COMPUTATION AND PLOTTING OF LIQUIDUS ISOTHERMS IN MULTICOMPONENT SILICATE SYSTEMS

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Abstract

Machine plotting of computed two-dimensional projections of isotherms on liquidus boundaries in multicomponent silicate systems has been coded in FORTRAN for an IBM 7094 computer and a CALCOMP digital plotter. Specimen results, using data of a twelve-component rock system (average granite plus water), are presented.

Introduction

A practical method for computing liquidus relationships in multicomponent binary salt systems using only the data of each of the constituent binary systems (Smith, 1965) has been simplified for use with multicomponent silicate systems (Smith, 1964). The rationale in dealing with salt systems starts with an assumption of ideally ionic behavior of the component binary compounds and the programs of computation determine and use empirical parameters which correct for non-ideal behaviour. On the other hand, the rationale for silicate systems starts with an assumption of ideally molecular behaviour of the component complex compounds and the programmes of computation in an analogous way correct for non-ideal behaviour. Thus the computer programmes for silicate systems are simpler because there need be no provision for various combinations of valency and common ions. In addition the compositions may be in weight fractions of silicate compounds instead of mole fractions of ions.

Several computer programmes (in FORTRAN II language) based on this method have been written and are being assembled into a system of optional routines. One of the most useful of the constituent programmes computes the temperature at regular compositional points on the liquidus of any component, the compositional variables being the weight fractions of any two of the other components while keeping the weight fractions of the remaining components constant. Although a table of such values contains all the necessary information for displaying the projection of a liquidus boundary from hyperspace to one of the three-component planes, the positioning of isotherms by graphical interpolation involves a considerable amount of further work. Accordingly, a change in the programme was made such that the output is a table of compositional points for isotherms in ten degree intervals. A CALCOMP digital plotter, controlled off-line by tape data output from the 7094 computer, became available at this time and a sequence of new routines was added to the programme to command the plotter to draw the computed isotherms.

METHOD

For programming generalization, the components are assumed to be in order such that the first three define the compositional plane to which the computed data are to be projected, and the invariant placement of these three components in the plotted compositional triangle is component 1 at the lower left corner, component 2 at the lower right corner, and component 3 at the upper corner.

A list of compositions corresponding in order to the selected components is inserted as data. The programme uses the values of the fourth and following compositions as constants and computes values of the first three as variables whose sum is constant.

The programme of computation outlined previously (Smith, 1964) is used with only minor changes up to the point at which temperatures at regular intervals of projected composition are computed on the liquidus surface of each of the first three components. In the earlier programmes, the results were printed as three tables of projected compositions and corresponding temperatures, but in the current programmes, the results are stored and used to generate reverse tables of temperatures at ten-degree intervals and corresponding lists of projected compositions. These compositional points can be used to construct a projection of the three liquidus phase boundaries, contoured with their respective isothermal lines.

Machine drawing of the computed isotherms was tested with a CALCOMP digital plotter and found to be satisfactory. The details of transformation of the compositional tables, for the isotherms to appear within a triangular boundary and in the proper sense relative to the three corners, are not difficult to programme but are too complex to describe in a few words. This part of the programme was designed to be fairly general in that machine drawing would be in a triangle of any shape, size, and position on the page.

There is a specific provision in the programme for making a correction for pressure if water is one of the components and the other components of the system are dominantly albite, orthoclase, and quartz. The approximate pressure in order to hold the given water concentration in the silicate liquid at the liquidus temperature is computed using an empirical function (Smith, 1963, p. 264) and the effect of this pressure on raising the liquidus temperature is computed assuming a linear function and using a coefficient read with the data. This routine is skipped automatically unless a control number is in a specific data field. It is quite useful for comparing computed and measured liquidus data for hydrous silicate systems which have been studied at pressures equal to the water vapour pressure of the silicate liquid.

Computer Programmes

Programmes for the above computations were written in FORTRAN II language and run on an IBM 7094 computer. It would be preferable to use the FORTRAN IV language under IBSYS monitor control, but the CALCOMP plotter routines compatible with this scheme are not yet available here. The table-generating programme was translated into FORTRAN IV and the plotting programme will be translated in the near future. Copies of the FORTRAN programmes and column-binary compiled decks are available on request.

Specimen Results

A complex system of unusual interest to petrologists is granite–water. As a rather rough approximation, this can be treated as binary by assuming that the silicate composition is cotectic. Alternatively, it has been considered to be similar to the quaternary system albite–orthoclase–quartz–water by assuming that the other mineral components of granite can safely be neglected. However, the quantitative effects of anorthite in the system is not small because anorthite raises the liquidus temperature of albite but at the same time lowers the liquidus temperature of the other major minerals (Smith, 1963, p. 215; 1964). Each of the other minor mineral components of granite would be expected to lower the liquidus temperatures of the major minerals. Therefore a better approximation of the granite–water system would be the normative composition of granite, including all minor but not trace components, plus water. Since there are only three major mineral components, albite, orthoclase, and quartz, their liquidus surfaces, also binary and ternary cotectic relationships between them, are of first importance.

The average composition of granite (Daly, 1933) was converted into the following normative minerals and corresponding weight fractions of the anhydrous assemblage:

Albite	0.29684	Mn-Pyroxene	0.00223
Orthoclase	0.24485	Corundum	0.01143
Quartz	0.28720	Magnetite	0.02295
Anorthite	0.08702	Ilmenite	0.00747
Enstatite	0.02209	Apatite	0.00454
Fe-Pyroxene	0.01338		

Together with water this 12-component system was found to be suitable for at least preliminary computation of the liquidus surfaces of the first three minerals. There are enough reliable data on liquidus temperatures in binary systems to allow calculation of many of the three parameters required for the liquidus function of the major minerals. The rest were approximated by analogy, neglecting the residual error because the concentration of the minerals involved is small.

The binary liquidus parameters were computed by programme LIQPAR (Smith, 1965) using primary data in the literature. A detailed discussion of these parameters, the propagation of their errors into the final results, and further refinements of the computation method are left for later communication.

Computer runs were made using the programmes described above, with the weight fraction of water at 0.00, 0.02, 0.04, 0.06, 0.08, and 0.10, and the granite mineral components making up the remainder, each time projecting the albite, orthoclase, and quartz liquidus isotherms. The quality of the plotter output is indicated in Fig. 1 which was prepared

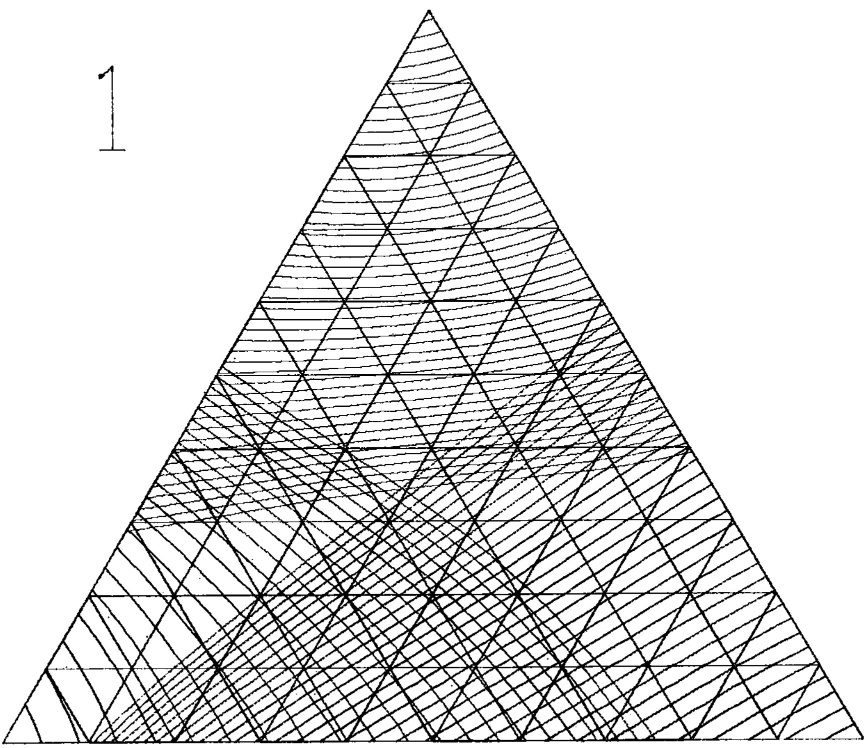

FIG. 1. Photo-copy of machine drawing of projected isotherms of albite (lower left corner), orthoclase (lower right corner), and quartz (upper corner) in the multicomponent mineral system described in the text, and at a weight fraction of 0.10 water. The length of sides of the triangle in the drawing is ten inches.

from a photostat of the machine drawing. A tracing (Fig. 2) was made of the same drawing, adding cotectic lines defined by isothermal intersections, suppressing metastable parts of isotherms, and showing computed values of compositional points. Finally, the projected binary cotectic lines of the six plots were superimposed (Fig. 3) to show the effect of increasing concentration of water on the thermal valleys of the granite–water system.

A diagram of ternary liquidus relationships in multicomponent systems, projected as described above, cannot be used to predict the course of the liquid during crystallization of a selected composition because the compositional invariancies assumed for the diagram no longer obtain. The computed surfaces give the temperature values above which the system would contain no crystalline phase and below which one or other of albite (in plagioclase), orthoclase, or quartz would be present, at the vapour pressure of the given water concentration in the complex silicate liquid.

The fact that the computed trace of the albite–orthoclase–quartz

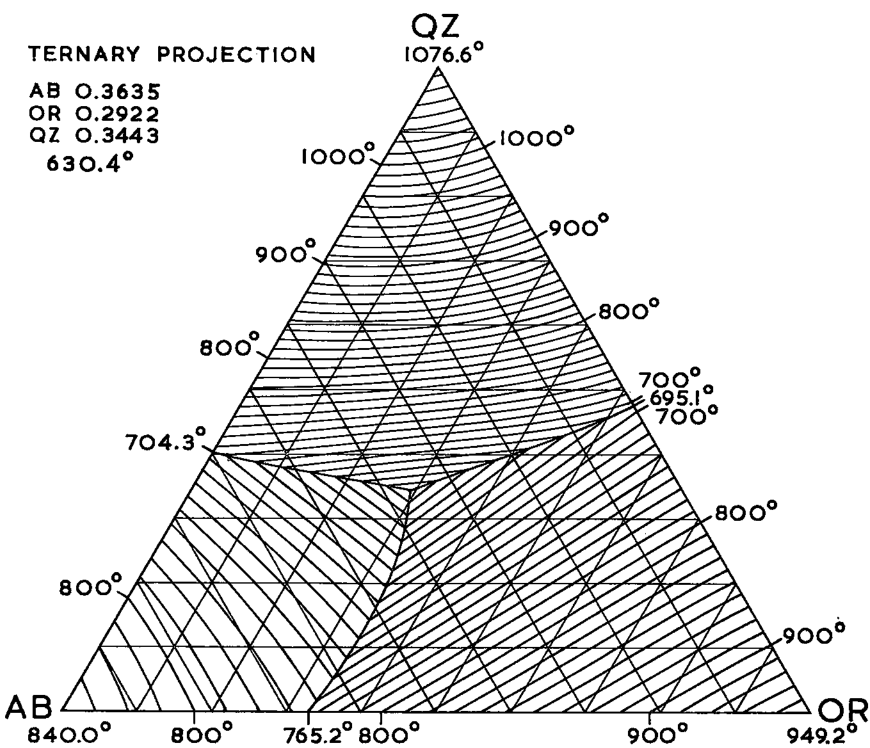

FIG. 2. Tracing of fields of isotherms from the machine drawing shown in Fig. 1, with added cotectic joins and computed numerical values.

ternary cotectic point for granite with variable water concentration very nearly intersects the compositional point of average granite (Smith, 1964) is in accord with Bowen's classical hypothesis of the origin of magmas of granitic composition. It has no direct bearing, however, on the determination of the geological process by which the low melting temperature liquid is formed.

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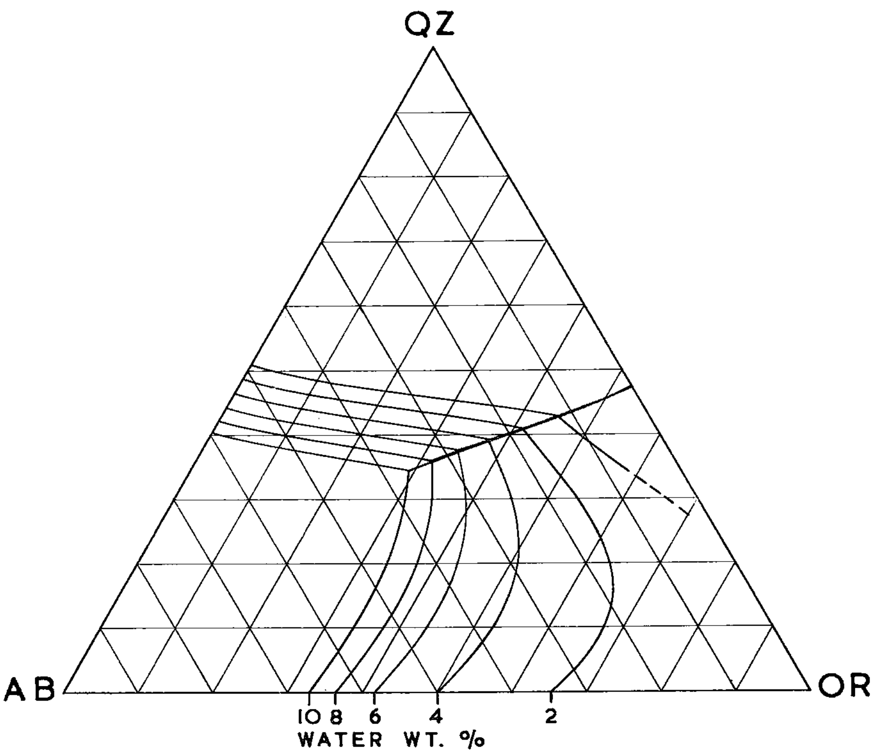

Fig. 3. Cotectic joins, as in Fig. 2, from six machine drawings superimposed to show the effect of variable weight fraction of water. (At zero concentration of water the computed projected isotherms show no intersection of the albite and orthoclase liquidus surfaces near the albite-orthoclase join.)

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