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VERTEXVIEW: AN INTERACTIVE PROGRAM TO ANALYZE AND PLOT PETROLOGICAL PHASE DIAGRAMS

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Abstract—VERTEXVIEW is an interactive microcomputer program that permits interactive analysis, editing, and plotting of petrological phase diagrams. It has been designed as a menu-driven Microsoft Windows application to allow inspection of a large variety of calculated phase diagrams such as ternary chemographies, Schreinemaker projections and mixed-variable phase diagrams. Different windows, menus, and options are available depending on the kind of phase diagram provided in the input file. General commands include the *Copy*, *Save*, *List*, and *Print* commands, and different zoom options are provided. The program also provides single and/or multiple selection of invariant and univariant elements in Schreinemaker projections. Flexibility, ease of operation and on-line help make it ideal for both teaching and research. © 1997 Elsevier Science Ltd

Key Words: Phase diagrams, Metamorphic petrology, Interactive graphics.

INTRODUCTION

With the aid of personal computers, phase equilibrium calculations have become routine work in many aspects of metamorphic petrology (e.g. Perkins, Essene, and Wall, 1987; Perkins, Brown, and Berman, 1986; Powell and Holland, 1988; Brown, Berman, and Perkins, 1989; Connolly, 1990). Most packages include computer-driven graphics to produce on-screen and printed phase diagrams, but interactive analysis is frequently not supported.

With this problem in mind, we have developed VERTEXVIEW, a Microsoft® Windows™ application to perform interactive analysis, plotting, and editing of petrological phase diagrams. The program should serve on several levels. As a research tool, VERTEXVIEW allows rapid analysis of phase diagrams which may be edited to produce camera-ready output. As a teaching aid, its interactive nature and on-line help provide an useful insight into the kind of problems which are related to phase-equilibria calculation and analysis.

VERTEXVIEW has been designed specifically to read the plot file structure of VERTEX (Connolly, 1990). VERTEX can be used to calculate a great variety of phase diagrams, including: composition phase diagrams (ternary chemographies), Schreinemaker projections (such as P–T–X_f–μ_i diagrams, where X_f is the composition, that is the molar fraction, of a stable fluid phase and μ_i is the chemical potential of the ith component in the system), mixed variable diagrams (P–T–X_i diagrams, where X_i is the composition of a system expressed by the molar fraction of its ith component), and stability fields. Further, VERTEX can be used to compute equilibria involving solution phases using the pseudocompound approximation of Connolly (1990). VERTEX is part of a collection of FORTRAN 77 programs (PeRpLeX) for computing multidimensional phase diagrams and general thermodynamic calculations. Source codes of the PeRpLeX package are available from the second author or via the Internet (http://www.erdw.ethz.ch/~jamie/perplex.html) and may be easily compiled to generate applications running on a variety of platforms, including Microsoft® Windows™. VERTEXVIEW is modelled after the PeRpLeX PostScript® plotting program PSVDRAW, which can be used to produce high quality editable PostScript® images of the diagram calculated with VERTEX.

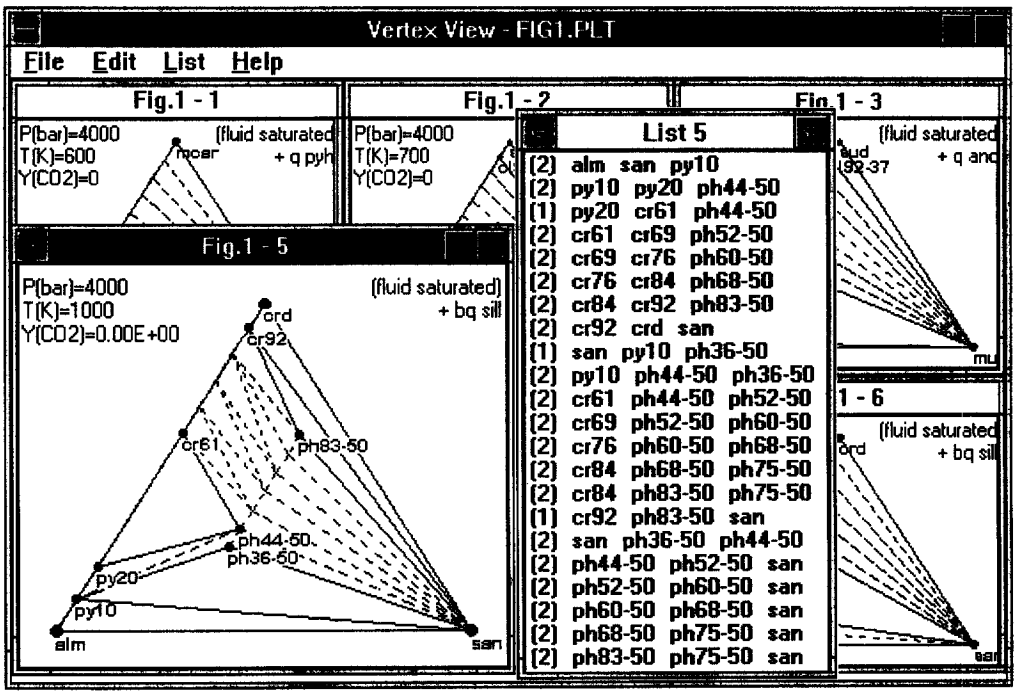

Figure 1. VERTEXVIEW full-screen image of isobaric-isothermal MgO-FeO-$KAlO_2$ composition phase diagrams for system K_2O-MgO-FeO-Al_2O_3-SiO_2-H_2O. Chemographies were computed with component saturation hierarchy H_2O-SiO_2-Al_2O_3, so that H_2O, α-quartz (or β-quartz) and pyrophyllite (or andalusite, kyanite, or sillimanite, according to different P–T sectioning values) are phases in excess, as given at top-right of each *Plot* window. P, T, $X(CO_2)$ conditions for each diagram are indicated at top-left corner of window. The *Plot* window labelled "Fig.1–5" has been enlarged to show details discussed in text. "List 5" window summarizes both three-phase and two-phase assemblages plotted in that chemography. Abbreviations of endmembers different from Kretz (1983), and occurring in the "Fig.1–5" and "List 5" windows are: bq: β-quartz, san: K-feldspar, sill: sillimanite. Abbreviations of pseudocompounds in same windows are: cr##: Mg-Fe cordierite solution, ph##-##: phlogopite-annite-eastonite-siderophyllite solution, py##: pyrope-almandine solution. See Appendix for notations of solid solutions and phase equilibria.

PROGRAM STRUCTURE AND HARDWARE/ SOFTWARE REQUIREMENTS

VERTEXVIEW has been coded in Microsoft® Visual Basic 3.0. The distribution package consists of two self-extracting archives plus an unzipped SETUP.TXT file with setup instructions. The first archive includes the following files: README.TXT (documentation), VERTEXV.EXE (the executable program), VERTEXV.HLP (on-line help facility), and some ancillary files. The second archive provides input files to test that the program has been properly installed.

Equipment with the following minimum system attributes is required or recommended. Hardware: IBM-PC or compatible 80386 processor with 4 Mbytes RAM, a VGA card and a "mouse" or other pointing device. A 80486 processor with 8 or more Mbytes RAM (recommended) will strongly increase execution speed. Software: MS-DOS 5.0 or later and Microsoft® Windows™ 3.1 or later. Although this release also runs with Windows®95 and Windows®NT, a forthcoming release will be specifically setup as a 32-bit application. A record of user comments and upgrade notices is mantained by the first author at his Internet URL (http://www.dmp.unito.it/castelli.html).

VERTEXVIEW conforms to the standard Microsoft® Windows™ and accesses all facilities of the Microsoft® Windows environment. After starting the program and opening a file, different *Plot* windows, "child" windows, menus, and options are available from the main window depending on the kind of phase diagram provided in the input file. A detailed on-line help about windows, commands, and options is also provided. General commands are arranged in drop-down menus and include: (1) the *Copy* and *Save* commands to copy to the "clipboard" or to a bitmap file the content of *Plot* window(s); (2) the *Print* command to plot the current content of *Plot* window(s) and of some "child" windows; and (3) the *Print Setup* command to customize any printer/plotter device supported by the current Microsoft®Windows release. It is worth mentioning that, after interactive analysis of the phase diagram (see the next section and Examples A–C), appropriate selections with the *Print Setup* command can be used to "print" the content of the

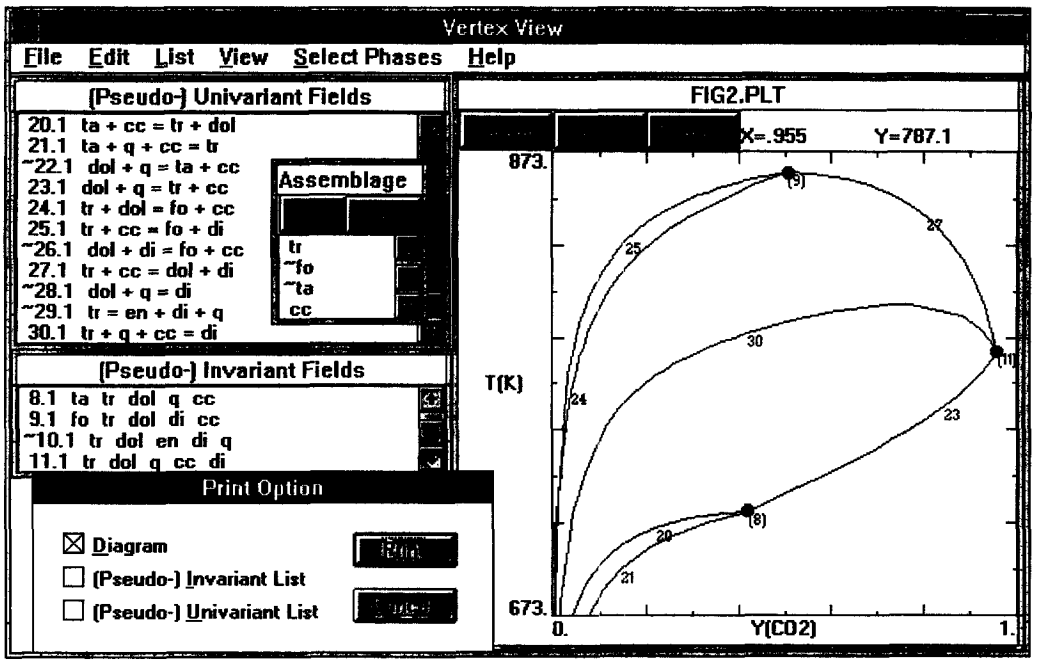

Figure 2. VERTEXVIEW full-screen image of T–$X(CO_2)$ Schreinemakers projection for the CaO-MgO-SiO_2-H_2O-CO_2 system at P = 2000 bars. Four windows (*FIG2.PLT*, *(Pseudo-) Invariant Fields*, *(Pseudo-) Univariant Fields* and *Assemblage*) and one dialog box (*Print Option*) are open at same time. Phase fields within phase diagram of *Plot* window are drawn as solid curves (univariant elements) and full dots (invariant elements), respectively. To right of *Default*, *Previous* and *Redraw* command buttons, given X and Y values correspond to those of invariant assemblage (11) tremolite + dolomite + quartz + calcite + diopside. Elements of phase diagram are listed and labelled in *List* windows (equilibrium equations are written such that the high-T assemblages are written on right side of equilibrium; see Appendix for notation of phase equilibria). Abbreviation of endmembers different from Kretz (1983) are: cc: calcite, m: magnesite, q: α-quartz, ta: talc. *Plot* window shows stability field of tremolite + calcite assemblage, which has been automatically determined by selecting (i.e. double-clicking with mouse) two phases in *Assemblage* window of *Select Phase* menu. This field is contoured by the 25, 27, 23 and 21 univariant equilibria (note that no tilde characters occurs in front of them in *List* window). *Print Option* dialog box has been left open to show multiple options of *Print* command.

Plot window(s) to an high-quality editable PostScript® file.

As many as six composition phase diagrams (see Example A) may be shown simultaneously in separate *Plot* windows. Each *Plot* window is resizable with the mouse and includes a ternary chemography, as well as some computational parameters. Phase assemblages plotted in each *Plot* window are also listed in a separate "child" window that may be inspected using the commands of the *List* Menu.

Schreinemaker projections are also shown in a *Plot* window, whereas two "child" windows list the (pseudo-)invariant and (pseudo-)univariant fields (Connolly, 1990), respectively (see Example B). Appropriate labelling of invariant and univariant elements is provided in both the *Plot* window and the *List* windows. In the *Plot* window, back and forward zoom facilities include mouse-driven sizing boxes, command buttons, and numeric input of x/y values in text boxes. Coordinates within the diagram are listed, as a function of the mouse position, at the top-right corner of the *Plot* window.

The *View* menu includes commands to facilitate on-screen interpretation of the plot by including/excluding univariant and invariant fields, and labels from the plot.

Commands of the *Select Phases* menu aid with further analysis of the calculated projection. At the user's option, one or more phases (among those included in the calculation) may be selected from a list to be (1) constrained as an assemblage, (2) included in any assemblage, or (3) excluded from any assemblage (see the *Assemblage* window in Figure 2).

Management of mixed-variable phase diagrams is similar to that of Schreinemaker projections (see Example C), although the *Select Phases* menu is not provided in the current release.

WORKING EXAMPLES

Examples A-C show three simple applications of the program. For clarity and editorial convenience, we have chosen examples involving a small number of phases, equilibria, and solution models. Note

that Figures 1–3 are screen images and thus lower in quality than output generated by the VERTEXVIEW *Print* command.

Example A

Isobaric–isothermal composition phase diagrams in the KFMASH system (equation of state and thermodynamic data from Holland and Powell, 1990) are shown in Figure 1. The thermodynamic composition space has been reduced to the MgO-FeO-$KAlO_2$ ternary by specification of the component saturation hierarchy H_2O, SiO_2, Al_2O_3 (Connolly, 1990). The *Plot* window labelled "Fig.1–5" has been enlarged to show both stable assemblages at $P = 4$ kb, $T = 1000$ K and the use of the *Resize* option in VERTEXVIEW. In "Fig.1–5", there are three stable three-phase assemblages (K-feldspar-biotite-garnet, K-feldspar-phlogopite-cordierite and garnet-cordierite-biotite), which define triangular regions (drawn with heavier lines in printed output). Dashed tie-lines (lighter tie-lines in the printed output) are used to define the fields of two-phase assemblages (such as sanidine-cordierite) in which mineral(s) exhibit solid solution (see Appendix for notations of solution models and phase equilibria).

Example B

This example is a T-$X(CO_2)$ Schreinemaker projection calculated in the CaO-MgO-SiO_2-H_2O-CO_2 system at constant pressure. Phase relationships were calculated using the equation of state and the thermodynamic data of Holland and Powell (1990), and included the following compounds: calcite, dolomite, diopside, enstatite, forsterite, magnesite, quartz, talc, and tremolite. The complete topology of this system (e.g. Kerrick, 1974, fig. 14) is not shown in Figure 2, but instead results obtained by applying the *Assemblage* command of the *Select Phases* menu. This option has been used to outline the stability field of the tremolite + calcite assemblage. The stability T-$X(CO_2)$ field of this assemblage has been obtained by selecting both tremolite and calcite in the *Assemblage* window, and is defined by the invariant and univariant elements given in the *Plot* window, which are automatically indicated in the *List* windows.

Schreinemaker projections including phases which exhibit solid solutions have a similar layout and may be inspected using the same commands and options. In addition to notation of invariant/univariant equilibria discussed in the Appendix, appropriate drawing is used in the *Plot* window to

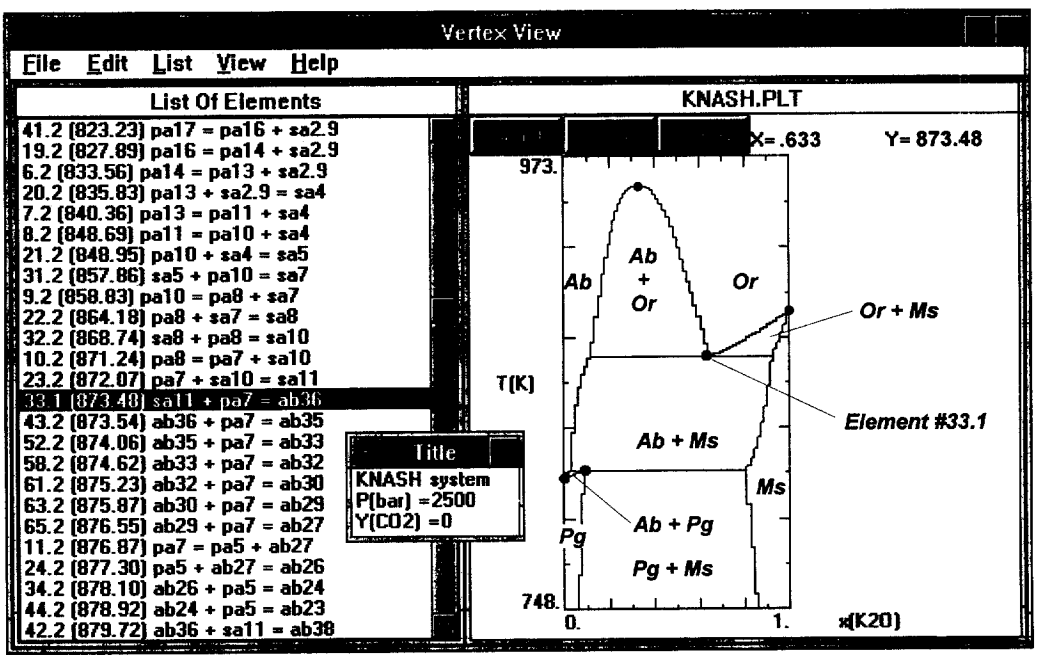

Figure 3. VERTEXVIEW full-screen image of mixed-variable phase diagram. Isobaric phase diagram of *Plot* window depicts T versus $K_2O/(K_2O + Na_2O)$ phase relationships between alkali feldspars and micas at $P = 2500$ bars after sequential projection through saturated components H_2O, SiO_2, and Al_2O_3. *List* window to left shows elements of diagram with increasing temperature (equilibrium equations are written such that high-T assemblages are written on right side of equilibrium). Abbreviation of endmembers different from Kretz (1983) are: san: K-feldspar (sanidine or orthoclase), sill: sillimanite, ta: talc. Abbreviations of pseudocompounds are: pa##: muscovite-paragonite solution, sa##: Na-K feldspar solution (Ab-rich side), ab##: K-Na feldspar solution (Or-rich side). Labels in italics have been added during final editing of figure. See Appendix for equilibrium and solid solution notation.

recognize those elements which contain solution phases modelled by pseudocompounds. True univariant and invariant elements are drawn as thick curves and large full dots, respectively. Pseudoinvariant and pseudounivariant elements are drawn as small full dots and dashed curves, respectively. The same scheme is supported in the printed outputs.

Example C

An example of a VERTEXVIEW application to a mixed-variable phase diagram calculation is shown in Figure 3, where phase relationships in the KNASH system are given at constant pressure as a function of temperature and $K_2O/(K_2O + Na_2O)$ ratio. The phase diagram was calculated with the equation of state and thermodynamic data of Holland and Powell (1990), and indicates the one-phase to two-phase assemblages as a function of temperature and composition of the sequential projection through SiO_2 and Al_2O_3 components. To inspect the diagram and recognize elements, the pointer device may be moved within the diagram at the temperature of interest. For example, the invariant reaction assemblage albite + muscovite = orthoclase is defined by the eutectoid element 33.1 occurrring at $T = 873.48$ K and $X(K_2O) = 0.633$. This reaction is labelled 33.1 ($sa_{11} + pa_7 = ab_{36}$) in the *List* window. According to the pseudocompound notation, this is a true invariant equilibrium consisting of albite (of composition $sa_{11}ab_{89}$), orthoclase ($sa_{64}ab_{36}$), and muscovite (pa_7ms_{93}). In the same *List* window, the six elements listed after #33.1 (labels are: 43.2, 52.2, 58.2, 61.2, 63.2, 65.2) contour a portion of the $Or_{ss} = Or_{ss} + Ms$ pseudounivariant continuous reaction (orthoclase varying from $sa_{64}ab_{36}$ to $sa_{73}ab_{27}$) in the range $873.48 < T < 876.55$ K. See the Appendix for notation of equilibrium reactions and solid solutions.

SUMMARY

VERTEXVIEW performs interactive analysis and plotting of calculated phase diagrams. The types of diagrams supported by the program include: composition phase diagrams (chemographies), Schreinemaker projections (two-dimensional diagrams in which the invariant and univariant phase relations of a multicomponent system are projected as a function of two of its potentials) and mixed-variable phase diagrams (diagrams in which compositional variables of the system are plotted against a potential variable). Its layout, menu-driven commands, and options have proven ideal for graduate and undergraduate courses in petrology. Sets of practical exercises may be arranged to describe changes which take place, in the kind and number of phases, as a function of potential variables of a system. In addition, the interactive nature and commands of the *Select Phases* menu makes the understanding of Schreinemaker projections straightforward. For these reasons, advanced users and researchers may easily and rapidly inspect complex petrological problems.

The VERTEXVIEW plot file format is currently that generated by VERTEX (see Appendix). However, appropriate routines can be easily created to handle plot files generated by other thermodynamic calculators.

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APPENDIX

Abbreviations, Solid Solution Models and Notation

In VERTEXVIEW phase diagrams, names of pure end-members and pseudocompounds are given with the format and abbreviations entered in the thermodynamic data

input files used by VERTEX. Most of the abbreviations are according to Kretz (1983), but some shorter names are used to make pseudocompound labelling shorter, and are maintained in VERTEXVIEW to keep consistency of phase notation.

Mineral solutions occurring in Examples A and C were modelled with pseudocompounds (Connolly, 1990), using the ideal models listed in Connolly and others' (1994) and Berman's (1990) solution model for garnet. For solution models with only one independent mixing site, the notation for pseudocompounds consists of an abbreviated end-member name followed by its molar proportion in the pseudocompound. For example, in the *Plot* window labelled "Fig.1–5" of Figure 1, py10 and py20 are pseudocompounds containing 10 and 20 mol% pyrope-component along the binary pyrope-almandine, respectively. The pseudocompound notation for multisite solution models is more complex. As an example, ph44-50, in the same *Plot* window (Figure 1), is a biotite (phlogopite-annite-eastonite-siderophyllite solution) where 44 corresponds to X_{Mg} value and $50 = 1 - X_{Ts}$ (i.e. the value of the Tschermaks exchange vector), respectively.

Notation of phase equilibria

In Schreinemaker projections and mixed-variable phase diagrams (Figures 2 and 3), equilibrium labels in the *List* windows consist of a two-part numerical identifier, separated by a dot. The first number is the equilibrium index, which is be used to identify the invariant and univariant equilibrium in the *Plot* window. The second number is a flag which indicates the true variance of the field. If the flag is 1, the apparent and true variance of the assemblage are the same. If the flag is 2, then at least two compounds present in the assemblage represent the same solution, and the true variance of the equilibrium is greater than the apparent variance. The *List* window of Example C (i.e. "List Of Elements" in Figure 3) shows the use of this notation.

An integer flag is also used to specify the type of assemblages in composition phase diagrams (see the "List 5" *List* window of Figure 1). In this case the flag is (1) when the assemblage is invariant (as the san-py10-ph36-50 assemblage of Figure 1). If the flag is (2), the assemblage is part of a high variance, heterogeneous phase, region in which two or more of the pseudocompounds represent a homogeneous solution phase. For example, the pseudocompound assemblage cr92-crd-san is a two-phase assemblage consisting of K-feldspar and cordierite (where X_{Mg} in cordierite may be estimated from the averaged composition of the cr92 and crd pseudocompounds, i.e. $X_{Mg}=96$). Situations not included in Chemography 5 of 11 are: the flag is (0), if the assemblage consists entirely of stoichiometric compounds; the flag is (3) when the assemblage is part of a homogeneous phase region; and the flag is (4) if the assemblage contains two or more phases of an immiscible solution.

Input file format

The input file to VERTEXVIEW is an ASCII text-formatted file consisting of different segments generated by VERTEX during calculation of the phase diagram. The following is a short description of segments used to construct the "Fig.1–5" composition phase diagram of example A (Figure 1). Full details about the format of input file to VERTEXVIEW are included in the PeRpLeX package and are available on request. The first segment defines: the type of diagram to be plotted; the saturated phase components due to the saturation hierarchy H_2O, SiO_2, Al_2O_3; all phases (true compounds and pseudocompounds) included in the KFMASH system. The second segment lists the compositional coordinates of the phases which may be plotted in the FeO-MgO-$KAlO_2$ composition diagram. The third segment contains: the stable two-phase and three-phase assemblages for that system at P = 4000 bars, T = 1000 K and $X(CO_2)$ = 0; phases and species which define the buffering or component saturation surfaces (H_2O, β-quartz and sillimanite) at the specified P, T, $X(CO_2)$ conditions.