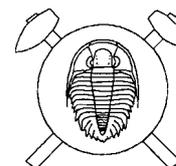


NORMAN, a QuickBasic programme for petrochemical re-calculation of whole-rock major-element analyses on IBM PC



NORMAN, program pro petrochemické přepočty analýz hlavních prvků na IBM PC (Czech summary)

(4 text-figs)

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NORMAN is a Microsoft QuickBasic 4.5 package designed for handling and recalculation of whole-rock major-element data from igneous and metamorphic rocks on PC compatible computers. It is capable of computing parameters of the most common normative calculation schemes, including CIPW and Catanorm. The core of the system consists of modules to handle the import, editing and saving of the major-element analyses, as well as browsing, saving and exporting the computed results.

The calculation algorithms are: (1) nearly independent QuickBasic programmes ("standard modules"), and (2) plain text calculation scripts ("user-defined functions") that may contain variables referring to the original data, to constants as well as to parameters calculated by other standard modules and user-defined functions.

The advantage of the chosen approach is the simplicity, availability and open architecture that enables an average user not only to follow, but also, if need be, to modify the algorithms applied to his data.

Key words: BASIC, CIPW, geochemistry, norms, petrology, recalculation, software

Introduction

The interpretation of whole-rock geochemical data from igneous and metamorphic rocks often requires complex and time-consuming calculations. Nowadays, these are routinely performed on a personal computer using dedicated software (e. g. MinCalc – Melín – Kunst 1992, NewPet – Clarke 1993, MinPet – Richard 1995). However, unless either sufficiently detailed documentation is provided, or the user has a fairly good skill in the particular programming language, it is complicated to figure out exactly which algorithm has been employed by the author. Moreover, any modifications to the original algorithm are usually difficult or even impossible as it is not a common practice to make the source code available to the public, especially for commercial programmes.

To eliminate this major drawback and to give the user an opportunity to tailor the algorithms, a new package for

recalculation of major-element analyses, named NORMAN, has been developed. It consists of several core modules designed for importing and editing of the input data, selecting an appropriate calculation scheme, display, printing and saving the output data. The calculation algorithms are stored in small, nearly independent modules with a simple structure. Currently modules are available for calculation of the CIPW norm (including the modification with biotite and hornblende; Hutchison 1974, 1975), Niggli molecular norm (Catanorm; Hutchison 1974 and references therein), improved Mesonorm for granitoid rocks (Mielke – Winkler 1979), Niggli's values (Niggli 1948), multicationic parameters of the French authors (De la Roche *et al.* 1980; Debon – Le Fort 1983, 1988), chemical approximation to the modal QAPF classification for the igneous rocks (Q'–ANOR, Strec-keisen – Le Maitre 1979), major-element based tectonic discrimination of granitoids (Maniar – Piccoli 1989) and several others (Tables 1–2).

Table 1. Overview of the available standard modules.

Menu item ¹	Default suffix ²	Module name	Calculation scheme (reference)
Granit.mesonorm	.MEZ	MEZONORM.EXE	Improved granite mesonorm (Mielke – Winkler 1979)
Kohler-Raaz	.KOH	KOHLER.EXE	(Köhler – Raaz 1951)
C. I. P. W.	.CPW	CIPW.EXE	CIPW norm (Hutchison 1974, 1975 and references therein)
C. I. P. W. with Hb & Bi	.CPH	CIPWHB.EXE	Modified CIPW with hornblende and biotite (Hutchison 1975)
Catanorm	.KTN	KATANORM.EXE	Niggli's molecular norm (Catanorm) (Hutchison 1974 and references therein)
De La Roche	.RCH	LAROCHE.EXE	R ₁ –R ₂ multicationic values (De la Roche <i>et al.</i> 1980)
Debon-Le Fort	.DLF	DEBON.EXE	(Debon – Le Fort 1983, 1988)
Niggli	.NGL	NIGGLI.EXE	Niggli's values (Niggli 1948)
Miscellany	.MSC	PETRCALC.EXE	Various petrochemical indexes, such as total iron as FeO, mg number, agpaite index, molar A/NK and A/CNK, AFM values (Irvine – Baragar 1971), differentiation index (Larsen 1938), solidification index

¹ as they appear on the menu "Calculations"

² default suffix of the ASCII-saved results, that is also used as reference in the user-defined functions

Table 2. List of the available user-defined functions.

Menu item ¹	Default suffix	Module name	Calculation scheme (reference)
Q'-ANOR	.STR	STR.DEF	Chemical approximation to the modal QAPF classification scheme (Streckeisen – Le Maitre 1979)
Maniar – Piccoli	.MAN	MAN.DEF	Major-element based classification of granitoids (Maniar – Piccoli 1989)
Zircon saturation	.ZWH	ZWH.DEF	Zircon solubility in crustal melts at 750 °C (Watson – Harrison 1983)
Apatite saturation	.AWH	AWH.DEF	Apatite solubility in leucocratic melts at 750 °C (Harrison – Watson 1984)
CIPW-based values	.PAR	PAR.DEF	sum of salic and femic normative minerals from the CIPW norm; differentiation index (Thornton – Tuttle 1960)
Catanorm from CIPW	.KFC	KFC.DEF	Catanorm from CIPW by coefficients (Hutchison 1975)
Mode from CIPW	.MFC	MFC.DEF	Mode from CIPW by coefficients (Hutchison 1975)
Alkaline Sylvester	.ALK	ALK.DEF	Discrimination between alkaline granite, calc-alkaline granite, and strongly peraluminous granite with SiO ₂ > 68 % (Sylvester 1989)

¹ as they appear in the menu “Calculations User defined”

The description of NORMAN given here is only brief as the details are set in the user’s guide provided with the programme (Janoušek 1999).

System specifications

An overview of the NORMAN package is shown in Figure 1. The core of the system (MAIN.EXE), calls specialised modules handling input/output operations and calculation of the results (DIRECT.EXE, SAVE.EXE and CALC.EXE). NORMAN can import major-element data as dBase *.DBF files, NewPet *.ROC files (Clarke 1993) and several mutations of ASCII files. The input data can be edited, and, or, entered from the keyboard using the built-in editor. If desired, the modified data set can be saved into *.DBF, *.ROC or ASCII files.

The calculation algorithms are of two types: (a) “standard modules”, or compiled, stand-alone QuickBasic routines, and (b) “user-defined functions”, or plain text scripts defining formulae using basic arithmetic operators, raw major-element data, constants, and various parameters calculated by the other modules.

As soon as they are computed, the results can be displayed and printed either individually, analysis by analysis, or in the form of a table. The data set may be browsed, searched, its subsets selected and their basic statistical parameters shown. The results can be saved as dBase or ASCII files, as well as comma-delimited files compatible with NewPet. At the moment, NORMAN has no plotting capabilities but, to obtain the graphic output, the results can be imported either to NewPet (utilising its generic plots) or to a professional programme, such as Microsoft Excel or Grapher.

Considerable attention has been paid to the installation module (INSTALL.EXE) that makes it possible not only to configure the package (including the installation and de-installation of standard modules and user-defined functions) but also to edit the calculation scripts used by the user-defined functions (*.DEF files). Although these can be prepared using any word processor, the editor built into the installation module enables a more comfortable entry of the arguments from menus, taking care of the correct syntax.

Standard modules

These are compiled QuickBasic 4.5 programmes, independent of the rest of the package. The only exceptions are several variables reserved by the system and three arrays utilised for input of the major-element analyses (either raw major-element data or atomic proportions) and output of the calculated results. Figure 2 shows an example of a simple standard module designed for calculation of multicationic parameters after (Debon – Le Fort 1983, 1988).

In these standard modules, typically a cycle is run for all the samples (from 1 to *pocet*), the calculation algorithm performed and the results transferred to the output array (*w()*). Should an error to be encountered, an error code, together with the information concerning in which module and at which sample it occurred, is passed to the core of the system and the corresponding error message is displayed. An overview of the available standard modules is given in the Table 1.

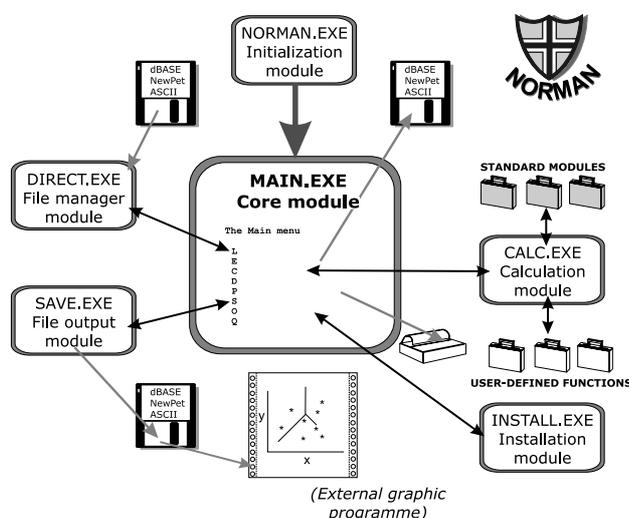


Fig. 1. An overview of the NORMAN package.

User-defined functions

An ASCII calculation script, or user-defined function, can call other user-defined functions, standard modules and its own, previously-evaluated parameters. Computation of the user-defined functions is slower than for the standard modules, as for each parameter of the particular function, the formula needs to be interpreted and the necessary modules called. Meanwhile, all the provisional results are stored temporarily on the hard disc to enable

recursive calling of the calculation module. Although at a cost, a major advantage of the user-defined functions is that a user does not need any programming knowledge to be able to understand their operation or to even modify them. Hence development of user-defined functions, especially if aided by the editor built in the installation module, is trouble-free.

The user-defined functions may contain basic arithmetic operators (+ - * / ^ and brackets), reference to raw major-element data (e. g. % SiO_2), atomic proportions

```
'$INCLUDE: 'NORDEF.BI'
REM * Debon and Le Fort (1988): Bull. Mineral., 111, 493-510 *

ON ERROR GOTO Handler

FOR y = 1 TO pocet
  si = r(1, y): ti = r(2, y): al = r(3, y): fe3 = r(4, y): fe2 = r(5, y)
  mn = r(6, y): mg = r(7, y): ca = r(8, y): na = r(9, y): k = r(10, y)
  H2O = r(11, y): co2 = r(13, y): p = r(12, y)

  REM Q
    w(1, y) = CINT(si / 3 - (k + na + 2 * ca / 3))
    q = w(1, y)
  REM P
    w(2, y) = k - (na + ca)
  REM A
    w(3, y) = al - (k + na + 2 * ca)
  REM B
    w(4, y) = fe2 + fe3 + mg + ti
    b = w(4, y)
  REM F
    w(5, y) = 555 - (q + b)
    f = w(5, y)

    w(6, y) = na + k
    w(7, y) = k / (na + k)
    w(8, y) = mg / (fe2 + fe3 + mg)

  REM Recalc to 100%
    suma = q + b + f

    w(9, y) = q / suma * 100
    w(10, y) = b / suma * 100
    w(11, y) = f / suma * 100

NEXT y
CHAIN "calc"

Handler:
erro = 6
kde = y
```

Cycle for all the samples

Assign atomic proportions *1000 stored in $r()$ to variables si , ti , etc. for better understanding the algorithm

The algorithm itself; typically the only part of the module to be altered. Results are assigned to the array $w()$. The parameter names are given in a configuration file

Return to the calculation module

Simple error handler returning the error code and location at which the error occurred

Fig. 2. Example of BASIC code of a simple standard module: DEBON.EXE, used for calculation of multicationic parameters after (Debon – Le Fort 1983, 1988).

(e. g. % *Si*), constants (molecular weights: e. g. *WSiO₂*, atomic weights: e. g. *WSi*, various user-defined constants: e. g. *pi*, factors to recalculate weight % oxide to weight % element and vice versa: e. g. *fFeO*, *fFe2*) and parameters calculated by other modules. To refer to standard modules and user-defined functions, each is assigned a unique three letter identifier. For instance, the reference to parameter “anorthite” from the CIPW norm would be “An[CPW]”. These three letters are also used as the default suffix for saving ASCII results of the given calculation scheme.

The concept of the user-defined functions is best demonstrated with an example. A user-defined function STR.DEF (Fig. 3) calculates the Q'–ANOR parameters (Streckeisen – Le Maitre 1979), containing reference solely to parameters of the Granite Mesonorm [MEZ] (Mielke – Winkler 1979) combined by arithmetic operators.

A more complicated case is given in Figure 4: the user-defined function MAN.DEF performs calculations necessary for the geotectonic classification of granitoids after Maniar – Piccoli (1989), referring to the param-

eters computed by a standard module PETRCALC (e. g. *FeOt [MSC]*), parameters calculated earlier by the same function (e. g. *@sum1[MAN]*) as well as to raw major-element data (e. g. % *MgO*). The list of currently available user-defined functions is given in Table 2.

Hardware requirements, availability and future development

Although minimal hardware requirements of NORMAN are IBM PC compatible computer with MS-DOS 5 or higher, about 1 MB free hard disc space and EGA, VGA or Hercules compatible graphic card, it will run on quicker machines under MS Windows 95/98, preferably in full-screen DOS regime. This programme, including the necessary documentation (both in HTML and a Microsoft Word file) together with source files of all the standard modules, is available free of charge. These can be obtained either via Internet (at <http://www.geocities.com/vjanousek.geo/Norman>) or on request from the author. At the moment, NORMAN's calculation algorithms are being ported into a new environment that is based on

```
*Chemical classification for igneous rocks after Streckeisen & Le Maitre (1979)
Q' = 100 * Quartz[MEZ] / (Quartz[MEZ] + Orthoclase[MEZ] + Albite[MEZ] +
Anorthite[MEZ])
ANOR = 100 * Anorthite[MEZ] / (Orthoclase[MEZ] + Anorthite[MEZ])
```

Q' and ANOR are computed from parameters returned by the standard module MEZONORM.EXE, as indicated by the corresponding default suffix “MEZ” in the square brackets (see Table 1)

Fig. 3. Example of a function definition file for a user-defined function: STR.DEF that calculates Q'–ANOR parameters after (Streckeisen – Le Maitre 1979) from the improved Mesonorm for granitoid rocks (Mielke – Winkler 1979).

```
*Tectonic classification of granitoids (Maniar & Piccoli 1989)
FeOtot = FeOt[MSC]
FeOMgO = FeOt[MSC] + %MgO
FeO\FeOMgO = FeOt[MSC] / FeOMgO[MAN]
A\NK = A\NK[MSC]
A\CNK = A\CNK[MSC]
@sum1 = %Al2O3 + %Na2O + %K2O + %MgO + FeOt[MSC]
A1 = 100 * (%Al2O3 + %Na2O + %K2O) / @sum1[MAN]
F1 = 100 * FeOt[MSC] / @sum1[MAN]
M1 = 100 * %MgO/@sum1[MAN]
@sum2 = %Al2O3 + %Na2O + %K2O + %MgO + FeOt[MSC] + %CaO
A2 = 100 * (%Al2O3 + %Na2O + %K2O)/@sum2[MAN]
F2 = 100 * (FeOt[MSC]+%MgO)/@sum2[MAN]
C2 = 100 * %CaO/@sum2[MAN]
```

weight % MgO
(a constant)

Calling standard module
PETCALC.EXE (default
suffix “MSC”; Table 1)

Calling a parameter
calculated earlier by the
same module (MAN.DEF)

Parameters whose name starts with “@” are temporary and will not be shown when the results are being displayed sample by sample

Fig. 4. More complicated user-defined function: MAN.DEF for major-element based tectonic discrimination of granitoids (Maniar – Piccoli 1989). This function refers not only to parameters of a standard module (PETRCALC.EXE) but also to its own, temporary parameters calculated earlier (*@sum1*, *@sum2*) and to raw major-element data (% *MgO*).

the freeware statistical language R (Ihaka – Gentleman 1996). The intention is to build eventually a platform-independent system with high-level plotting capabilities.

Conclusions

NORMAN provides a simple, but versatile addition to the available PC software for petrochemical and normative recalculations of major-element analyses from igneous and metamorphic rocks. Its open architecture should enable an average user with little programming knowledge to understand, and, if need be, also to modify the built-in calculation algorithms. This philosophy, together with the availability of the package, is believed to be appealing enough to encourage other geochemists to produce new modules and to further expand the system.

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NORMAN, program pro petrochemické přepočty analýz hlavních prvků na IBM PC

Pro kalkulaci petrochemických a normativních přepočtů analýz hlavních prvků vyvřelých a metamorfovaných hornin se běžně používá speciálního softwaru. Velkou nevýhodou bývá, že je obvykle obtížné vysledovat, jaký výpočetní algoritmus byl užít, a ještě těžší či zcela nemožné tyto algoritmy jakýmkoli způsobem modifikovat.

Vývoj nového softwaru tedy vedla snaha vytvořit programový balík, ve kterém by byly použité algoritmy snadno dostupné, pochopitelné a případně i modifikovatelné průměrným uživatelem. Vzniklý produkt, nazvaný NORMAN, představuje soubor několika základních modulů pro import, editaci a ukládání analýz hlavních prvků, výběr výpočetního postupu, zobrazení, prohlédávání, tisk a ukládání vypočtených parametrů. Podporované vstupní a výstupní formáty zahrnují dBase (*.DBF), několik variant textových souborů a formát používaný oblíbeným programem NewPet (*.ROC).

K jádru systému přistupuje množství výpočetních modulů (obstarávající výpočet celé řady normativních hodnot, včetně CIPW normy a Katanormy), jež jsou dvojího typu: (1) *standardní moduly*, neboli nezávislé BASICové programy, přejímající z jádra systému pouze vstupní data (analýzy hlavních prvků) a vracející spočtené parametry, a (2) *uživatelské funkce*, tedy textové předpisy, vyjadřující běžné matematické operace s konstantami (např. molekulové a atomové hmotnosti) a proměnnými (vypočtenými jinými výpočetními moduly).

