Case study

PHASS99: A software program for retrieving and decoding the radiometric ages of igneous rocks from the international database IGBADAT

CrossMark

Ali T. Al-Mishwat

Department of Earth and Environmental Sciences, Kuwait University, P.O. Box 5969, 13060, Kuwait

ABSTRACT

PHASS99 is a FORTRAN program designed to retrieve and decode radiometric and other physical age information of igneous rocks contained in the international database IGBADAT (Igneous Base Data File). In the database, ages are stored in a proprietary format using mnemonic representations. The program can handle up to 99 ages in an igneous rock specimen and caters to forty radiometric age systems. The radiometric age alphanumeric strings assigned to each specimen description in the database consist of four components: the numeric age and its exponential modifier, a four-character mnemonic method identification, a two-character mnemonic name of analysed material, and the reference number in the rock group bibliography vector. For each specimen, the program searches for radiometric age strings, extracts them, parses them, decodes the different age components, and converts them to high-level English equivalents. IGBADAT and similarly-structured files are used for input. The output includes three files: a flat raw ASCII text file containing retrieved radiometric age information, a generic spreadsheet-compatible file for data import to spreadsheets, and an error file. PHASS99 builds on the old program TSTPHA (Test Physical Age) decoder program and expands greatly its capabilities. PHASS99 is simple, user friendly, fast, efficient, and does not require users to have knowledge of programing.

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1. Introduction

This paper introduces to earth scientists a simple, yet powerful, FORTRAN software program designed to retrieve geochronological information from the international IGBADAT database, for use in petrogenesis research. The program is fast, efficient, and demands no programming skills by users. Below is a short description of the IGBA (Igneous Base) system, the IGBADAT database, and DECIGB (Decode Igneous Base). In this contribution, 'radiometric' and 'physical' age adjectives are used interchangeably.

Since the late 1990s, the present author has been involved in a campaign to expand programs and libraries in IGBA software packages. Results include extensive enhancements and additional capabilities (Al-Mishwat, 1997). The PHASS99 program described in this contribution is one such development towards this objective.

1.1. IGBA

The IGBA petrologic database was originally developed by Chayes and Brandle (1974) in the Carnegie Institution of Washington D.C.

and formally published by Chayes (1985). The history of the IGBA system is found in Chayes (1990). Li and Chayes (1983) and Chayes (1987) described the design and generation of the database. The IGBA system contains the database IGBADAT and its associated packages of FORTRAN software programs for input into, and output from the IGBA databases and for their maintenance. The system also contains a bibliographic reference data file of the literature sources. Readers are referred to Chayes (1983), Brandle (1994) and IGCP (1984) for information on the proprietary syntax, grammar and vocabulary of IGBA. In the 1990s, IGBADAT moved to the Internet platform (Brandle and Nagy, 1995a; Brandle et al., 1997).

1.2. IGBADAT

IGBADAT is a repository of published information on igneous rocks from many regions (Chayes, 1985). It contains petrological, lithological, mineralogical, geochemical, geochronological, stratigraphical data, and other ancillary information. This wealth of data is of interest to many researchers of igneous rocks (Nishiwaki and Brandle, 2007), but it has not been sufficiently utilized as a result of the lack of appropriate software programs. This contribution focuses on the geochronological component of specimen

descriptions in the IGBADAT database.

IGBADAT is supervised by the International Union of Geological Sciences (IUGS), Commission on Systematics in Petrology (Subcommission on Data Bases in Petrology), and housed in the National Geophysical Data Center (World Data Center A) in Boulder, Colorado (USA).

The current version of GBADAT has information on more than 25,000 specimens of plutonic and volcanic rocks from all over the world, and contains in excess of three million records.

The IGBADAT information base is specimen-based. Published age information extracted for each sample from the literature is contained in a specimen description which includes detailed information on the specimen. Each specimen description consists of three records (A, B and C records) as presented in Supplementary material A. Records A and B are a one line each with the name of the geological rock unit and major element chemistry clearly indicated, while record C is a multi-line containing all other information.

Record C contains the bulk of information on the specimen. It is represented by C records in specimen descriptions in Supplementary material A. Different types of information constituting record C are separated by colons. Radiometric age information is located between the second and third colons, and after the first semicolon in this range. Stratigraphic ages, if reported in sample description, occupy the position between the second colon and the first semicolon in the range (Al-Mishwat, 1997).

1.3. DECIGB

The DECIGB package is one of the IGBA system packages (Chayes, 1986, 1988). It is a library containing a set of FORTRAN subroutine programs designed to decode age and other types of information. The library is accessed by many decoding modules for IGBA databases, one of which is PHASS99.

The embryonic algorithm for core codes and search engines in the DECIGB package was developed as a rudimentary tool containing small code module units (Chayes, 1986). Le Maitre and Chayes (1985) commented briefly on the decoding of IGBADAT.

2. PHASS99 program

2.1. General description

The IGBA system DECIGB package (Chayes, 1988) is composed of a large number of individual FORTRAN programs and an associated decoding library designed for the sole purpose of decoding various types of information contained in IGBADAT and similar databases. Previous decoding of radiometric and other physical ages was accomplished by the TSTPHA program in the DECIGB package, which is the predecessor to PHASS99. PHASS99 is far more encompassing and superior to TSTPHA, due to its expanded capabilities and added functionalities. Table 1 lists the differences between PHASS99 and TSTPHA.

The radiometric age in a specimen description consists of an alphanumeric string which supplies all information requisite for characterization of that age. Strings are identified, retrieved, parsed and their mnemonic representations are converted to high-level English counterparts. Supplementary material A shows a small IGBA database containing descriptions for eight specimens. Fictitious ages are used to illustrate the diversity of age methods and information.

2.2. Radiometric ages

IGBADAT and databases of similar structure, such as KAYDER (Unan, 1983, 1993) rely heavily on the use of mnemonic

Table 1
Comparison between features of TSTPHA (Chayes, 1986) and PHASS99 (Al-Mishwat, this paper).

	(Chayes)	(Al-Mishwat)
Platform	Mainframe-DEC	PC-WINDOWS
Number of specimens	Not specified	300 000
Number of Age Systems	10	40
Number of ages/specimen	5	99
Spreadsheet	N	Y
Style of Decoding	Mnemonic	English
Library	Separate	Bundled
Error file	N	Y

Table 2
List of radiometric and other physical age methods handled by PHASS99. Chayes (1983) methods are tagged by asterisks.

	MNEMONICS	ENGLISH EQUIVALENTS
01*	???	UNKNOWN METHOD
02*	OTHR	OTHER METHODS
03*	MGNT	MAGNETIC STRIPING
04*	FSTR	FISSION TRACK
05*	ISKR	ISOCHRON
06*	CN14	CARBON-NITROGEN
07	SN73	^{147}SAMARIUM–^{143}NEODYMIUM
08	SN62	^{146}SAMARIUM–^{142}NEODYMIUM
09*	DMNS	DEPLETED MANTLE ND-SM
10	CHUR	CONDRITIC-NORMALIZED
11*	RS87	RUBIDIUM–STRONTIUM
12	RSMI	RB-SR MINERAL ISOCHRON
13	UTH	GENERAL URANIUM–THORIUM
14	UT40	^{234}URANIUM–^{230}THORIUM
15*	UPB	GENERAL URANIUM-LEAD
16	UP86	^{238}URANIUM–^{206}LEAD
17	UP57	^{235}URANIUM–^{207}LEAD
18	TP28	^{232}THORIUM–^{208}LEAD
19	TR06	^{230}THORIUM–^{226}RADIUM
20	PP76	^{207}LEAD–^{206}LEAD
21*	KAR	POTASSIUM–ARGON
22	AA09	ARGON–ARGON
23	KC40	POTASSIUM–CALCIUM
24	LH76	LUTETIUM–HAFNIUM
25	RO87	RHENIUM–OSMIUM
27	HT82	HAFNIUM–TUNGSTEN
28	HFND	HAFNIUM–NEODYMIUM
29	LC38	LANTHANUM–CERIUM
30	FC55	IRON–COBALT
31	MC53	MANGANESSE–CHROMIUM
32	IX29	IODINE–XENON
33	XEXE	XENON–XENON
34	CA36	CHLORINE–ARGON
35	BEAL	BERYLLIUM–ALUMINUM
36	BB10	BERYLLIUM–BORON
37	PTOS	PLATINUM–OSMIUM
38	LB38	LANTHANUM–BARIUM
36	HUTH	HELIUM/URANIUM–THORIUM
39	HEPB	HELIUM–LEAD
40	PT10	PALLADIUM–THORIUM

* is used to indicate age systems by the older age decoder TSTPHA.

representations for specifying age components. Table 2 presents the radiometric age mnemonic alphanumeric strings treated by the PHASS99 decoder, along with their corresponding geochronological equivalents. The majority of methods listed show only names of elements, but elements involved in more than one decay scheme also have their mass numbers included (e.g. U–Pb–Th systems).

A radiometric age is composed of the following four components:

1. An age number with its exponential modifier (e.g. 4567E5). Age decodes to 456.7My.
2. An age method 4-character mnemonic string identifying the age method used, e. g. SMND. SMND decodes to the Samarium-Neodymium isochron method.
3. A 2-character mnemonic string for the material analysed, e.g. T1. T1 decodes to zircon.
4. A digit between 1 and 10 showing the position of reference of source publication in the bibliography list vector of rock groups.

These four components in the alphanumerical strings are separated by the separators '-', '/' and ','.

Below are two examples of radiometric alphanumeric age strings:

:; 25E6-KAR/WR,1;2E6-UPB/QD,2:
(Without a stratigraphic age.)
:MIOC,1;22E6-KAR/NE,1;5E6-LB38/WR,7;234E5-BB10/QD,1:
(With a stratigraphic age.)

Chayes (1983) and Brandle (1994) may be referenced for full lists of IGBA mnemonics and their corresponding high-level English equivalents. The mnemonics, syntax, grammar and vocabulary of the IGBA system are also found on the Internet at the site:

http://www.ige.csic.es/sdbp/structur.txt

The basic and limited Chayes and Brandle (1974) version of the age decoder TSTPHA, allows only five physical ages for each specimen. Only ten physical age methods were handled by the software search engine. The PHASS99 version of the decoder program allows up to forty physical age methods and permits each specimen to have up to 99 ages, hence the program's acronym name PHASS99.

3. Expansion of the IGBA age program

This section describes the most important enhancements in PHASS99. Differences between the two decoder programs, TSTPHA and PHASS99, are summarized in Table 1 and described below.

3.1. Migration to PC-WINDOWS platforms

The development of personal desktop computers and WINDOWS programming platforms in the mid 1980s, opened new opportunities for fast and readily-accessible large scientific computations. A significant advancement in PHASS99 is the transformation of the IGBA system files and packages from DEC mainframe computers to desktop and laptop computers using Microsoft WINDOWS. This migration requires conversion of the DEC FORTRAN codes into WINDOWS FORTRAN. This major change made IGBADAT and IGBA system available to a wide user community. Modern source code algorithms, programming strategies, fast compilation, linkage and execution, and accessibility accompanied this step. Such a development constitutes a major advancement for the IGBA system. PHASS99 is compiled under the LAHEY-FUJITSU FORTRAN 95 Compiler (SHASTA) Version 7.50.01.

3.2. Large ensemble of radiometric isotopic systems

Incorporation of a large number of radiometric age systems in PHASS99 is a very significant development. This important improvement in the program also allows extensive radiometric age information coverage of ages of igneous rocks. Rapid technological advancement in mass spectrometers and proliferation in the literature of age determination of igneous rocks since the late 1980s, have produced a voluminous amount of age determinations, from single mineral and whole rock samples. An example is the production of zircon age determinations by high-precision U and Pb chronometers.

Thirty-six of the age methods are radiometric chronometers. In Table 2, the age methods tagged with asterisks are those of Chayes (1985), and the remaining age methods are introduced in this contribution. Four of the age systems listed are non-radiometric, and include, for example, magnetic striping and fission track ages.

Most age methods are derived by the radiometric isochron method. Many of these methods are well established and have been in use for many decades, such as the Rb–Sr, Sm–Nd and U–Pb isotopic systems. Other modern radiometric methods have been used with success, such as the Al–Mg and Hf–W methods. The majority of isochron systems are relatively new approaches and include relatively recent systems, such as the Mn–Cr isotopic chronometer. In addition, a large number of systems have been recognized recently and are under various stages of verification or utilization. Among these systems are the I–Xe and the La–Ba methods.

Recently Cook et al. (2014) discussed the Os–W decay, as a possible chronometer, and Smye et al. (2014) characterized the U–Th–Pb systematics of allanite for use in geochronology.

3.3. Large number of ages per sample

PHASS99 can handle up to 99 ages per specimen, when compared with only five ages per sample in the previous software version (TSTPHA). This enhanced capability allows PHASS99 to work with the radiometric systems currently available to earth scientists. Although samples do not currently contain the maximum of 99 ages, PHASS99 will be able to handle such a situation in the future.

3.4. Spreadsheet capability

Spreadsheets have been used for the last three decades as an integral part of scientific investigations, as tools for storage of voluminous data and information, and for the manipulation of data mathematically, statistically and graphically. The DEC version of TSTPHA was developed before spreadsheets came on the scene in the late 1980s.

An important feature in PHASS99 is its ability to generate output files compatible with spreadsheet programs, such as EXCEL. The output file is a generic type space-delimited output file. Spreadsheet numerical and graphical techniques can perform complex computational tasks and produce publication-ready illustrations for research in igneous rock geochronology.

3.5. High-level english output

Extraction and decoding programs in the DEC mainframe version of the IGBA decoding software package DECIGB (Chayes, 1988), accept information on igneous rocks only in mnemonic formats. Working with mnemonics can be challenging for users translating mnemonic codes manually, to meaningful high-level English equivalents. A visual reference of IGBA vocabulary proprietary lists is a tedious and lengthy process and is prone to error. PHASS99 alleviates all of these shortcomings in TSTPHA, by generating result output files containing mnemonics and their corresponding high-level English representations through transparent electronic translation. The spreadsheet-compatible file contains only English text. Supplementary material B shows such results, and Supplementary material C shows a spreadsheet-compatible output file of specimens in Supplementary material A. Supplementary material D is an EXCEL spreadsheet file containing results from Supplementary material A in spreadsheet format.

3.6. Circumvention of compilation and linking

The Chayes DECIGB (Chayes, 1986, 1988) version of the IGBA software system includes the IGBA decode library. It requires separate compilation, linking and insertion into the compiled version for the radiometric age program TSTPHA. This is followed by the creation of an executable (.exe) file of the decoder. This is a task that only experienced programmers can perform. PHASS99 obviates the need for these steps and offers users a convenient, user-friendly, simple one-click bundled application tool. Pertinent subroutines from the DECIGB (Chayes, 1988) and other subroutines created and added by the present author were inserted into PHASS99 to create one consolidated, and robust stand-alone program, resulting in an application that requires no programming skills.

3.7. Error files

An extra advantage presented to users by PHASS99 during its execution, is the generation of an output error file that directs them to locations of faulty information in input files and conflicts (i.e. bugs) in the program. Consequently, the user can correct these errors in order to successfully execute the program. Users might experience difficulties in the absence of such assistance, especially when interfacing with large databases like IGBADAT.

3.8. Comprehensive debugging of age decoder and library

Over the last three decades, the author did extensive debugging of the entire IGBA system package programs and libraries. The accuracy of IGBA programs, among them PHASS99, was serially improved and numerous errors were removed. Chayes and Nagy (1994) performed a similar correction of errors in the database.

4. Mechanics and flow of PHASS99 execution

Fig. 1 is a flow chart showing the operation of PHASS99. User interaction with the program is minimal and interfacing is easy. First, the program is launched at the system command prompt or by clicking its icon on the desktop. After the program launches, the only action required by the user is to enter the names of files. Appendix A is a 'READ.ME' file describing PHASS99 aspects and requirements for its operation. Appendix B is an 'INSTRUCTION MANUAL' for program use.

PHASS99 reads an input file, launches the decoder search engine, extracts physical age alphanumeric strings, decodes mnemonic information to high-level English equivalents, generates the three output files and prints them.

The first generated output file is an ASCII text (.DAT) file containing age dates. The second generated output file is a space-delimited spreadsheet-compatible (.DAT) file which can be imported into a spreadsheet program like EXCEL. The content of this file is highlighted, copied, and pasted into a spreadsheet. The third output file generated is an ASCII text (.DAT) file containing error messages that might be produced during execution of PHASS99.

For convenience, the PHASS99 program executable file (PHASS99.exe) and input files should reside on the computer desktop or in a dedicated folder; otherwise, proper paths should be set to declare file locations.

5. Examples of input and output files

Supplementary material A shows a sample data file (IGAGD. DAT) structured according to IGBA system proprietary rules. The output results file (IGAGR.DAT) is displayed in Supplementary
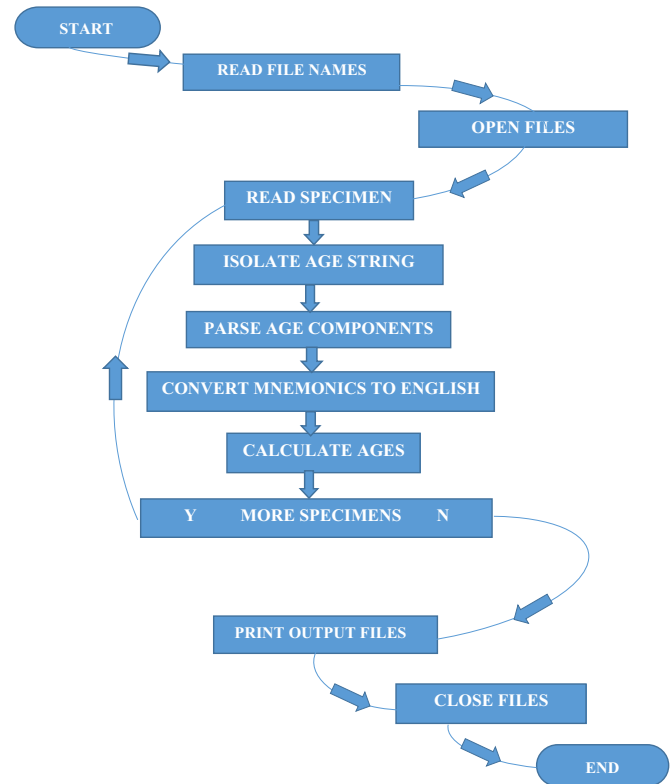

Fig. 1. PHASS99 process flow chart.

material B which shows raw text decoded age mnemonics along with their English equivalents. Supplementary material C (IGAGRS. DAT) is a space-delimited spreadsheet-ready output file. Its content is readily and easily blocked, copied, and finally pasted into a spreadsheet (e.g. EXCEL). This allows users to take advantage of spreadsheets capabilities such as mathematical and statistical manipulation, and production of high-quality and publication-ready graphical illustrations. Supplementary material D is a spreadsheet (IGAGS.XLSX) displaying results from file IGAGD.DAT in spreadsheet format. Supplementary material E (IGERROR.DAT) displays error messages generated by PHASS99.

Supplementary material F is a second input data file (FULL99. DAT) in which one sample (CGA C) contains more than ninety nine ages. Supplementary material G is spreadsheet file FULL99.XLSX, containing the maximum 99 age entries.

Potential users are encouraged to test PHASS99 on the sample data provided and on IGBADAT itself. In the two sample data files provided, some information is deliberately faked so as to produce error messages in the error file. Furthermore, users should assemble their own IGBA-structured files and subject them to PHASS99 processing. By so doing, they can verify the integrity of the PHASS99 program because the input radiometric age information is known.

6. Discussion and conclusions

This study describes PHASS99, an IGBA system program designed to retrieve and decode radiometric and other physical age information from igneous rocks in the international database IGBADAT, and similar databases. It also describes developments and enhancements introduced in the program over its predecessor, the TSTPHA decoder.

PHASS99 offers significant overhaul modifications which led to its migration to the WINDOWS environment on PC and laptop

computers. It allows the accommodation of a large number (99) of radiometric and physical ages per specimen, a large number of isotopic chronometers (40), reduction of mnemonic representations of age components to English- language equivalents, and obviating the need for FORTRAN compiling-linking procedures. All of these improvements, among others, resulted in a powerful stand-alone application tool that is user-friendly during the extraction and decoding of radiometric and physical ages from IG-BADAT (and similar data bases).

Several attempts have been made in the past to popularize IGBADAT (Brandle and Nagy, 1995b). Torley and McBirney (2002) pointed out the need of the earth science community, to explore the wealth of information stored in IGBADAT. PHASS99 optimized and simplified dramatically, the task of retrieving radiometric ages from the database; another step towards data mining of IGBADAT and increasing awareness of its advantages. The aim of this study was to enhance the ease of using the IGBADAT international igneous rock database. Such retrieval tasks were accomplished by incorporating developments and enhancements in TSTPHA, the early simple version of Chayes and Brandle (1974), and their collaborators.

Similar future contributions have been planned and will address other types of information in IGBADAT, such as the chemical composition of igneous rocks and their geography.

Acknowledgments

An earlier version of this manuscript was reviewed critically by Mike Duane, Linda Smith and Rao Divi. They are hereby acknowledged.

Appendix A

PHASS99 'READ.ME'

This is a 'READ.ME' file for the PHASS99 FORTRAN decoder program. It describes briefly the software program and acquaints users with it.

PHASS99 is designed specifically to extract and decode radiometric ages of igneous rocks from the international database IG-BADAT. The program is an expanded version of TSTPHA (Chayes, 1985). It includes more capabilities and functionality.

Each igneous rock (plutonic or volcanic) is stored in IGBADAT as a description. Information storage in each description follows rules of the IGBA system (Chayes, 1983; Chayes and Brandle, 1974), which possesses its proprietary vocabulary, grammar, and syntax. Mnemonic representation is utilized to describe information retrieved from the literature. C records within a description carry stratigraphic and geochronologic age data, among other geological and petrological information.

An igneous rock radiometric age is composed of a numeric age and its exponential modifier, a radiometric method (4-character mnemonics), analysed material (2-character mnemonics) and a reference number in the bibliography vector for the rock group. Decoding produces intelligible high-level English text.

Upon execution, PHASS99 targets geochronological data, isolates age alphanumeric strings, parses them, converts them to English and prints them. Output for each rock includes numeric age, radiometric method used (e. g. potassium-argon) and material analysed (e.g. biotite), and position of reference in the bibliography list vector.

Several output files are generated, of which one file is spreadsheet-ready. Data in this file can be blocked and exported to a spreadsheet like EXCEL, and pasted in it. This spreadsheet file allows users to take advantage of spreadsheet capabilities (Chayes, 1985; Chayes, 1983; Chayes and Brandle, 1974).

PHASS99 includes many debugging and tracing statements which can be activated, should users wish to modify the program to suit their own needs.

Limits of PHASS99 are as follows:

1. Maximum number of specimens in a data file=300,000 specimens.
2. Maximum number of radiometric ages in a specimen=99 ages.
3. Maximum length of a file name (including extension)=20 characters.

Appendix B

PHASS99 'INSTRUCTION MANUAL'

This is an 'INSTUCTION MANUAL' containing instructions to be followed by users of the PHASS99 FORTRAN decoder software program.

Prior to running the PHASS99 program, a location must be specified for installing the program executable version (PHASS99. EXE) and input files. For simplicity, all files should be placed on the computer desktop. An icon will be created to symbolize PHASS99. Clicking on the icon starts program execution. A user can also place files in any folder or subfolder. In this case, proper paths must be set and declared on the system command prompt during launching of PHASS99.

In addition, an input IGBA-structured file (e.g. IGBADAT.DAT) must exist on the computer beforehand. Care must be exercised to ensure input files are structured strictly according to IGBA rules (Chayes, 1983).

Furthermore, it is recommended that the computer monitor screen is set to maximum size allowable for the program to display properly PHASS99 screen banners. Monitor displays will not appeal aesthetically if screens are not set properly. However, this feature is only pictorial and will not affect computational results or output files.

PHASS99 accepts ASCII text data files (file.DAT) without tabs, record breaks, RETURNS or formatting different from the IGBA format (Chayes, 1983).

Execution of PHASS99 is simple and proceeds as follows:

1. Launch PHASS99 from the desktop icon or the system command prompt. Follow instructions.
2. User is prompted for a name of an input file. User responds by declaring an input file name, like IGBADAT.DAT.
3. User is prompted for a name of a results file. User responds by declaring a results file name (e.g. 1.DAT).
4. User is prompted for a name of a spreadsheet-compatible file. User responds by declaring a spreadsheet-compatible file name (e.g. 2.DAT).
5. User is prompted for a name of an error file. User responds by declaring an error file name (e.g. 3.DAT).
6. Content of the spreadsheet-compatible file is highlighted, blocked and pasted into a spreadsheet.
7. The PHASS99 'error file' should be consulted for error messages after each run of the program.

Notes:

1. Occasional imperfect appearance of data columns or error messages in results and error files is dependent on choice of editor used for viewing them, as well as font used and letter case.
2. Should execution of PHASS99 terminates prematurely, check input data file first for consistency of data and correctness of data structure (i.e. IGBA rules).
3. For any inquiries contact: lemonfather@yahoo.com

Appendix C. Supplementary material

Supplementary data associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.cageo.2016.02.023.

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