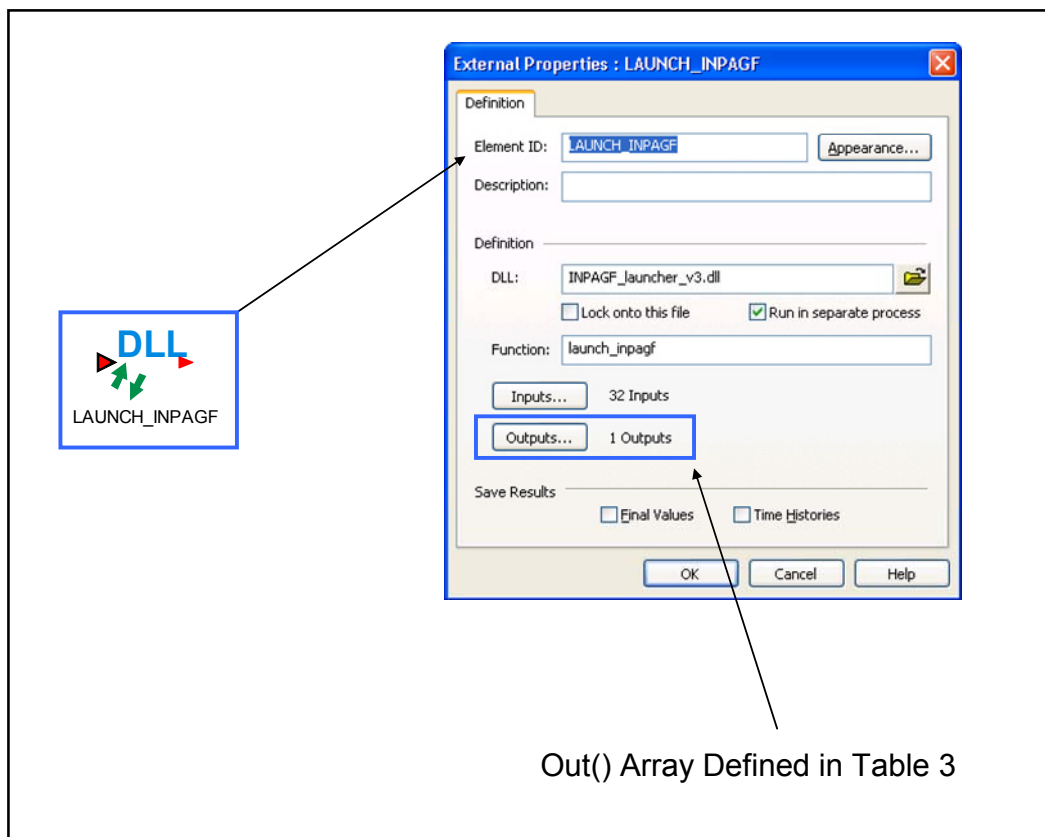


Figure 5: External DLL Element in GoldSim™ linking out() array to INPAGF_Launcher DLL

The output blocks and values are listed in Table 3 in the order that the GoldSim.exe and External DLL element expects to receive them. The GoldSim.exe calls the METHOD and reads the entire out() array at each call. The out() array is over written for each METHOD call. Refer to the GoldSim Users Manual Appendix C (p. 534, GoldSim Technology Group LLC, 2006) for further details on linking DLLs with the GoldSim.exe.

Table 3: INPAGF_Launcher DLL Output Array

out () Array	Value	Description
Method = 2		
out(1)	3.0	DLL Version
Method = 2		
out(1)	$32 + (2 \times \text{number of RN's})$	Expected values in the in() array
out(2)	$(\text{number of RN's} \times 200) + 200$	Expected out() array size
Method = 2		
out(1)	2.0	Start RN flux (total) output (value of 2 = 2-D table)
out(2)	T	number of timesteps
out(3)	R	number of columns
out(4) -	Timestep values	row labels
out(3+T)		
out(*) -	RN number	column labels (integer values between 1 and the total number of RNs)
out(*+R)		
out(*) -	RN Concentrations	concentration values passed by row
out(*+T*R)		

2.4.2. Output Files Read by INPAGF_Launcher DLL

The INPAGF_Launcher DLL reads the concentration output created by INPAG-F. Table 4 lists the INPAG-F output file by INPAG-F version.

Table 4: Versions of INPAG-F output files that can be read by INPAGF_Launcher

INPAG-F Version	Output File	Description
INPAGF.EXE	BASEFF.FLX	INPAG-F output that contains the radionuclide concentration for selected output times.
INPAGFL.EXE	BASEFF.FLX	INPAG-FL output that contains the radionuclide concentration for selected output times.

2.4.3. INPAGF_Launcher Output Subroutines

The INPAGF_Launcher DLL reads the INPAG-F output file using a series of calls to subroutines. The first call is to execute the specified version of the INPAGF.exe for the input file generated by the DLL (see Section 2.3 for Input Specifications). Next the output file is read and the data is passed back to the GoldSim.exe. The order of operations are listed below:

1. SYSTEM
2. Read INPAG-F Output files
3. Load out() array
4. Pass out() array to GoldSim.exe
5. Clean-up and exit

The DLL reads the values contained in the output file created by INPAG-F. The source code is included in the attached CD ROM, as listed in Appendix A.

2.5. Data Files

Sections 2.3 and 2.4 describe the format of the RN.dat input file and the required output data file as dictated by the versions of INPAG-F. The INPAGF_Launcher DLL writes one debug data file, scratch_f.txt. This is an ASCII text file that echo's the input and output arrays and prints out check points during the DLL execution that can be used to debug the input/output operations.

2.6. Defaults

There are no defaults. The INPAGF_Launcher DLL must receive the entire in() array or it will not run.

2.7. Errors

General error detection is not provided with the DLL. Table 5 lists common error messages generated by the DLL and the GoldSim.exe and some possible causes.

Table 5: Common DLL Error Messages

Error Message	Possible Cause(s)
The model cannot be run. LAUNCH_INPAGF: \\Near_Field_Calcuations\\INPAG_Calcuations\\Run_INPAG_F Could not load the DLL INPAGN_launcher_v3.dll	DLL is not in the Local Directory
	RN.DAT specified incorrectly
	in() array specified incorrectly
The model cannot be run. External element \\Near_Field_Calcuations\\INPAG_Calcuations\\Run_INPAG_F\\LAUNCH_INPAGF must have at least 1 output	No output defined in GoldSim.exe model file for the DLL external element.
The model cannot be run. External element\\INPAG_Calcuations\\Run_INPAG_F\\LAUNCH_INPAGF input arguments do not match; External function is expecting 85 inputs, 86 arguments are defined in GoldSim™	in() array specified with incorrect number of elements.
The model cannot be run. Dimensions do not match for output of external element \\INPAG_Calcuations\\Run_INPAG_F\\LAUNCH_INPAGF	The DLL passes a 2-D table to the GoldSim.exe and the external element must have the correct type selected.
\\INPAG_Calcuations\\Run_INPAG_F\\LAUNCH_INPAGF Win32Exception caught: at address 0x	DLL Error
Visual Fortran run-time error: Forrtl:severe(2): file not found, unit 95,	Rn.dat file is not in local directory
Visual Fortran run-time error: Forrtl:severe(2): file not found, unit 9,	Rn.dat file is not in local directory
Visual Fortran run-time error: Forrtl:severe(2): file not found, unit 12,	*.FLX file not in local directory.
	selected version of INPAGF.EXE did not execute successfully
	selected version of INPAGF is not found in the local directory
	Input file did not execute; errors in input file data

2.8. Hardware/Software Environments

The minimal hardware configuration to run INPAGF_Launcher DLL is a computer equipped with a Windows 32-bit or 64-bit operating system (e.g., Windows XP). INPAGF_Launcher DLL is developed as a dynamic link library (DLL) that must be called by another application. The software, GoldSim.exe (GoldSim Technology Group LLC, 2006), is required to operate the DLL. In addition, at least one version of INPAG-F (listed in Table 2) is required for the successful execution of the DLL.

3. INSTALLATION AND TEST CASES

3.1. Installation

Before installing the INPAGF_Launcher software, the user must ensure that a Windows operating system is installed on the target platform (see Section 2.8 Hardware/Software Specifications). The INPAGF_Launcher software is installed by placing a copy of the software on the hard-drive of a computer. The installation and test cases described herein assume that GoldSim™ (e.g. GoldSim™ Version 9.21 or later) is installed on the target machine. In addition, at least one version of INPAG-F (listed in Table 2) must be installed in the local directory to which the DLL and test cases are executed.

3.2. Test Cases

A test case is provided in Appendix A. Following the steps listed in Table 6 will provide evidence that the DLL is operating correctly once installed and that the functional requirements are satisfied. The test looks at the normal or expected operation of the DLL and has been developed to show a comparison of the resulting tables.

Table 6: Steps for Installation and Testing

Step	Description	Verification Results
1	Copy the INPAGF_Launcher_v3.dll, RN_No_Daughter.DAT file, the test BASENF.FLX file and INPAGF_Launcher_DLLv3_Test_Case .gsm from the Appendix A directories on the CD media to a test directory on a workstation or desktop computer	Files appears in directory
2	Copy an executable version of INPAG-F (listed in Table 2) on the local computer that contains INPAGF_Launcher_v3.dll, INPAGF_Launcher_DLLv3_Test_Case.gsm, and the BASENF.FLX file.	File(s) appears in directory on the local computer.
3	Rename RN_Daughter.DAT to RN.DAT	File appears in directory.
4	Launch GoldSim™ v9.21 (or later)	GoldSim™ is launched
5	Open the file INPAGF_Launcher_DLLv3_Test_Case.gsm in GoldSim™	File opens.

Table 6: Continued.

Step	Description	Verification Results
6	Select the version of INPAG-F by selecting 0 or 1 for the element "INPAG_F_Type" in the INPAGF_Launcher_DLLv3_Test_Case.gsm file	N/A
7	Run the file by selecting /Model/Run Model from the pull-down menus.	GoldSim™ Run Controller appears. Dialog box appears with query, "Starting a new simulation will destroy your existing results. Are you sure you want to run again?"
8	Select "Yes" to dialog box query.	Dialog box appears stating "Simulation Complete!"
9	Click "OK" in dialog box.	Dialog box disappears. Run Controller may also disappear depending upon GoldSim™ option settings.
10	Verify that the contents of the results tables match the output for test file results in Appendix A.3.	Results match.
11	Repeat Steps 6-10 for each version of INPAG-F	N/A

Please note that the values contained in the test case, INPAGF_Launcher_v3_DLL.gsm, should not be used for any other purpose than as an example. The values do not necessarily represent a real repository system and are only default values used in an example model. In addition, the test case is set up for multiple realizations. Single realizations should be run to compare the results to the results from stand alone INPAG-F .exe runs.

One additional test case has been included in Appendix A on the attached CD ROM. This case can be used to link both INPAGF_Launcher.DLL and INPAGN_Launcher.DLL (Mattie and Kalinich, 2007) to a single GoldSim.exe model file and execute both in series. The INPAG-N code is used to simulation source term and near field transport and the INPAG-F code is used to simulation far field transport. They were created to work in series and therefore it would be desirable to run a probabilistic simulation using both codes.

4. SUMMARY

The objective of this document is to provide a guide for using the INPAGF_Launcher DLL software package with GoldSim.exe. The test cases included with this manual was based upon a hypothetical performance assessment model constructed by Sandia National Laboratories as part of a technology transfer program funded by the Taiwan ICP Phase II - Technology Transfer for Interim Dry Storage and Final Disposal of Spent Nuclear Fuel under a WFO Funds-in agreement contract between Sandia and Lockheed Martin. This work supports DOE/RW international leadership in geologic disposal of spent nuclear fuels and radioactive waste and working item IN-SNL-DD23, "Technology Transfer for Geologic Repository Science and Performance Assessment", under the AIT/TECRO Joint Standing Committee for Civil Nuclear Cooperation. Sandia National has over 30 years experience in assessing radioactive waste disposal and at the time of this publication is providing assistance internationally in a number of areas relevant to the safety assessment of radioactive waste disposal systems.

The SNL developed software enables INER to perform probabilistic simulations for safety analysis and performance assessment of geologic disposal of commercial spent nuclear fuel. The report guides a user through the steps necessary to use the software and presents a successful test case demonstrating the paradigm of coupling deterministic codes to a contemporary probabilistic software application. The effort was the result of a cooperative technology transfer project between Sandia National Laboratories and the Institute of Nuclear Energy Research (INER) in Taiwan for the preliminary assessment of a potential SNF waste repository in Taiwan. However, this software package can be easily modified to model site specific conditions for assessments of other potential radioactive waste repositories.

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APPENDIX A: SOURCE CODE AND TEST CASES

The source code and example GoldSim™ model file discussed in this document are stored on the Compact Disc (CD) distributed with this SAND report, and are also available for download at <http://www.sandia.gov/icp/>.

A.0 Test Cases

INPAGF_Launcher_DLLv3_GSv921_Test_Case.gsm
INPAGN_INPAGF_Launcher_DLLs_v3_GSv921_Test_Case.gsm
INPAGN_Launcher_v3.DLL
BASENF.FLX

A.1 INPAGF_Launcher_v3.DLL and Source Code

Launch_inpagf_v003.f90
INPAGF_Launcher_v3.DLL

A.2 RN.DAT

RN_No_Daughter.DAT
RN_Daughter.DAT

A.3 INPAG-F Test Case Results

INPAGF_BASEFF.FLX
INPAGFL_BASEFF.FLX

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