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INFOREX Information Retrieval System: Analysis and Processing of Experimental Data on Phase Equilibria in Igneous Rocks

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Abstract—The most recent version of the INFOREX database (INFOREX 4.0, 1996), which includes experimental data on crystal–melt equilibria and a package of programs for their analysis and processing, is presented. The database contains the results of 186 studies (about 7000 experiments and more than 9600 phase compositions) and is currently the most complete information system in the field of experimental petrology of igneous rocks. The main options of INFOREX can be divided into the information, retrieval, and applied (*Petrological Calculations*) categories. The computational functions include: (1) calculation of regression coefficients describing mineral–melt equilibria for olivine, plagioclase, three varieties of pyroxenes and spinellids: a total of 28 geothermometers; (2) calculation of the Fe^{3+}/Fe^{2+} ratio in experimental glasses for nine models; (3) calculation of the H_2O solubility in melts for water-saturated experiments for three models; and (4) auxiliary calculations, including the projection of glass compositions onto ternary diagrams. The paper presents examples of using the INFOREX system to analyze the high-pressure cotectic melts *Ol–Opx–Cpx* and equilibrium isotherms between melts and amphibole under water-saturated conditions.

INTRODUCTION

Numerous experimental studies of phase equilibria in synthetic and natural silicate systems have yielded enormous amounts of data on the conditions of quench experiments and the phase compositions of their products. According to our estimates, the overall number of subliquidus high-temperature experiments alone is at least 10 000; these are approximately equaled in number by microprobe analyses of the phases (crystals and quench glasses) synthesized in these experiments. In order to make efficient use of this vast experimental information in petrological and geochemical investigations, it is necessary to analyze hundreds of publications and assess the reliability of the data presented therein.

This problem is particularly urgent in computer modeling of magmatic equilibria based on calibrations that simultaneously include data from hundreds and thousands of experiments (Nielsen, 1990; Weaver and Langmuir, 1990; Ariskin *et al*., 1993; Ghiorso and Sack, 1995). Furthermore, petrological reconstructions rely heavily on phase diagrams, geothermobarometers, and correlations, which must incorporate experimental data so as to compare empirical relationships and extrapolations proposed by various workers and to evaluate their accuracy. To accomplish these tasks, it is essential to have rapid access to the available information and to be able to filter the data by major-element criteria (magma composition) and experimental conditions, including duration, temperature, pressure, f_{O_2} and volatile conditions. Apparently, a resolution of these issues could be found in a global computer system that would accumulate the experimental information available on phase equilibria of igneous rocks and provide an opportunity to assess the data for reliability.

A few years ago, we started working on such a system (Ariskin *et al.*, 1992) and recently presented the INFOREX 3.0 database developed for IBM-compatible personal computers running MS-DOS (Meshalkin and Ariskin, 1996; Ariskin *et al*., 1996). In addition to experimental information, this package includes a user-friendly multifunctional *Data Base Management System* (DBMS) (Meshalkin *et al.*, 1996), which proved to be very efficient in practice (Ariskin and Nikolaev, 1995; Almeev and Ariskin, 1996; Ariskin and Nikolaev, 1996). This prompted us to integrate a number of new functions into the user interface for solving some applied petrological problems. This paper will give the most complete description of the experimental data set included in the INFOREX version 4.0 (1996) and a few examples of its use.

BRIEF DESCRIPTION OF THE INFOREX SYSTEM

Here, the term *system* is used to refer to both the database and the built-in module that processes the user-requested information retrieved from the base. This may be regarded as the first and essential step toward creating a petrological expert system that can both analyze experimental data and use the results to simulate phase equilibria and test various computer-generated models.

File Structure and Hierarchy

The INFOREX database is based on text files with tabulated compositions of experimentally synthesized phases. The top-level files hold references and run conditions. The master file, containing experimental conditions (CONDIT.EXP) (Meshalkin *et al.*, 1996), is divided into fixed fields that include: reference number, experiment number, rock name, address of the starting material composition, flag for the presence or absence of volatile components, pressure, temperature, oxygen fugacity, experiment duration, and container type. The last seven fields serve to identify the phase assemblages (glass, olivine, garnet, etc.), with flags indicating the availability of microprobe analyses. With certain exceptions (for sulfides, carbonates, and metals), the composition files are formatted uniformly and contain the contents of 12 major oxides in the order: SiO_2, TiO_2, Al_2O_3, FeO (total), MnO, MgO, CaO, Na_2O, K_2O, P_2O_5, Cr_2O_3, and H_2O. A separate file stores additional information on hydrous experiments: compositions of the volatile components and, if present, of the fluid phases (H_2O, CO_2, and H_2) in weight and mole percent.

Statistics of Experimental Data

As of April 1996, the database contains information reported in 186 works, such as papers, books, and dissertations, between 1962 and 1995, as well as some unpublished information that was available to us (Fig. 1a). Of the 6900 experiments incorporated into the database, more than 80% relate to natural rocks; 4580 experiments were performed at dry conditions, and the rest were conducted in the presence of H_2O and/or CO_2. The high-pressure experiments account for no more than 40%. Figures 1c and 1d show the distribution of the experiments as a function of pressure and temperature. The total number of microprobe-determined phase compositions is 9618, and the most representative data are available for quench glasses (3634), olivine (1442), plagioclase (1026), and high-calcium pyroxene (914) (Fig. 1b).

A special data set of the INFOREX system includes 298 glass compositions with known ferric–ferrous ratios (Nikolaev *et al.*, 1996). For 94 hydrous experiments, direct water determinations are given, in addition to the major-element concentrations in quench glasses (Almeev and Ariskin, 1996).

Main DBMS Options

The concept of the INFOREX DBMS consists in the idea that we create not so much a “store” of some potentially useful information as a working system designed to solve both traditional and current petrological problems. In the future, this system may become a part of a more general package that, in addition to the database and retrieval software, would include various computer models of phase equilibria applicable to closed and open geochemical systems. Thus, the main DBMS options can be classified into the *information* (1, 2, 3, and 6), *searching* (4 and 5), and *applied* (7) categories:

(1) System Configuration;

(2) General System Information;

(3) View / Edit / Input Data Files;

(4) Selecting Experimental Conditions;

(5) Setting Phase Assemblages;

(6) Exchange INFOREX Data; and

(7) Petrological Calculations.

The first six options were detailed in our previous papers (Meshalkin *et al.*, 1996; Meshalkin and Ariskin, 1996; Ariskin *et al.*, 1996), so here we shall only describe several new features that have been added to the DBMS during the last few months. These include particularly new capabilities of the search procedure, which operates in two stages that involve the selection of run conditions (4) and the definition of the set of liquidus phases (5).

Option (4) has now been supplemented so that it is possible to choose water-saturated and/or water-undersaturated experiments and to save records containing water determinations in melts to a separate file; an analogous search is possible for experiments with known ferric–ferrous ratios in quench glasses. Additionally, the glass compositions are now constrained not only by the oxide contents (SiO_2, Al_2O_3, CaO, Na_2O + K_2O, TiO_2, FeO, and MgO) and characteristic ratios (FeO/MgO and Mg/(Mg + Fe)), but also by dividing the data into three magmatic series (tholeiitic, subalkaline, and alkaline) based on the (Na_2O + K_2O)–SiO_2 diagram shown in Fig. 2 (*Klassifikatsiya i nomenklatura* ..., 1981).

When setting the phase assemblages [option (5)], it is now possible to specify more exactly the set of liquidus phases, selecting only those runs that have glass compositions in equilibrium with a desired mineral (e.g., plagioclase: *Pl–Liq*, *Ol–Pl–Liq*, *Ol–Pl–Cpx–Liq*, etc.), with a mineral assemblage (e.g., *Ol–Opx–Cpx–Liq*), or experiments involving the compositions of two desired phases (olivine–melt, orthopyroxene–garnet, etc.). This additional capability is geared to the needs of petrologists developing mineral–melt geothermometers, two-mineral geobarometers, or attempting to classify the compositions of liquids produced by partial melting of peridotite.

Despite the large amount of information analyzed, the search procedures of the INFOREX DBMS run on a PC of 486 class or higher and take only a few seconds. The search results are saved as conveniently usable files formatted in tabular form, which can be easily integrated into standard graphic software.

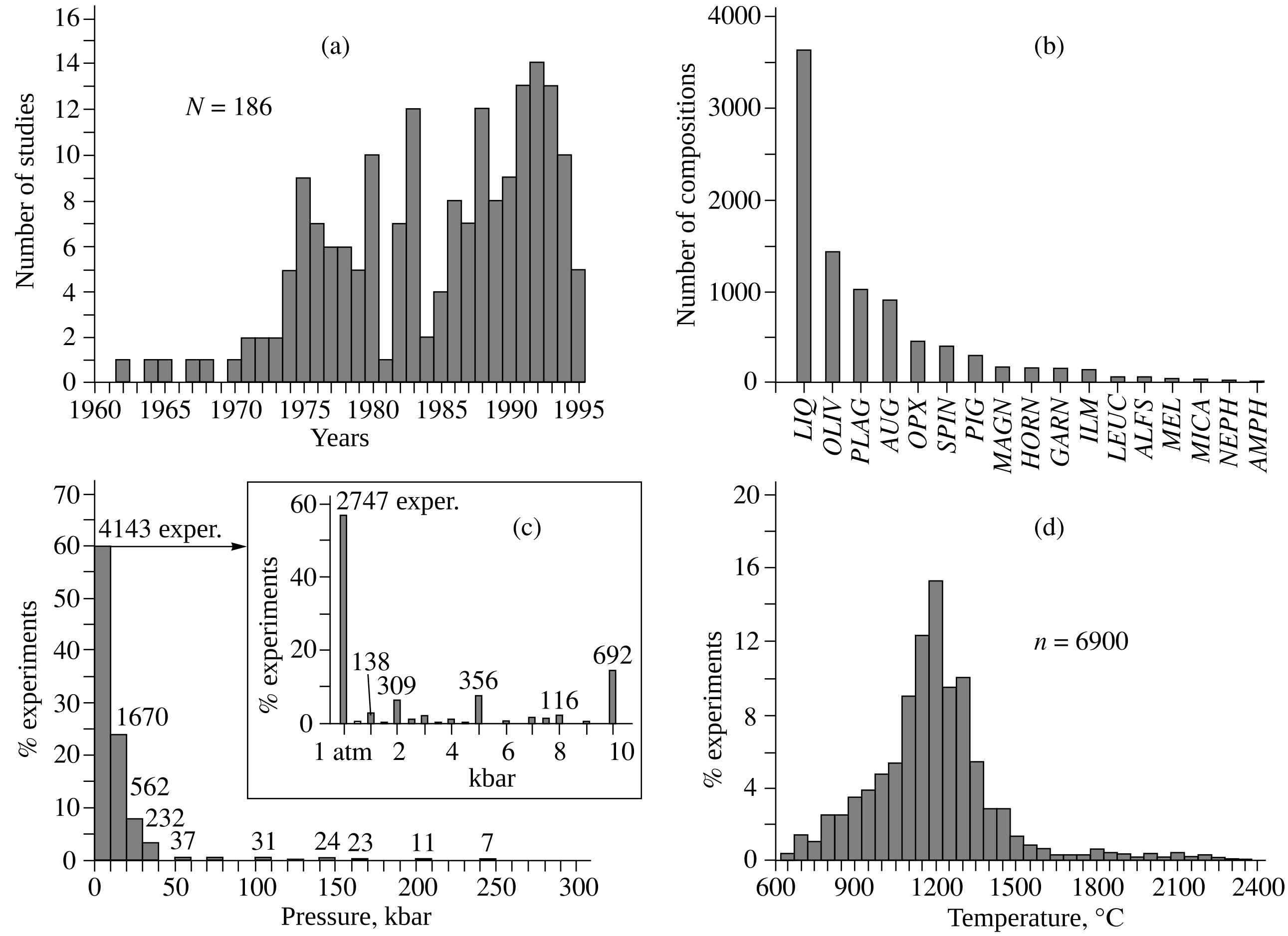

Fig. 1. Statistics of experimental data available in the INFOREX 4.0 (1996) database.
Distribution of the number of studies in terms of year of publication (a), phase compositions (b), and experimental pressure (c) and temperature (d). Phase symbols are as used in the database (Meshalkin *et al.*, 1996).

PETROLOGICAL CALCULATIONS

In the research conducted by our group, the principal function of the INFOREX system is to prepare data for developing mineral–melt geothermometers with the subsequent integration of these relationships into the COMAGMAT package of petrological programs, designed to simulate phase equilibria in magmatic melts (Ariskin *et al.*, 1993). At the same time, the solution of this specific task frequently involves a number of practical petrological tasks concerning the division of iron into the ferric and ferrous oxidation states, estimation of oxygen fugacity and water content in the melt, various major-element recalculations, including projection of glass compositions onto pseudoternary diagrams, construction of concentration plots, and so on. The need for additional programming aimed at automating all these procedures led to the creation of a special routine of the INFOREX database called *Petrological Calculations*. Its structure and main functions are shown in Fig. 3.

The *Petrological Calculations* include: (1) *Calculation of Regression Coefficients* describing mineral–melt equilibria for olivine, plagioclase, three varieties of pyroxenes and spinellids: a total of 28 geothermometers; (2) *Calculation of the* Fe^{3+}/Fe^{2+} *Ratio* in experimental glasses according to nine models (Sack *et al.*, 1980; Kilinc *et al.*, 1983; Kress and Carmichael, 1988; Borisov and Shapkin, 1989; Kress and Carmichael, 1991; Mysen, 1991; and three models in Nikolaev *et al.*, 1996); (3) *Calculation of* H_2O *Solubility* in melts for water-saturated experiments according to three models (Burnham, 1994; Dixon *et al.*, 1995; Almeev and Ariskin, 1996); and (4) *Auxiliary Calculations*, including the normalization of glass compositions to 100% (for dry and hydrous systems) and their projection onto ternary diagrams, such as *Ol–Pl–Qtz* and *Qtz–An–Ab*.

These functions require the same procedure for all types of calculations: at first, the user browses through the list of search-generated initial data files, selects one such file, and sets the type of calculation (1–4); if necessary, the model parameters are specified. After that, control is transferred to the program, which creates an output file. The user can view the computational results

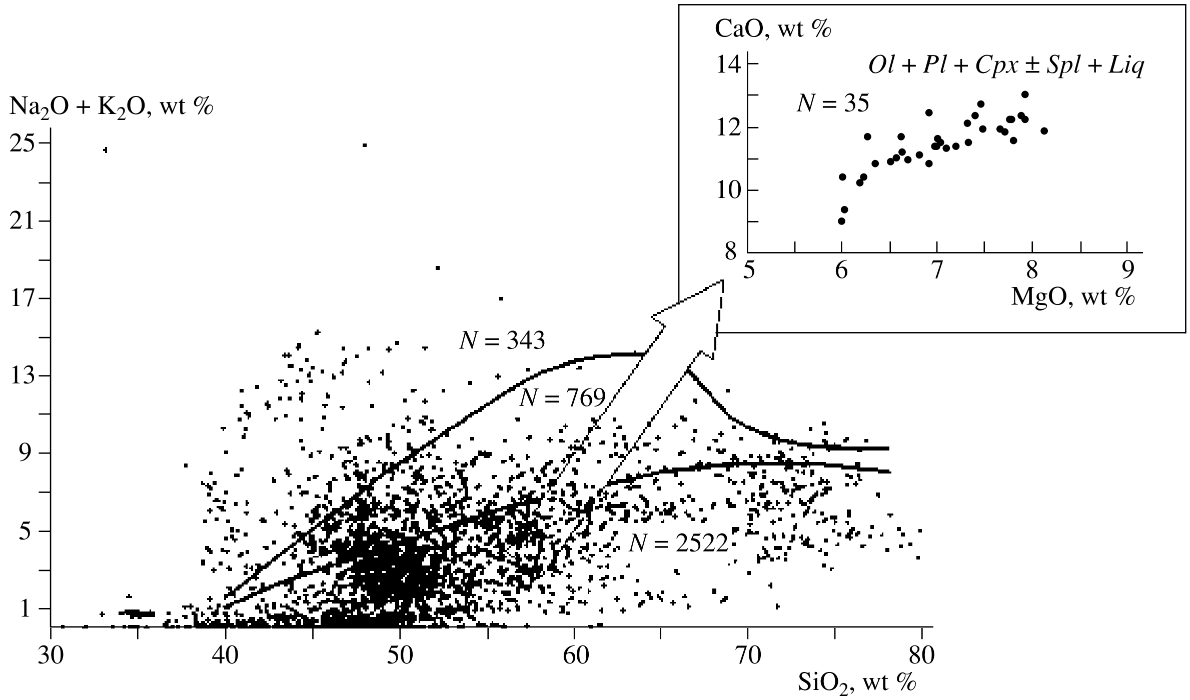

Fig. 2. Division of glass compositions into conventional tholeiitic, subalkaline, and alkaline series (*Klassifikatsiya i nomenklatura,* 1981). Inset shows an additional sampling of "tholeiitic glasses" obtained in 1 atm experiments of more than 24 h duration, with olivine, plagioclase, and high-Ca pyroxene (±*Spl*) present on the liquidus. This assemblage coexists only with melts containing at least 8% MgO.

within the DBMS, compare them with those obtained earlier, print them, and, if necessary, run the calculation procedure again with new initial data or model parameters.

This paper will not consider examples of creating melt–mineral geothermometers, analyzing redox equilibria, or calculating the water content in quench glasses: the reader is referred to papers specially devoted to these subjects (Ariskin and Nikolaev, 1996; Ariskin *et al.*, 1996; Almeev and Ariskin, 1996; Nikolaev *et al.*, 1996). Here we illustrate the efficiency of the INFOREX system using new options that make it possible to analyze the pattern of cotectic lines depending on pressure and temperature in certain petrologically important projections.

Analysis of Ol–Opx–Cpx Cotectic Melts at High Pressure

For example, consider the results of high-pressure experiments on Mg-rich basalts and peridotites. The *query* is formulated as follows: we need to find runs conducted on samples of natural and similar synthetic ultrabasites and basites at pressures of 10–20 kbar (dry conditions) in the temperature range 1250–1450°C. Additional search attributes include: experiment duration must be at least 12 h, and the experiment products must be high-magnesia glasses ($Mg^{\#} > 0.65$) whose compositions correspond to equilibrium with the lherzolite assemblage *Ol–Opx–Cpx* ± *Spl*. In response to this query, the INFOREX database produced 75 experiments matching these criteria: these runs represent 13 studies, conducted between 1977 and 1996 (Mysen and Kushiro, 1977; Takahashi and Kushiro, 1983; Fujii and Scarfe, 1985; Takahashi, 1986; Falloon and Green, 1987; Falloon *et al.*, 1988; Bartels *et al.*, 1991; Kinzler and Grove, 1992; Hirose and Kushiro, 1993; Falloon *et al.*, 1994; Baker and Stopler, 1994; Baker *et al.*, 1995; Kushiro, 1996).

The *Petrological Problem* is to construct a generalized equation describing the compositional shift of the *Ol–Opx–Cpx–Liq* cotectic melt as a function of temperature and pressure. To accomplish this, we chose the *Auxiliary Calculations* option (Fig. 3) and recalculated the 75 glass compositions to the *Ol*, *Pl*, and *Qtz* components according to the procedure of Walker *et al.*, (1979). This is the routine procedure used by petrologists to project multicomponent compositions onto pseudoternary diagrams (in this case, *Ol–Pl–Qtz*) so as to visualize them on a plane. The INFOREX program enables the user to process these data in a linear model of the form:[1]

$$T, °C = aP, \text{kbar} + b\ln X_{Ol} + c\ln X_{Pl} + d, \tag{1}$$

where a, b, c, and d are regression coefficients. The regression parameters and their standard deviations cal-

[1] For multiphase equilibria, such descriptions (sublinear models) are extremely common among petrologists, particularly when developing computer programs for calculating phase equilibria (Longhi, 1991, 1995; Kinzler and Grove, 1992; Yang *et al.*, 1996).

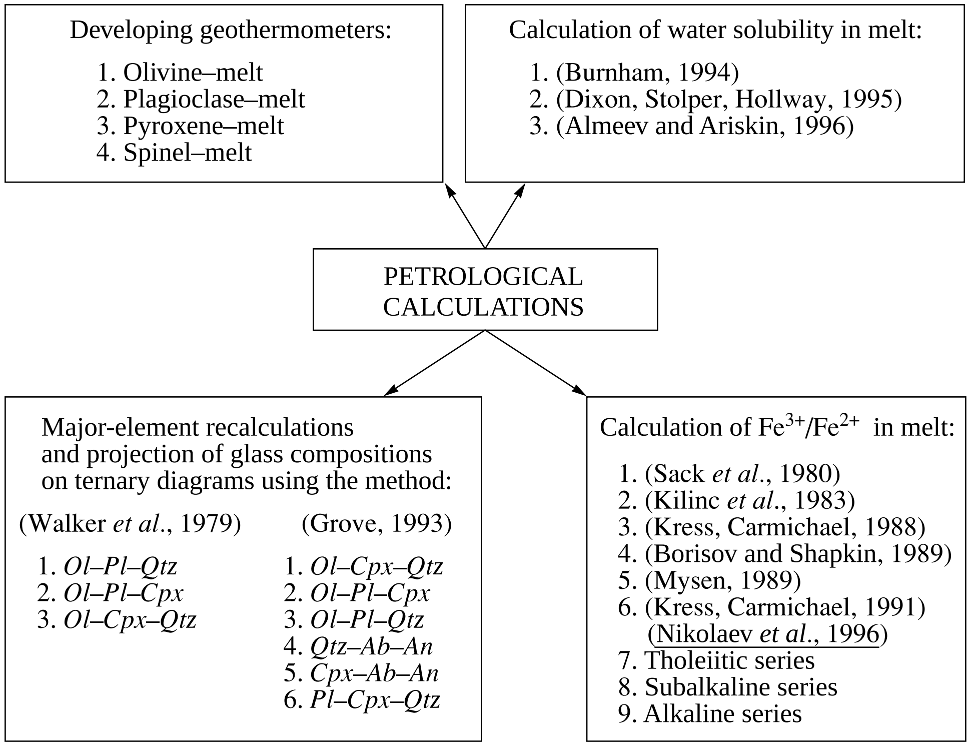

Fig. 3. Block diagram showing the main functions of the *Petrological Calculations* module.

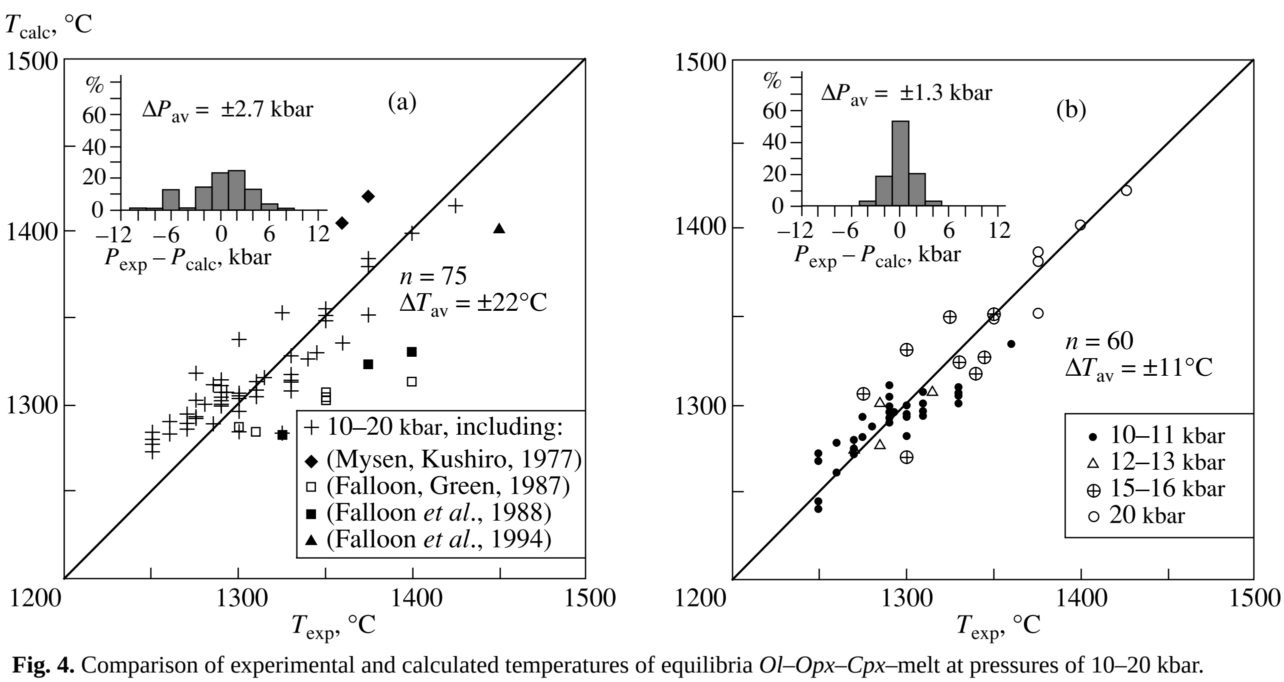

Fig. 4. Comparison of experimental and calculated temperatures of equilibria *Ol–Opx–Cpx*–melt at pressures of 10–20 kbar. Calculations were performed according to equation (1) using parameters in the table: (a) total data set of glass compositions extracted from the database; (b) the same data set excluding the experiments of Mysen and Kushiro (1977) and Falloon *et al.*, (1987–1994) (see the main text of the paper). The histograms represent the accuracy of solving the inverse problem for pressure.

culated for the compositions retrieved from the base are presented in the table.

These parameters can be used to determine the accuracy with which equation (1) reproduces the values of experimental temperatures and to assess whether this equation can be used for barometry at a known melt composition and equilibrium temperature. These data are shown in Fig. 4a and, at first sight, indicate that the accuracy is fairly high: the average deviations of the calculated temperatures and pressures from the experi-

Regression coefficients for the equation of high-pressure equilibrium *Ol–Opx–Cpx*–melt (1) and equation of amphibole liquidus under water-saturated conditions (2)

Parameters	*Ol–Opx–Cpx*–melt, P = 10–20 kbar, T = 1250–1450°C		Amphibole–melt, P = 2–6.9 kbar, T = 800–1000°C
	n = 75	n = 60	n = 59
a	8.14 (1.39)	8.65(0.77)	–71.47(9.63)
b	7.91 (23.84)	34.86(13.30)	–159.28(38.75)
c	–82.60 (15.56)	–99.10(10.05)	668.93(50.44)
d	1171.49 (37.99)	1170.89(21.40)	1317.39(65.32)

Note: Standard deviations (1σ) are given in parentheses.

mental ones are ±22.4°C and ±2.75 kbar, respectively. However, a close examination of 15 points with maximum deviations (45–87°C and 5–10 kbar) reveals that 13 of them represent results obtained in one laboratory (Falloon and Green, 1987; Falloon *et al.*, 1988; Falloon *et al.*, 1994), and the remaining two relate to early experiments on peridotite melting (Mysen and Kushiro, 1977), which were later revised on several occasions.

In our opinion, these discrepancies may point to the presence of systematic, possibly methodical, differences in the results obtained in the Australian laboratory (Falloon *et al.*, 1987–1994) from the data of other investigators (Takahashi and Kushiro, 1983; Fujii and Scarfe, 1985; Takahashi, 1986; Bartels *et al.*, 1991; Kinzler and Grove, 1992; Hirose and Kushiro, 1993; Baker and Stolper, 1994; Baker *et al.*, 1995; Kushiro, 1996). This conclusion does not indicate unambiguously which experiments yield the most accurate results, but practical considerations suggest that in constructing the liquidus equation (1), it would be useful to exclude the data of those 15 experiments that show the greatest deviations during the solution of the inverse problem.

This opportunity is provided by a special option of the INFOREX system, enabling all experiments representing a particular study to be filtered out (Meshalkin and Ariskin, 1996). Resorting to this option, we excluded from consideration the data of Mysen and Kushiro (1977), Falloon and Green (1987), Falloon *et al.*, (1988), and Falloon *et al.*, (1994); the regression parameters for compositions extracted with this filter and obtained in the 60 "more accurate" experiments are also given in the table. These results show better agreement between the data and appreciably increased precision in solving the inverse problem (Fig. 4b).

We have discussed this example in detail because it graphically demonstrates the potential of the INFOREX database as an *expert system*. Statistical processing of large amounts of information without carefully examining the data is likely to produce inadequately accurate dependencies. The INFOREX system

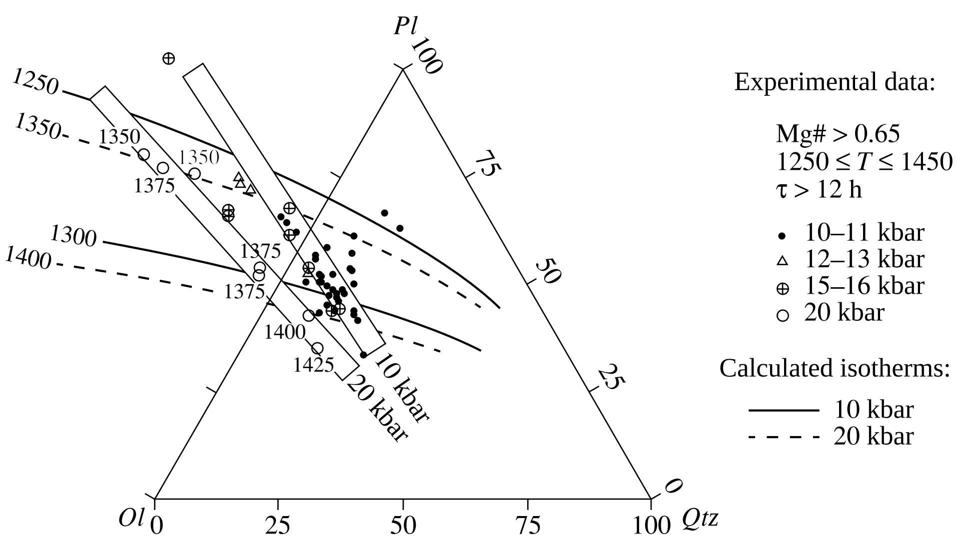

Fig. 5. Composition of experimental glasses and calculated isotherms of high-pressure equilibrium *Ol–Opx–Cpx*–melt in the "barometric" projection *Ol–Pl–Qtz*. Recalculation to normative components was performed using the method of Walker *et al.*, (1979). Attempts to graphically project natural compositions onto this diagram may lead to errors in estimating pressure of about 5–7 kbar.

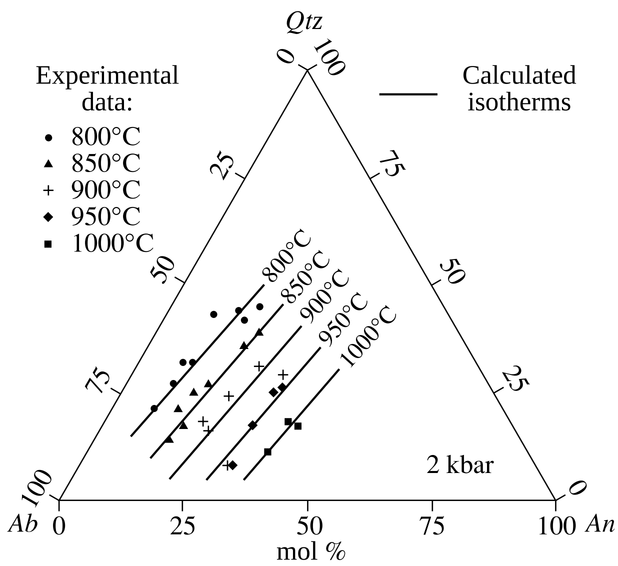

Fig. 6. Composition of experimental glasses and calculated isotherms of amphibole–melt equilibrium under water-saturated conditions (P = 2 kbar).

The glass compositions were projected onto the quartz–anorthite–albite plane using normative components calculated according to the method of Grove (1993).

allows the user to experiment with matching various data by constructing and analyzing regression equations (Ariskin and Nikolaev, 1996; Ariskin *et al.*, 1996).

The above analysis also has practical significance. In Fig. 5, the compositions of 60 high-pressure cotectic melts *Ol–Opx–Cpx* are projected onto the *Ol–Pl–Qtz* plane. Petrological interest in this projection arises from its barometric potentialities, because some investigators have repeatedly demonstrated that the olivine–pyroxene equilibrium lines are appreciably shifted toward the *Ol* corner with increasing pressure (Takahashi, 1986; Kinzler and Grove, 1992; Hirose and Kushiro, 1993; Baker *et al.*, 1995); this shift is schematically shown in Fig. 5. Using equation (1), we calculated the equilibrium isotherms *Ol–Opx–Cpx–Liq* at pressures of 10 kbar (1250 and 1300°C) and 20 kbar (1350 and 1400°C) and superposed them on this scheme. The data presented show that, in attempts to graphically project the natural or calculated compositions of basaltic melts onto this diagram without considering the temperature of the assumed equilibrium with residual lherzolite, the error in estimating the pressure may be as high as 5–7 kbar.

Calculation of Isotherms of Melt Saturation in Amphibole

To provide another illustration of using the INFOREX database, we shall analyze the results of water-saturated experiments. The purpose of our query is to find all runs conducted on natural and synthetic samples at pressures of 1–10 kbar in the presence of excess water (vapor phase) subject to two additional conditions: (1) the data on the composition of the melt are available, and (2) the composition includes the final phase assemblage of high-calcium amphibole (hornblende). No constraints are imposed on the experiment duration.

In the INFOREX database, these match criteria are met by 158 experiments published in 10 papers. The distribution of pressures is as follows: 66 experiments were carried out at pressures of 1–2.5 kbar, 63 at 3–5.2 kbar, and 29 at 7–10 kbar. These experiments bracket the temperature range 675–1050°C, with glass compositions varying from basaltic andesite to rhyolite (52–80% SiO_2). The melts retrieved correspond to equilibria with various assemblages, which include—in addition to amphibole—plagioclase, olivine, orthopyroxene, augite, magnetite, ilmenite, biotite, apatite, and some other minerals. To further analyze these data, we selected the most representative studies (Beard and Lofgren, 1991; Luhr, 1990; Sisson and Grove, 1993) conducted at pressures of 2 kbar (28 experiments), 4 kbar (19 experiments), and 6.9 kbar (12 experiments). The petrological problem was to use this set to construct the liquidus equation for amphibole and estimate the effect of temperature and pressure on the composition of a melt in equilibrium with hornblende.

For this purpose, we again chose the *Auxiliary Calculations* option (Fig. 3) and analyzed nine methods of recalculating glass compositions in order to find a projection, in which the desired relationships are seen most clearly. The best result was obtained with Grove's method, which was used to project the compositions onto the *Qtz–An–Ab* (quartz–anorthite–albite) plane; this is not surprising, if we consider that the experimental glasses are, on average, of dacite composition. After that, the data of 59 selected experiments were processed according to the linear model:

$$T,\ ^\circ\mathrm{C} = a\ln P,\ \mathrm{bar} + bX_{Qtz} + cX_{An} + d, \qquad (2)$$

where a, b, c, and d are regression coefficients (table). During the solution of the inverse problem according to equation (2), the experimental values of temperature and pressure were reproduced within ±19.4°C and ±1111 bar (average deviations); this appears to be a good result, if we consider the large amount of methodical uncertainties associated with hydrous experiments and glass quenching. Figure 6 shows five isotherms calculated at a pressure of 2 kbar according to equation (2) using parameters in the table. These data clearly demonstrate that our liquidus equation for amphibole faithfully reproduces the shift of the melt compositions into the field enriched in quartz and albite with decreasing temperature. The estimates of water content in the melts according to the models of Burnham (1994) and Almeev and Ariskin (1996) vary within 4.2–6.0 and 5.5–7.2 wt % H_2O, respectively.

CONCLUSION

The INFOREX database with its built-in procedures of processing experimental information is a powerful new tool for petrological investigations. With this system, subliquidus experiments are searched and analyzed in a matter of seconds, and a user who is experienced at using the base will have to spend only a few hours to develop the most accurate mineral–melt geothermometers or liquidus equations for multiphase assemblages. The petrologist now has access to the results of about 7000 experiments on melting synthetic and natural samples, and about 10 000 compositions of experimental phases are available for testing geothermometers and various empirical dependencies. A new capability for working with experimental data is the calculation of water concentration in glasses for which there are no direct determinations of H_2O content. The database is systematically updated annually.

At the same time, it is somewhat disconcerting to see that the INFOREX system is being introduced into petrological research at an unreasonably slow pace. Scientists still tend to use traditional computer models of fractionation, melting, and other algorithms designed to solve certain specialized petrological problems. The question of the accuracy and applicability of the programs is commonly ignored or regarded as the developer's sole responsibility. Such an approach to computer modeling appears to be inadequate. As we see it, any direct application of computer models to natural rocks and minerals is possible only after these models are tested on experimental data covering that field of magma compositions that is of interest to each particular petrologist or geochemist. The INFOREX system offers unique opportunities to accomplish this task.

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