

## COMAGMAT: A FORTRAN PROGRAM TO MODEL MAGMA DIFFERENTIATION PROCESSES

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**Abstract**—The purpose of this paper is to present a general model (COMAGMAT) for the calculation of equilibrium temperatures and phase relations at a given extent of crystallization or melting in natural magmatic systems. This model is based on a set of empirical expressions that describe mineral–melt equilibria for major and trace elements in terms of pressure (up to 12 kbar), temperature, and liquid compositions for systems ranging from primitive basalts to dacites. These expressions are in the form of empirically calibrated mineral–melt geothermometers for Olivine, Augite, Pigeonite (Opx), Plagioclase, Ilmenite, and Magnetite used to develop the algorithm simulating multiply saturated magmatic melts. The results of the program are in the form of calculated liquid lines of descent, plus the equilibrium mineral proportions and compositions. The phase equilibria calculations form the core of a model that allows the user to simulate processes ranging from simple isobaric crystallization to in situ differentiation processes resulted from crystal settling, and polybaric fractionation.

**Key Words:** Igneous differentiation, Fractionation, Phase equilibria, Simulation, Basalt.

### INTRODUCTION

One of the main goals of experimental petrology during the last 15 years has been the development of computer models designed to simulate numerically igneous differentiation processes for natural systems. The majority of these programs are based on, and limited by, data from melting experiments and are intended primarily to simulate crystallization of terrestrial basalts (Nathan and Van Kirk, 1978; Nielsen and Dungan, 1983; Frenkel and Ariskin, 1984; Ghiorso, 1985; Ariskin and coworkers, 1987, 1988, 1990, 1992; Weaver and Langmuir, 1990). Recently, several attempts have been undertaken to model more complex igneous processes, such as assimilation (Ghiorso and Carmichael, 1985; Nielsen, 1985, 1990), “continuous melting” (Langmuir, Klein, and Plank, 1991), or in situ differentiation of layered intrusions (Frenkel and others, 1989). The purpose of this paper is to present COMAGMAT, a program designed to model igneous processes in magma chambers at pressures up to 12 kbar (Ariskin and others, 1992).

Earlier versions of COMAGMAT (RTRK and THOLEMAG) have been applied to:

- (1) Simulating the dynamics of the layering formation of Siberian differential sills (Frenkel and others, 1989);
- (2) Calculation of estimates of primary mineral compositions in cumulative rocks of basic intrusions (Barmina and others, 1989);

- (3) Interpretation of the petrogenesis of andesite-basaltic series of Eastern Kamchatka (Barmina, Ariskin, and Frenkel, 1989; Barmina, Ariskin, and Kolesov, 1992);
- (4) Computer barometry of the MORB glass compositions from the Atlantic mid-ocean ridge (Ariskin, Frenkel, and Tsekhonya, 1990).

### THERMODYNAMIC BACKGROUND

Any model designed to simulate magmatic processes must include an algorithm for the calculation of mineral–melt equilibrium at a given set of independent parameters of state. This problem is equivalent to the search for an extreme of one of the thermodynamic potentials. There are two ways of approaching this problem. One solution is to base the algorithms on the convex programming theory to determine the minimum of the free energy surface (Ghiorso, 1985). This method is arguably the most general and could be used to describe the entire range of natural systems. The approach, however, faces difficulties related to the requirement of a single set of accurate models for mineral and melt activity composition relationships applicable to the entire range.

A second solution type is largely independent of this problem. This approach takes advantage of numerical solutions of nonlinear empirical equations that describe mineral–melt equilibria and mass action law, combined with the mass balance constraints for a whole system composition. This approach allows us to see different activity models for each mineral–melt

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system to describe and simulate phase equilibria, even within the framework of the single system of equilibrium equations. One can achieve an acceptable level of accuracy using the second solution type, although as a rule, the mineral–melt expressions are accurate for only a limited range of composition (Nielsen and Dungan, 1983; Weaver and Langmuir, 1990). In the model described here we combined an empirical approach with the basic thermodynamic considerations of Frenkel and Ariskin (1984) into a hybrid algorithm.

#### CALCULATION OF MINERAL–MELT EQUILIBRIA USING THERMOMETRY, EQUILIBRATION, AND MELTING/CRYSTALLIZATION CONSTRAINTS

##### *Calculation of the equilibria melt–crystal mixtures assuming constant mineral compositions*

The interaction between a solid phase  $s$  and the liquid  $l$  can be represented as a system of reactions producing the endmember minerals  $M_m^s$  ( $m$  from 1 to  $M_s$ ,  $s$  from 1 to  $S$ ) from the arbitrary selected components in the liquid phase  $L_k$  ( $k$  from 1 to  $K$ ):

$$\sum_{k=1}^K v_{km}^s L_k = M_m^s \quad (1)$$

where  $v_{km}^s$  are stoichiometric coefficients. The reactions yield equilibrium constants in the form:

$$K_m^s(P, T) = a_m^s / \prod_{k=1}^K v_{km}^s a_k^l \quad (2)$$

as a function of pressure  $P$  and temperature  $T$  with the component activities depending on concentrations in the liquid and solid phases

$$a_k^l = a_k^l(x_1^l \dots x_K^l), \quad a_m^s = a_m^s(x_1^s \dots x_{M_s}^s). \quad (3)$$

The thermodynamic form of the  $P$ – $T$  relationship of the equilibrium constants is familiar:

$$K_m^s = \exp(-\Delta G_m^s/RT),$$

$$\ln K_m^s = -(\Delta U_m^s + P \Delta V_m^s - T \Delta S_m^s)/RT \quad (4)$$

where  $\Delta G_m^s$ ,  $\Delta U_m^s$  and  $\Delta S_m^s$  are the changes in free energy, internal energy, volume, and entropy in the formation of a given component. If the activity–composition relations were known, for example for ideal or regular solutions, Equations (2)–(4) could be used to calculate the equilibrium based only on thermodynamic data from extensive extrapolation with respect to temperature and pressure of the system states. In fact, because of the marked nonideality of the melt, many petrologists prefer to use simple empirical relations to specify the mineral–melt equilibria:

$$\ln D_m^s = (A_m^s + \beta_m^s P)/T + B_m^s, \\ D_m^s = D_m^s(x_m^s; x_1^l \dots x_K^l). \quad (5)$$

The expressions used to describe mineral–melt equilibria based on these assumptions can be calibrated by least-squares regression from experimental data.

These expressions will be referred to here as geothermometers. The form of the function  $D_m^s$  may be more or less arbitrary, but the best fit with respect to the experimental data will be obtained if a model is used that accurately approximates the activity of mineral and melt components. If a system of geothermometers similar to (5) is available for all interest, the phase equilibria of a magmatic system can be calculated. These calculations require that the effective constants  $D_m^s$  approximates the equilibrium constant  $K_m^s$ .

The free energy for the mixture of phases of any composition (melt plus crystals) in a given initial state can be stated as:

$$G = \sum_{k=1}^K n_k^l \mu_k^l + \sum_{s=1}^S \sum_{m=1}^{M_s} n_m^s \mu_m^s. \quad (6)$$

In order to calculate the equilibrium state of the melt–crystal system, it is necessary to define the minimum  $G$  as a function of the molar quantity of the endmember minerals  $n_m^s$  and the chemical potentials  $\mu_m^s$ . To calculate equilibria, one should account for the mass balance constraints for each  $k$ -component

$$n_k = n_k^l + \sum_{s=1}^S \sum_{m=1}^{M_s} v_{km}^s n_m^s \quad (7)$$

and combining the Gibbs–Duhem relations with (4) and (7) obtain:

$$\partial G / \partial n_m^s = RT \ln[K_m^s(T)/K_m^s(T_m^s)] \quad (8)$$

where  $T$  is the real equilibrium temperature and  $T_m^s$  is the fictive equilibrium temperature relevant to a given endmember  $m$  in the phase  $s$  coexisting with the melt in the arbitrarily selected initial state. As was shown by Frenkel and Ariskin (1984), for a given set of empirical mineral–melt equilibria equations (e.g. Table 1), the expression (8) is equivalent to

$$\partial G / \partial n_m^s = R A_m^s (T/T_m^s - 1) \quad (9)$$

where  $T_m^s$  is a predicted equilibrium temperature (if phase  $s$  is presented in the liquidus assemblage) that can be derived from (5)

$$T_m^s = (A_m^s + \beta_m^s P)/(B_m^s - \ln D_m^s). \quad (10)$$

Values of  $A_m^s$  for silicate mineral–melt reactions are known to be more than 0 (the value of  $\beta_m^s$  is too small to change the sign). Therefore to minimize  $G$  from expression (9), it is necessary to increase the solid components in the system of the phase with the minimum predicted temperature (if  $n_m^s > 0$ ), and to decrease the proportion of the phase with the maximum predicted temperature (10).

A variety of computer algorithms to solve the phase equilibria of magmas at a given temperature or a fixed crystallinity can be constructed around Equation (9). For example the melting/crystallization model that is the core of the COMAGMAT program (Fig. 1), is dependent on the numerical procedure of adding/subtracting endmember minerals to the liquid phase in a free energy minimization algorithm. The MELTING/CRYSTALLIZATION procedure was

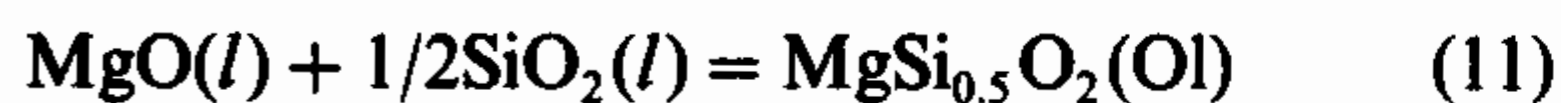


utilized in the program to calculate mineral–melt equilibria at a given bulk percent crystallized. In this program, the equilibrium temperature is unknown initially but may be derived as a result of the free energy minimization at a constant total crystallinity. This is the main difference between this approach and other magma crystallization models.

#### Equilibrium of melt–crystal mixtures with variable mineral compositions

In practice, the main  $G$ -minimization conditions (9)–(10) are not sufficient to equilibrate any phase assemblage. Rock-forming minerals are solid solutions, so that every increment of crystallization or dissolution of a constant composition phase would result in a new nonequilibrium state with regard to the partitioning of major and trace elements between minerals and coexisting melt. To address this problem we need an additional procedure that would reequilibrate the phase compositions after changes in their molar quantities.

In one of the simplest situations, Ol–melt equilibria can be described by the pair of reactions:



with the effective equilibrium constants (5) at atmospheric pressure

$$D_{\text{Fo}}^{\text{Ol}} = x_{\text{Fo}}^{\text{Ol}}/x_{\text{MgO}}^l(x_{\text{SiO}_2}^l)^{1/2} = \exp(A_{\text{Fo}}^{\text{Ol}}/T + B_{\text{Fo}}^{\text{Ol}}) \quad (13)$$

$$D_{\text{Fa}}^{\text{Ol}} = x_{\text{Fa}}^{\text{Ol}}/x_{\text{FeO}}^l(x_{\text{SiO}_2}^l)^{1/2} = \exp(A_{\text{Fa}}^{\text{Ol}}/T + B_{\text{Fa}}^{\text{Ol}}). \quad (14)$$

If a given nonequilibrium state is represented by the mixture of olivine crystals  $n_{\text{Ol}}$  (moles) of an arbitrary composition  $x_{\text{Fo}}^{\text{Ol}}$  and

$$n_l = \sum_{k=1}^K n_k^l$$

moles of the liquid phase with the composition defined only from the mass balance constraints (7),

one can calculate olivine–melt equilibria by the exchange reaction:



Using this reaction, one can quantify variations in the total molar quantities of MgO and FeO in the liquid and solid phase needed to equilibrate the mixture at a given olivine quantity  $n_{\text{Ol}}$ :

$$D_{\text{Fo}}^{\text{Ol}}(T) = (x_{\text{Fo}}^{\text{Ol}} - \Delta n_{\text{MgO}}^l/2n_{\text{Ol}})^{n_{\text{Ol}}} / (n_{\text{MgO}}^l + \Delta n_{\text{MgO}}^l)(x_{\text{SiO}_2}^l)^{1/2}. \quad (16)$$

Note, that to determine  $\Delta n_{\text{MgO}}^l$  from (16), the value of  $D_{\text{Fo}}^{\text{Ol}}(T)$  at the predicted temperature  $T$  must be known.

The equilibrium temperature and composition for olivine and coexisting melt at a given proportion of olivine crystals in the partly molten system, may be calculated in the following steps:

- (1) Assume an initial Ol composition  $x_{\text{Fo}}^{\text{Ol}(j)}$ , where  $j$  is the interaction constant, then on the basis of the mass balance constraints (7) calculate the initial liquid composition  $n_k^{(j)}$  for each component ( $k$ ).
- (2) Calculate the solid phase saturation temperature  $T_s^j$  from the initial liquid composition [using Eqs. (5), (10), (13), and (14)].
- (3) Solve Equation (16) for  $\Delta n_{\text{MgO}}^{(j)}$  and calculate a new liquid composition (keeping in mind  $\Delta n_{\text{FeO}}^{(j)} = -\Delta n_{\text{MgO}}^{(j)}$ ,  $n_{\text{MgO}}^{(j+1)} = n_{\text{MgO}}^{(j)} + \Delta n_{\text{MgO}}^{(j)}$ ,  $n_{\text{FeO}}^{(j+1)} = n_{\text{FeO}}^{(j)} + \Delta n_{\text{FeO}}^{(j)}$  and a new Ol composition  $x_{\text{Fo}}^{\text{Ol}(j+1)} = x_{\text{Fo}}^{\text{Ol}(j)} - \Delta n_{\text{MgO}}^{(j)}/2n_{\text{Ol}}$ ).
- (4) Calculate differences between the current and previous MgO and FeO contents in the melt. If the corrections are less than a given iteration limit  $\epsilon_j$ , go to step (6).
- (5) Repeat the calculations starting with steps (2).
- (6) Store or output the obtained values of  $T_{\text{Ol}}$  and phase compositions.

Table 1. Low-pressure mineral–melt geothermometer parameters used in COMAGMAT model ( $\ln D = A/T + B + d \ln X^{\text{liq}}$ )

Mineral	Calculated $D$	$A$	$B$	$d$	Ref.
Olivine ( $n = 71$ )	$x_{\text{Fo}}^{\text{Ol}}/x_{\text{MgO}}^l(x_{\text{SiO}_2}^l)^{1/2}$	5543	−2.32	0.210	Ariskin, Barmina, and Frenkel (1987)
	$x_{\text{Fa}}^{\text{Ol}}/x_{\text{FeO}}^l(x_{\text{SiO}_2}^l)^{1/2}$	6457	−4.22	0.084	
Augite ( $n = 25$ )	$x_{\text{En}}^{\text{Aug}}/x_{\text{MgO}}^l x_{\text{SiO}_2}^l$	8521	−5.16	—	<i>ibid.</i>
	$x_{\text{Fs}}^{\text{Aug}}/x_{\text{FeO}}^l x_{\text{SiO}_2}^l$	13,535	−9.87	—	
	$x_{\text{Wo}}^{\text{Aug}}/x_{\text{CaO}}^l x_{\text{SiO}_2}^l$	2408	−1.24	—	
	$x_{\text{AlO}_{1.5}}^{\text{Aug}}/x_{\text{AlO}_{1.5}}^l$	—	0.20	—	
Pigeonite ( $n = 18$ )	$x_{\text{En}}^{\text{Pig}}/x_{\text{MgO}}^l x_{\text{SiO}_2}^l$	8502	−4.74	—	<i>ibid.</i>
	$x_{\text{Fs}}^{\text{Pig}}/x_{\text{FeO}}^l x_{\text{SiO}_2}^l$	5865	−4.04	—	
	$x_{\text{Wo}}^{\text{Pig}}/x_{\text{CaO}}^l x_{\text{SiO}_2}^l$	4371	−4.02	—	
	$x_{\text{AlO}_{1.5}}^{\text{Pig}}/x_{\text{AlO}_{1.5}}^l$	—	0.10	—	
Plagioclase ( $n = 58$ )	$x_{\text{An}}^{\text{Pl}}/x_{\text{CaO}}^l(x_{\text{AlO}_{1.5}}^l)^2(x_{\text{SiO}_2}^l)^2$	10,641	−1.32	0.369	Ariskin and Barmina (1990)
	$x_{\text{Ab}}^{\text{Pl}}/x_{\text{NaAlO}_2}^l(x_{\text{SiO}_2}^l)^3$	11,683	−6.16	−0.119	

$X^{\text{liq}}$  is the molar ratio: Al/Si for Ol and (Na + K)Al/Si<sup>2</sup> for Pl.

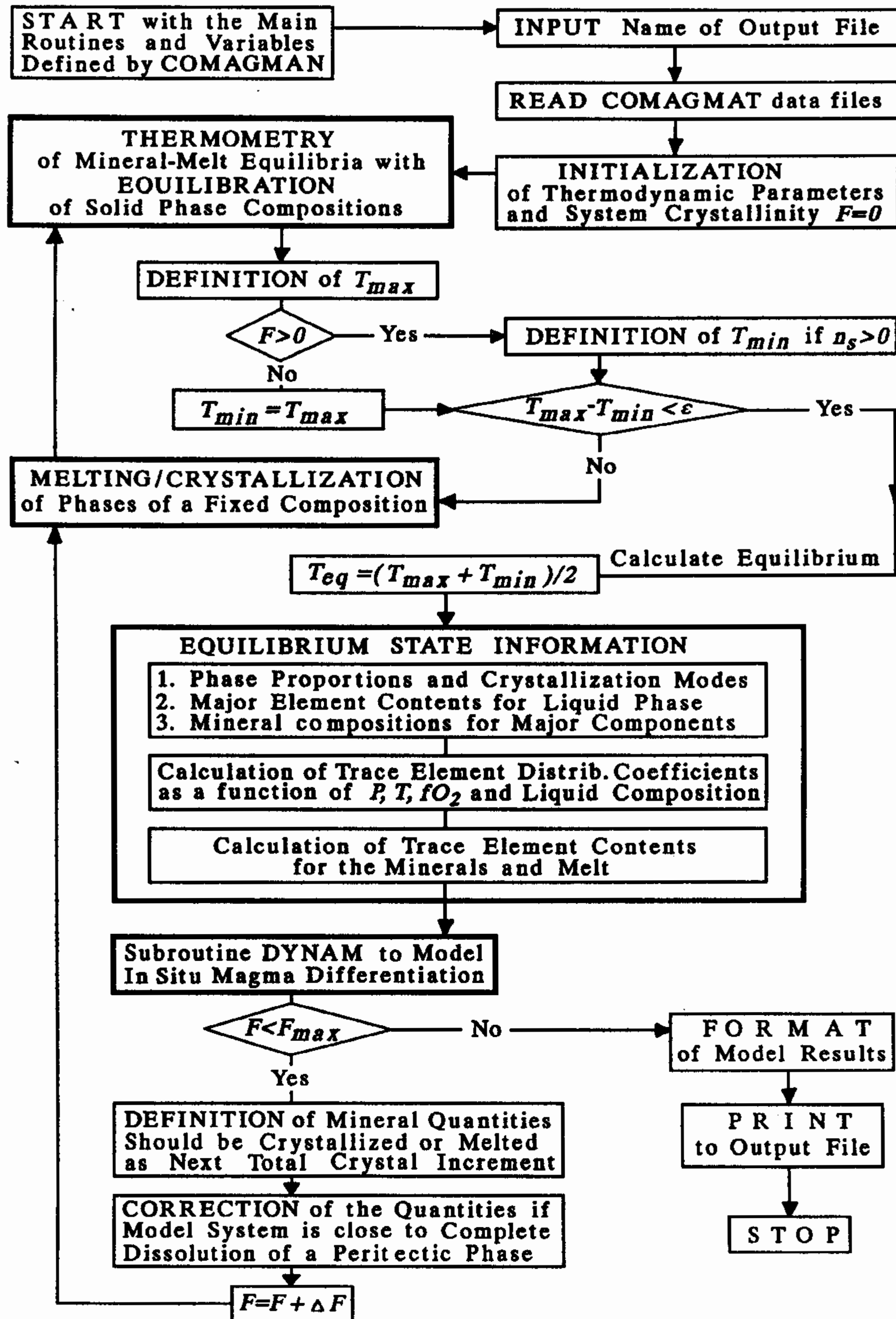


Figure 1. General flowchart of COMAGMAT. Model presented includes DYNAM subroutine to simulate the dynamics of in situ differentiation (Frenkel and others, 1989).

This algorithm may be applied to other mineral phases, and is particularly simple for analysis of systems saturated with respect to only one liquidus phase (e.g. Pl or Ol cumulates or the mantle at extremely high extents of melting). One can track the evolution of the liquid and mineral compositions as a consequence of equilibrium melting/crystallization if the technique is applied for sequentially decreasing or increasing contents of the phase of interest in the system.

Integration of the thermometry, equilibration, and melting/crystallization constraints allowed us to develop an algorithm for simulating the crystallization of natural cotectic assemblages (Ariskin and coworkers, 1987, 1988, 1990). A flowchart of the COMAGMAT program is shown in Figure 1. The main

iteration loops interact to simulate the equilibrium crystallization of melts coexisting with different mineral assemblages. Crystallization is modeled step by step as the total mode of crystals is increased. This circulation is paired with the recalculation of the mineral-melt equilibria at each step.

#### *Mineral-melt geothermometers*

The basic building blocks of the COMAGMAT model are a system of empirically calibrated equations that describe mineral-melt equilibria for Olivine, Plagioclase, Augite, Pigeonite, Orthopyroxene (Table 1) as well as for Ilmenite and Magnetite (17–21). These geothermometers have been calibrated using a database consisting of the results of published melting experiments conducted at 1 atm. Mineral



component activities were assumed to be equal to the mole fractions of the cations in a single site (ideal solution). Assumption of this simple model is that the effects of nonideality on mineral–melt equilibria are attributed primarily to the liquid phase.

When applied to trace-element partitioning, a two-lattice model for melt component activities effectively reduces the effects of the compositional dependence of mineral–melt distribution functions (Nielsen, 1985). A similar model was used as the basis for a number of mafic mineral–melt geothermometers included in the first COMAGMAT version (Ariskin, Barmina, and Frenkel, 1987). These expressions however, are applicable to a narrow range of melt composition. In an attempt to develop more accurate mineral–melt expressions covering a wider range of composition, we have determined that the addition of melt structural–chemical parameters such as Si/O, Al/Si, etc. to temperature  $T$  as independent variables in Equation (5) permits significantly improves the fit to the experimental data (see parameters for Ol and Pl geothermometers in Table 1).

It should be noted that the plagioclase–melt geothermometers from Table 1 have been derived using a minor but important modification of Nielsen's two lattice model (Ariskin and Barmina, 1990). In addition, a simple oxide model was used for the system of expressions describing appearance of titanium magnetite ( $\text{Fe}_3\text{O}_4/\text{Fe}_2\text{TiO}_4$ ) on the ferrobasalt melt liquidus (Ariskin and others, 1988):

$$(x_{\text{TiO}_2}/x_{\text{FeO}_{1.5}})^{\text{Mt}} = (x_{\text{TiO}_2}/x_{\text{FeO}_{1.5}})' \times \exp(19798/T - 14.76) \quad (17)$$

$$x_{\text{Fe}_3\text{O}_4}^{\text{Mt}} = 1/[2(x_{\text{TiO}_2}/x_{\text{FeO}_{1.5}})^{\text{Mt}} + 1] \quad (18)$$

$$x_{\text{Fe}_3\text{O}_4}^{\text{Mt}}/x_{\text{FeO}}^{\text{Mt}}(x_{\text{FeO}_{1.5}}^{\text{Mt}})^2 = \exp(34884/T - 14.97) \quad (19)$$

where total Fe was separated into ferric and ferrous forms by the relation given by Sack and others (1980). To simulate ilmenite ( $\text{Fe}_2\text{O}_3/\text{FeTiO}_3$ ) saturation conditions we used the two-lattice model equation of Nielsen and Dungan (1983):

$$x_{\text{FeTiO}_3}^{\text{Ilm}}/x_{\text{FeO}}^{\text{Ilm}}x_{\text{TiO}_2}^{\text{Ilm}} = \exp(8950/T - 3.30) \quad (20)$$

in combination with the empirical relations between magnetite and ilmenite compositions (Frenkel and others, 1989):

$$(x_{\text{Fe}_2\text{O}_3}/x_{\text{FeTiO}_3})^{\text{Ilm}} = (x_{\text{Fe}_3\text{O}_4}/x_{\text{Fe}_2\text{TiO}_4})^{\text{Mt}} \times \exp(-7732/T + 4.25). \quad (21)$$

Applying the geothermometers given in Table 1, one can invert the calculations by calculating mineral–melt equilibria temperatures for the initial database liquid compositions. Comparison of the calculated and experimental temperatures indicate an accuracy of  $\pm 10^\circ\text{C}$  ( $1\sigma$ ). A similar comparison of calculated and experimental mineral compositions indicate that Fo, An, En, and Wo contents can be predicted within 1–3 mol%. Application of the mineral–melt expressions derived for the COMAGMAT

model are limited primarily to tholeiitic and transitional systems, from magnesium basalts to dacite (45–60%  $\text{SiO}_2$ ,  $\text{Na}_2\text{O} + \text{K}_2\text{O} < 4\text{--}5\%$ ).

In a study of the accuracy of mineral–melt calculations, Weaver and Langmuir (1990) emphasized the effects of microprobe analytical uncertainties and interlaboratory differences on discrepancies in calculated temperatures. They reported that both the experimental techniques and the microprobe analytical procedures that usually are applied can each result in as much as a  $10\text{--}20^\circ\text{C}$  bias. However, the biases resulting from each of these techniques are independent of one another. Our analysis is in agreement with this conclusion. To evaluate the specific COMAGMAT geothermometers we calculated the temperatures of appearance of Ol, Pl, Aug, and Pig for the melt compositions from a set of experimental data that were not used in the calibration of the geothermometers (Grove and Juster, 1989; Juster and Grove, 1989; Thy, 1991; Thy, Lofgren, and Imsland, 1991). The results (Fig. 2) shows a good correlation of the COMAGMAT modeled temperatures with the experimental temperatures. There is however a slight shift for more alkalic compositions. Given the possibility of systematic compositional dependencies in the calculated temperatures, a special FUNLIQ subroutine has been included in the COMAGMAT program so that one can correct model values by inserting an empirically derived (i.e. from an independent set of experiments) offset in the calculated temperatures.

#### *Simulation of high-pressure phase equilibria*

To develop a high-pressure version of the COMAGMAT program, the empirical approach of Ariskin, Frenkel, and Tsekhonya (1990) based on the experimental data of Bender, Hodges, and Bence (1978) was applied. They determined that the pressure dependence of the crystallization temperatures ( $\partial T/\partial P$ ) for Ol and Pl were similar, and that the main result of increasing pressure was the expansion of the crystallization range for Augite relative to those of the other minerals. Using the Bender, Hodges, and Bence (1978) data, and the low-pressure mineral–melt geothermometers (Table 1), we selected empirical values of  $\beta_m^s$  [see Eq. (5)]. Application of this pressure correction reproduced the input data within  $15\text{--}20^\circ\text{C}$  from 1 atm up to 10–12 kbar. The results that fit the data with the least error were obtained using the optimal parameters of  $\beta_{\text{Fo,Fs}}^{\text{Ol}} = 2.4$ ,  $\beta_{\text{En,Fs,Wo}}^{\text{Aug}} = 2.8$ ,  $\beta_{\text{An}}^{\text{Pl}} = 2.0$ , and  $\beta_{\text{Ab}}^{\text{Pl}} = 4.0 \text{ cm}^3/\text{mol}$  with  $\text{Al}_2\text{O}_3$  in augite increasing by 0.7 wt%/kbar.

#### *Trace-element partitioning*

With the exception of Cr, trace-element contents in basaltic melts are known to have little influence on the liquidus temperatures and composition of the major mineral phases. Therefore trace-element partitioning calculations can be separated from the phase equilibria calculations. This does not indicate that major- and trace-element systematics are not to be



linked, only that the major element phase equilibria can be calculated independently of trace-element contents. The traditional approach to the description of mineral–melt partitioning is the single component distribution coefficients

$$D_i^{s/l} = C_i^s / C_i^l.$$

This approach is the simplest way to describe the available experimental and natural partitioning data. However, it is known that most trace elements  $D$  values are dependent strongly on the temperature, pressure, and phase composition. As noted, these dependencies can be reduced significantly by using a simple melt component activity model. In addition, the use of simulated equilibrium constants similar to those used for the major-element components (2, 5), in the place of simple element ratio partition coefficients also produces significantly improved accuracy (Gallahan and Nielsen, 1992; Nielsen, Gallahan, and Newberger, 1992). Unfortunately such an approach requires a large experimental database. For most systems, these data do not exist at present. Until

those data become available, use of partitioning expressions that have been corrected empirically for compositional dependence, temperature and pressure provides us with a more accurate method of describing trace-element behavior (Nielsen, 1992).

One of the major advantages of the approach used in COMAGMAT is the linkage between the major- and trace-element systematics. Calculation of the major-element mineral–melt equilibria controlled parameters, such as temperature and fractionating or melting mineral proportions, allows us to constrain the trace-element systematics. Stated simply the trace-element concentrations in the liquid and solid phases can be calculated as

$$C_i^l = C_i^0 n_o^{wt} / \left( n_i^{wt} + \sum_{s=1}^S D_i^{s/l} n_s^{wt} \right), \quad C_i^s = C_i^l D_i^{s/l} \quad (22)$$

where  $C_i^0$  is the initial bulk content of  $i$  element in the molten system,  $n_o^{wt}$  mass of the system,  $n_i^{wt}$  and  $n_s^{wt}$  are current masses of the melt and solid phases, with all masses calculated as part of the program. At present, the COMAGMAT software provides the option of

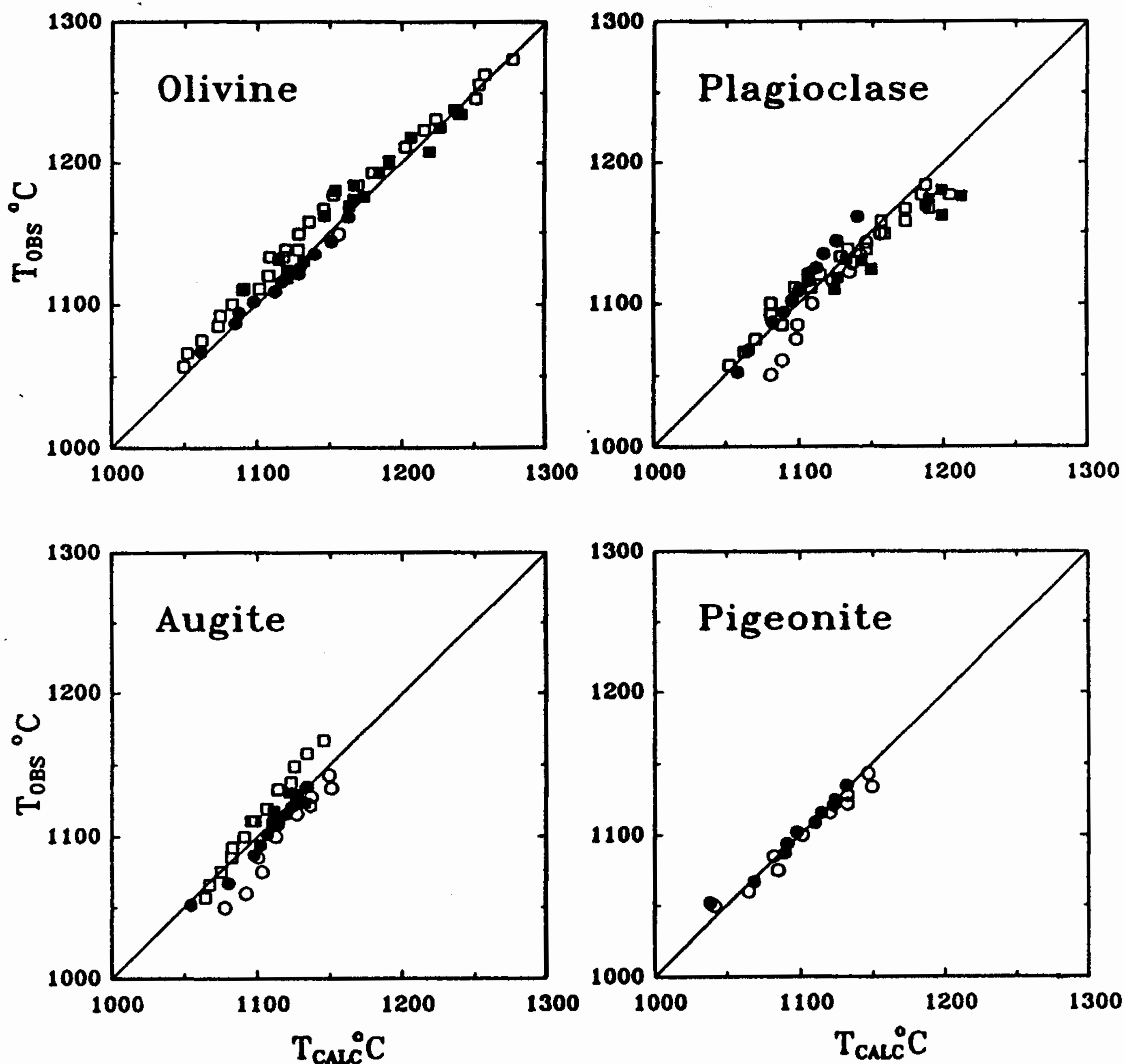


Figure 2. Comparison of mineral saturation temperatures observed in experiments with those calculated using mineral–melt geothermometers of COMAGMAT for same liquid compositions. (●) Grove and Juster (1989); (○) Juster and Grove (1989); (■) Thy (1991); (□) Thy, Lofgren, and Imsland (1991).



simulating the evolution of trace-element trends for the two following groups:

- (1) Mn, Ni, Co, Cr, Sc, V, Sr, Ba, Rb, Cu;
- (2) La, Ce, Nd, Sm, Eu, Gd, Dy, Er, Yb, Lu.

For elements and systems where the temperature or compositional dependencies are unknown, fixed values of the mineral–melt distribution coefficients are given in the “dicoef.dat” file (see Appendix). This usually is where there is insufficient data to calculate the dependencies. If the dependencies can be quantified, the partitioning behavior is calculated with the DISCO subroutine as a function of known intensive parameters. All values and dependencies of the partitioning behavior are calibrated from a set of experimental data summarized in Frenkel and others (1989) and Barmina, Ariskin, and Kolesov (1989b). To simulate the evolution of REE patterns in magmatic process we developed a system of equations based on regression of more than 200 values of silicate mineral–melt distribution coefficients. These expressions are given in terms of temperature, pressure, oxygen fugacity, and liquid composition (Table 2). A general equation to calculate REE partitioning is

$$\ln D_{\text{REE}}^{s/l} = a_0 + \{[a_1 + a_2(P - 1)]/T\} + a_3 \ln C_{\text{SiO}_2}^l + a_4 \ln N_{\text{REE}} \quad (23)$$

where  $P$  is pressure in bar,  $C_{\text{SiO}_2}^l$  is in wt% and  $N_{\text{REE}}$  is an ordinal number of the specific REE in the set from La to Lu ( $1 < N < 15$ ). Using the regression parameters from Table 2 (Barmina, Ariskin, and Kolesov, 1992) and REE distribution coefficients for ilmenite and magnetite (Nielsen, Gallahan, and Newberger, 1992) one can calculate the evolutionary trends of these elements in the liquid and solid phases for the complete set of rare earth elements.

#### *Simulation of equilibrium crystallization in basaltic magmas*

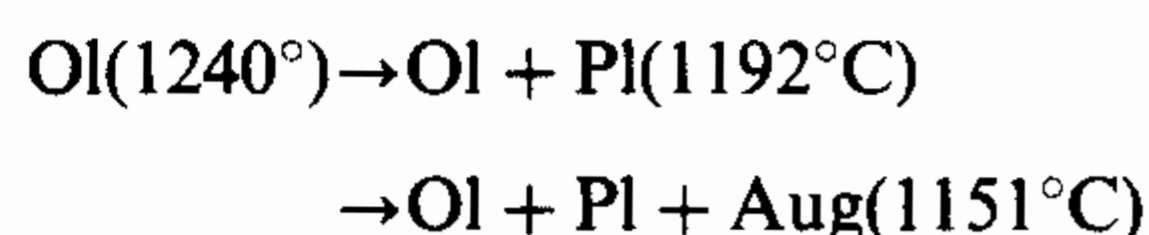
The algorithm discussed here is designed to simulate crystallization and liquid lines of descent for natural systems. Modeled major elements include Si–Ti–Al–Fe–Mg–Ca–Na–K and P. The program also simulates both open (12 oxygen buffers), and closed system differentiation with respect to oxygen at pressures up to 12 kbar. A FORTRAN-77 computer program applying the algorithm to the simulation of crystallization is available from the authors on disc. The modeling process may be calculated for systems ranging from basalt to dacite melts with a crystallization increment of 1–2 mol% of the initial system size up to a limit of 80–90% bulk percent crystallization.

As documented in the flowchart (Fig. 1), the initial conditions and simulation subroutines for the COMAGMAT program are contained in a series of setup files. These 8 data files include the desired model parameters (see “mainmenu.dat” in Appendix), initial major- and trace-element contents (“com-

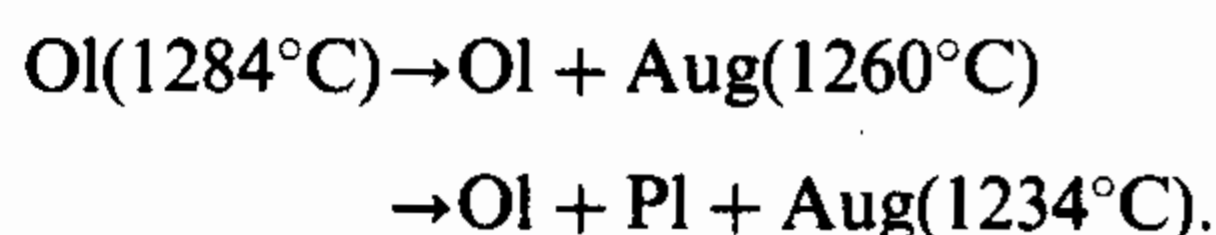
maj.dat” and “contra.dat”), distribution coefficients for trace elements (“dicoef.dat”), parameters of the mineral–melt geothermometers (“miners.dat”), equations describing 12 oxygen buffers (“oxybuf.dat”), the regression coefficients to correct calculated temperatures (“correc.dat”) as well as some dynamics parameters for modeling in situ differentiation (“intrus.dat”, see next section). The program COMAGMAN, which writes information into these setup files, is coded in C, for an IBM PC or compatible with DOS 3.0 or higher (Ariskin and others, 1992). The user interface is a menu-driven manager, with on-line help, built-in editor, and a procedure for opening data files for viewing or editing. After the input conditions are set, COMAGMAN allows the user to run the COMAGMAT program.

One can track each step of the calculations (corresponding to a given crystal increment) directly on the screen while the calculations are accumulating on file. After the calculations are complete, the formation will be written to an output file as a sequence of four tables containing phase proportions and compositions as a function of the total crystallinity, plus the equilibrium temperature defined for each step. COMAGMAT 3.0 software is linked to the graphics program PAINT for viewing the model results through a fixed set of preconfigured plots (Ariskin and others, 1992).

To illustrate the operation of the COMAGMAT program we present a comparison of calculated liquid lines of descent with those determined experimentally (Fig. 3). For this purpose we have selected the experiments of Thy (1991), conducted on the mildly alkalic lava SU106 at both low- and high-pressure conditions. The results of the calculations are, in general, close to the experimental results. The largest discrepancy is in the calculated Pl–melt temperatures, which were approximately 20°C high compared to the experimental temperatures. On the basis of this difference we can shift the temperature correction parameter for Pl and calculate a new equilibrium crystallization simulation for the SU106 melt at 1 atm and 10 kbar and the QFM buffer. The model results at 1 atm reproduce the experimentally determined sequence crystallization:



with liquid lines of descent close to those obtained by experiment (Fig. 3). The data from the 10 kbar simulation reproduce the expansion of the Aug stability field determined in the experiments



However, the calculated clinopyroxene-in temperature is about 40°C higher than in the experiments. The discrepancy seems to be the result partly of analytical limitations (Thy, 1991), but in any

Table 2. Regression constants for expressions describing REE distribution coefficients (Barmina, Ariskin, and Kolesov, 1992)

Mineral	Group	Initial information			Regression constants for Equation (23)					
		<i>P</i> (kbar)	<i>T</i> (°C)	Elements	<i>a</i> <sub>0</sub>	<i>a</i> <sub>1</sub>	<i>a</i> <sub>2</sub>	<i>a</i> <sub>3</sub>	<i>a</i> <sub>4</sub>	$\sigma(n)$
Olivine	LREE	0.001	1150–1414	Sm, Gd	–51.20 (15.63)	17,054 (5677)	—	8.24 (3.19)	1.08 (0.68)	0.41(22)
	HREE			Gd, Yb, Lu	–37.01 (5.50)	12,473 (1934)	—	4.07 (1.19)	3.54 (0.18)	0.26(38)
Augite	LREE	7.5–30	1050–1380	La, Ce, Nd, Sm, Gd	1.70 (4.70)	5432 (3778)	0.04 (0.04)	–1.79 (0.93)	0.34 (0.11)	0.25(16)
	HREE	7.5–20	1050–1300	Gd, Dy, Ho, Er, Yb, Lu	–9.12 (2.82)	–800 (1611)	0.15 (0.14)	2.52 (0.89)	–0.31 (0.19)	0.16(27)
Orthopyroxene	LREE	0.001	1169–1414	Ce, Sm, Gd	–19.63 (2.90)	21,891 (4309)	—	—	0.67 (0.31)	0.38(9)
	HREE			Gd, Yb	–24.29 (1.31)	22,995 (1969)	—	—	2.62 (0.30)	0.22(13)
Plagioclase	LREE	0.001	1150–1343	La, Ce, Nd, Sm, Gd	–1.63 (2.48)	4575 (1361)	—	–0.78 (0.78)	–0.49 (0.03)	0.18(65)
	HREE			Dy, Er, Lu	–11.37 (5.24)	–6951 (3088)	—	3.50 (1.71)	–0.56 (0.24)	0.22(35)

LREE and HREE are light and heavy rare earth elements (Gd is the dividing point). Standard deviation for each constant is given in parentheses below.  $\sigma(n)$  is the standard deviation for  $\ln D$  where  $n$  = number of points.



situation the COMAGMAT model pressure parameters may be corrected in the "miners.dat" file to fit the experimental data.

#### DYNAMIC BACKGROUND

The flowchart shown in Figure 1 includes the "DYNAM" subroutine, designed to model the dynamics of in situ crystallization. This routine was placed in this sequence so that after the phase equilibria had been determined for a given crystallinity, the modeled magma composition can be modified by addition or subtraction of the calculated equilibrium minerals and melt from the magma system. This enables the user to simulate a variety of igneous differentiation processes by changing the phase proportions and compositions during the evolution of the system. This approach is similar to that used for the simulation of fractional crystallization by several other investigators (Nielsen and Dungan,

1983; Ghiorso and Carmichael, 1985; Weaver and Langmuir, 1990). This technique also is useful for the construction of more sophisticated petrological models, such as those that simulate magma chamber recharge, assimilation, and eruption processes (Nielsen, 1985, 1990; Ghiorso and Carmichael, 1985). A common characteristic of most of these computer programs is that dynamics are calculated independently of space-time relationships or thermal constraints related to the actual physical mechanisms. Thus, these dynamics models could be referred as the "mass balance" based models.

In contrast, the "DYNAM" subroutine of COMAGMAT programs simulate a number of physical processes taking place simultaneously during in situ magma differentiation. These processes include loss of the heat of crystallization through the upper and lower margins of a tabular magma chamber, movement of solidification fronts into the magma body, crystal settling, together with the formation of

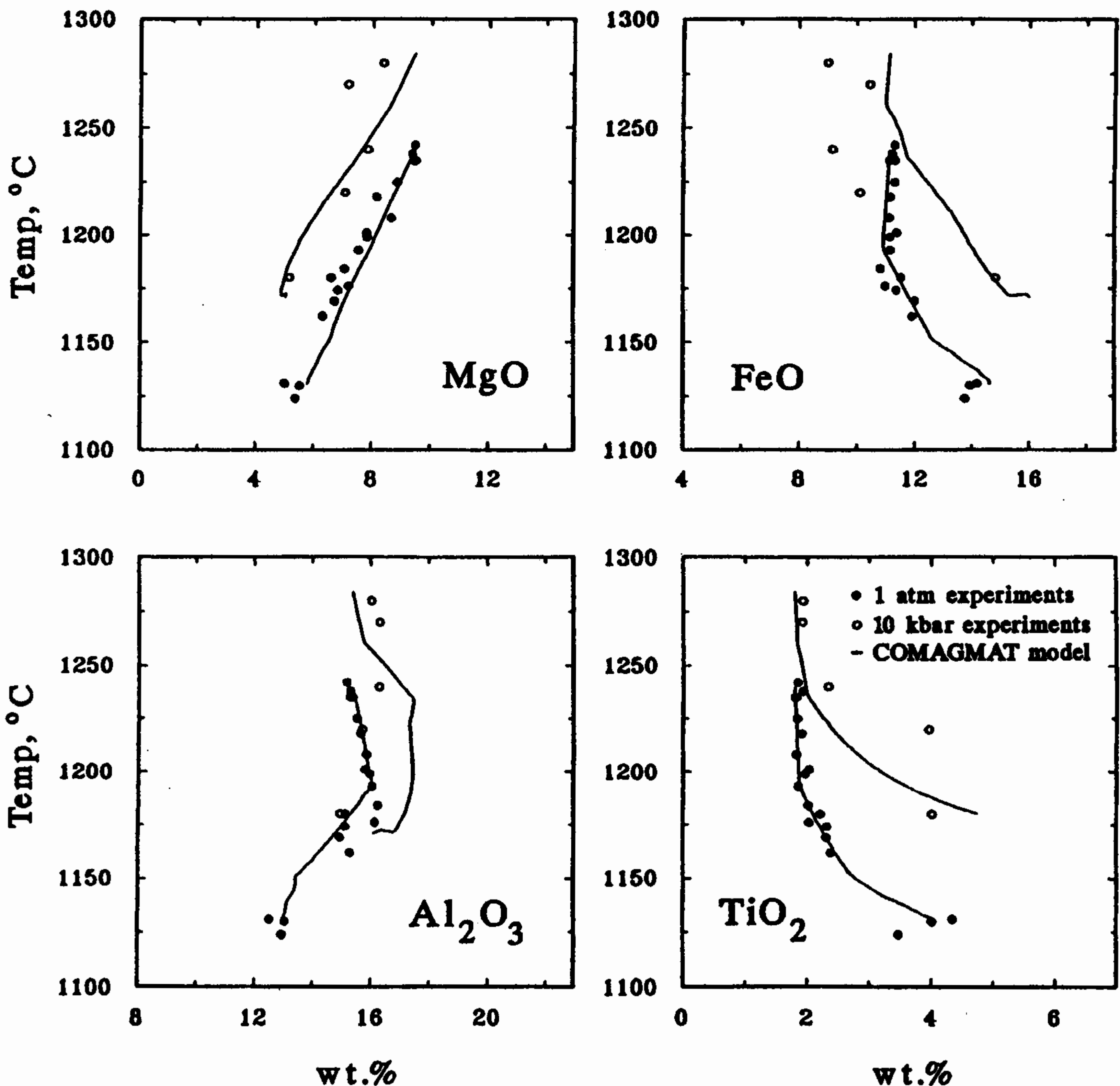


Figure 3. Comparison of temperature dependence of experimentally determined melt compositions (circles) with liquid lines of descent calculated using COMAGMAT program (curves). Experimental data are of Thy (1991). Calculations were conducted for melt of sample SU106 at QFM and total pressure of 1 atm and 10 kbar.



crystal-bonded (cumulus) and crystal-nonbonded (porphyric) aggregates, and the evolution of the primary mineral and trapped liquid compositions. The basic framework for this model and its full mathematical description are given in Frenkel and others (1989). In the example presented here, we will demonstrate how the equations that dictate the role of the dynamic processes in the "DYNAM" routine interact with the crystallization model discussed.

### THE CONVECTIVE-CUMULATIVE MODEL OF IN SITU DIFFERENTIATION

The main problem in simulating mineral-melt equilibria combined with heat-mass transfer in a magma chamber is to define the relationship between the increment of crystallization and the time needed to cool and crystallize the melt to a specific crystallinity. The development of an algorithm that will accurately model this link depends on the constraints selected for the assumed responsible physical mechanism. The convective-cumulative model described here for in situ differentiation was designed for the purpose simulating the formation process of the Siberian differentiated sills (Frenkel and others, 1989). This model is constrained by about 20 years of field work, petrography, geochemistry, and computer simulation. Perhaps the most important assumption that follows from this work is that the high efficiency of convection in 100–1000 m thick magma bodies makes them nearly uniform in temperature and composition up to the point where the magma chambers becomes filled with cumulates. This will result in fractionation of the magma, but not perfect fractional crystallization because of the effects of the presence of suspended crystals. Those solid phases are assumed to form near the upper boundary of chamber, then drop through the convecting magma body into a series of cumulates at the base of the magma body.

Note that convection is assumed not to prevent eventual settling of the suspended crystals. The dynamics of movement that are a consequence of the convective-cumulative model are illustrated schematically in Figure 4.

Frenkel and others (1989) proposed a number of semiempirical (as a result of previous works on simulating magma differentiation) constraints that approximate the convective-cumulative process with the aim of linking the dynamic equations with the basalt crystallization algorithm.

(1) Heat flux though by upper ( $U$ ) and lower ( $L$ ) boundaries of a convecting magma layer may be approximated by:

$$J_Q^U = \alpha_U / \sqrt{t}, \quad J_Q^L = \alpha_L / \sqrt{t} \quad (24)$$

where  $t$  is time, and  $\alpha_U$  and  $\alpha_L$  are empirical parameters are based on the heat capacity, density, and heat conductivity of the surrounding rocks as well as the temperature at the chamber boundaries. These fluxes should be partitioned in accordance with the assumption that the total heat removed from the magma chamber consists of the heat of cooling and crystallization of the convecting layer because of formation of the settling crystals (con), and the heat of crystallization from minerals formed in situ (ins):

$$J_Q^{U,L} = J_{con}^{U,L} + J_{ins}^{U,L}.$$

Therefore, within the upper crystallization zone,

$$J_{con}^U = 0, \quad J_{ins}^U = \alpha_U / \sqrt{t} \quad \text{when } t \leq t^*,$$

$$J_{con}^U = \alpha_U (\sqrt{t} - \sqrt{t^*}) / t, \quad J_{ins}^U = \alpha_U \sqrt{t^*} / t$$

when  $t > t^*$ ,

and within the lower crystallization zone

$$J_{con}^L = 0, \quad J_{ins}^L = \alpha_L / \sqrt{t} \quad (25)$$

where  $t^*$  is the duration of the initial chilling regime of solidification. The partitioning of the heat budget

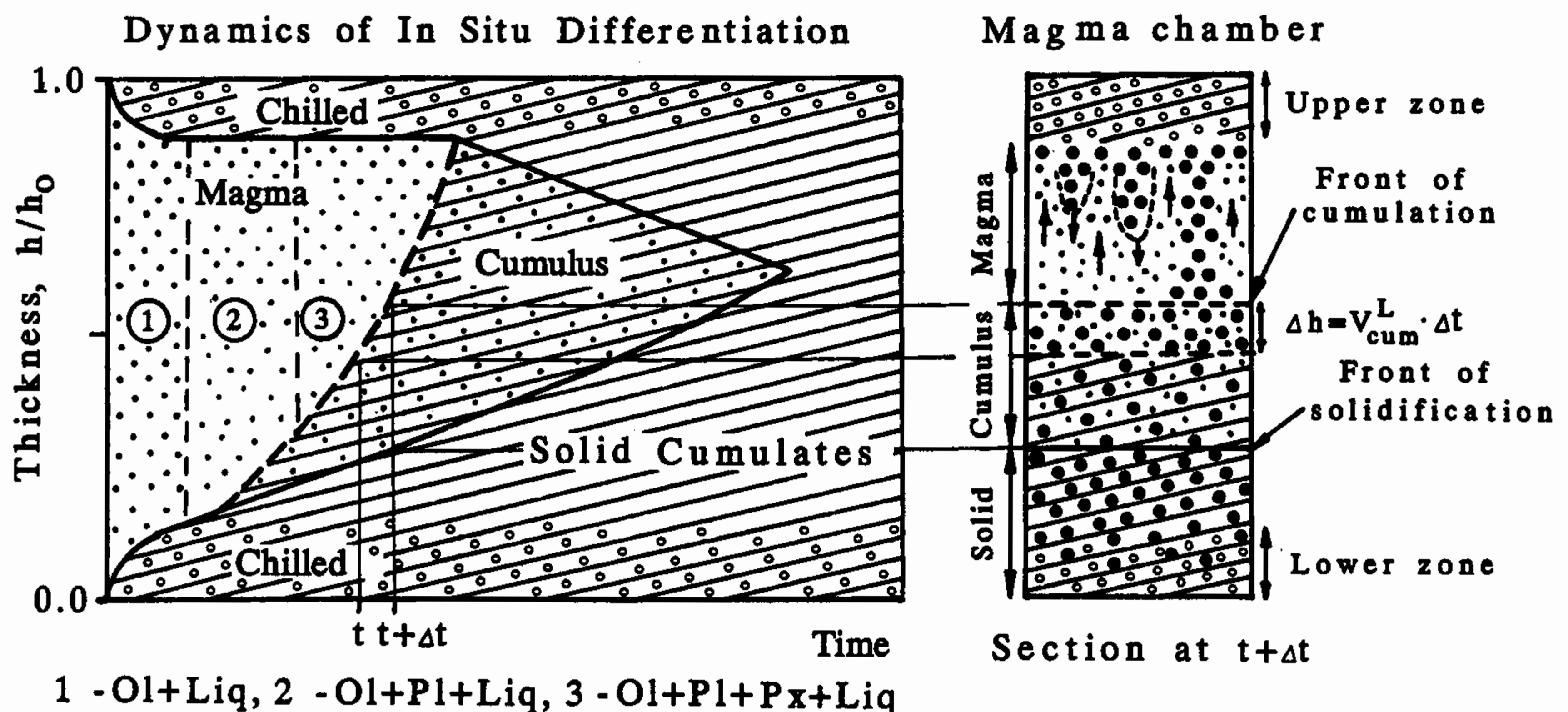


Figure 4. Dynamics of in situ magma differentiation assuming convective-cumulative model of Frenkel and others (1989). It is assumed that differentiation will stop after magma chamber is full of cumulates.



indicates that all crystals formed near the bottom layer and some of those formed near the upper crystallization zone are not involved in the main convection process.

(2) Using equation (25), one can calculate the fluxes of convective and in situ crystallized minerals generated at the upper and lower zones of crystallization as:

$$j_{\text{con}}^{U,L} = J_{\text{con}}^{U,L} / \lambda_{\text{mag}}, \quad j_{\text{ins}}^{U,L} = J_{\text{ins}}^{U,L} / \lambda_{\text{mag}} \quad (26)$$

where  $\lambda_{\text{mag}}$  is the heat of crystallization. The proportion of the crystals from the upper zone also can be defined from Equation (26).

(3) The flux of minerals generated in situ determines the rate of movement of the upper and lower boundaries of the convecting magma in the direction opposite to the heat fluxes:

$$V_{\text{ins}}^{U,L} = j_{\text{ins}}^{U,L} / (1 - F_{\text{cr}}^{U,L}) \quad (27)$$

where  $F_{\text{cr}}^U$  is a total crystal fraction for the convection magma, and  $F_{\text{cr}}^L$  is the crystallinity of a pile of mineral grains accumulated at the lower front as a result of crystal settling. For both situations

$$F_{\text{cr}}^U = \sum_{s=1}^S f_s^{\text{sus}}, \quad F_{\text{cr}}^L = \sum_{s=1}^S f_s^{\text{cum}} \quad (28)$$

where  $f_s^{\text{sus}}$  is the fraction of solids  $s$  suspended in the convecting magma (assumed to be in equilibrium), and  $f_s^{\text{cum}}$  is the fraction of the same phase, but within the lower zone cumulates (Frenkel and others, 1989):

$$f_s^{\text{cum}} = f_s^{\text{sus}} (1 - v_s / V_{\text{ins}}^L) \quad (29)$$

where  $v_s$  is the crystal settling velocity for each mineral (for settling phases,  $v_s$  and  $V_{\text{ins}}^L$  differ in sign).

(4)  $F_{\text{cr}}^U$  cannot be more than a maximum value,  $F_{\text{CR}}^L$ , the critical crystallinity. The approach of  $F_{\text{cr}}^U$  to  $F_{\text{CR}}^L$  signifies the appearance within the chamber of a layer composed of a crystal-bonded aggregate. At that point, the surface of the layer is torn away from the in situ crystallization front and becomes the boundary of the layer of the convecting magma layer (Fig. 4). In this situation, the vertical velocity of the lower accumulation front can be calculated from the expression (30) when  $F_{\text{cr}}^L = F_{\text{CR}}^L$

$$V_{\text{cum}}^L = \sum_{s=1}^S f_s^{\text{sus}} v_s / \left( F_{\text{CR}}^L - \sum_{s=1}^S f_s^{\text{sus}} \right) \quad (30)$$

In principle, when crystal flotation takes place, the cumulates may form at the upper boundary, but this example is not characteristic of trap intrusions.

(5) Given the constraints and assumptions, the model rock compositions can be calculated for  $k$  major or  $i$  trace elements taking into account the proportion and composition of the phases that constitute the chilled or accumulation units:

for the upper zone

$$C_{k,i}^U = f_{\text{mag}}^l C_{k,i}^l + \sum_{s=1}^S f_s^{\text{sus}} C_{k,i}^s \quad (31)$$

and for the lower zone

$$C_{k,i}^L = f_{\text{cum}}^l C_{k,i}^l + \sum_{s=1}^S f_s^{\text{cum}} C_{k,i}^s \quad (32)$$

where  $f_{\text{mag}}^l$  is the liquid fraction in the convection magma and  $f_{\text{cum}}^l$  is the fraction of the same liquid trapped in the model cumulates. The values of  $C_{k,i}^l$  and  $C_{k,i}^s$  represent, respectively, the liquid and solid phase compositions linked by the same mineral–melt equilibria.

#### Relationship between phase equilibria and dynamic parameters

The system of Equations (24)–(32) includes constraints on both thermodynamic ( $C_{k,i}^l$ ,  $C_{k,i}^s$ ,  $f_{\text{mag}}^l$ ,  $f_s^{\text{sus}}$ ) and dynamic ( $\alpha_{U,L}$ ,  $t^*$ ,  $v_s$ ,  $F_{\text{CR}}^L$ ,  $V_{\text{cum}}^L$ , etc.) parameters. Therefore, using these equations we can construct a model for in situ differentiation that combines the effects of both crystallization and crystal–melt dynamics on the calculated liquid lines of descent. The mechanics of this thermodynamic–dynamic integration (Fig. 1) is discussed in detail next.

Given the bulk composition and thickness  $H$  of a sheet magma body, the model begins by assuming the system is entirely liquid ( $F = 0$ ). Calculation of equilibrium crystallization proceeds up to the value  $F_{\text{int}}$ , the fraction of intratelluric phases. Beginning from  $F = F_{\text{int}}$ , the equilibrium state information is entered to the DYNAM subroutine with the initial time ( $t = 0$ ). The chilling duration ( $t^*$ ) defines the thickness of the upper and lower chilled zones:

$$\Delta h_{\text{ch}}^{U,L} = 2\alpha_{U,L} H / (1 - F_{\text{int}}) \lambda_{\text{mag}} \sqrt{t^*} \quad (33)$$

The formation of chilled zones along the margins results in a loss in the volume of the model magma system, both for the liquid and for the equilibrium solid phases. After correcting for that volume loss, the remaining melt further is crystallized incrementally (in terms of  $\Delta F$ ). The phase equilibria at a new % crystallinity then is calculated. Each forthcoming iteration through the DYNAM subroutine begins with the determination of the heat and crystal mass flux (25)–(26) as well as the time interval corresponded to the given  $\Delta F$ :

$$\Delta t = -\Delta F / j_{\text{con}}^U \quad (34)$$

From this information we can determine the phase compositions of the upper crystallization and lower accumulation zones (28)–(30) and calculate their thickness from the expression:

$$\Delta h_{U,L} = V_{\text{ins}}^{U,L} \Delta t.$$

Alternatively, if the accumulation front has been torn already from the crystallization front,

$$\Delta h_L = V_{\text{cum}}^L \Delta t. \quad (35)$$

If the thicknesses and bulk chemistry of the upper and lower zones are known, one can calculate the



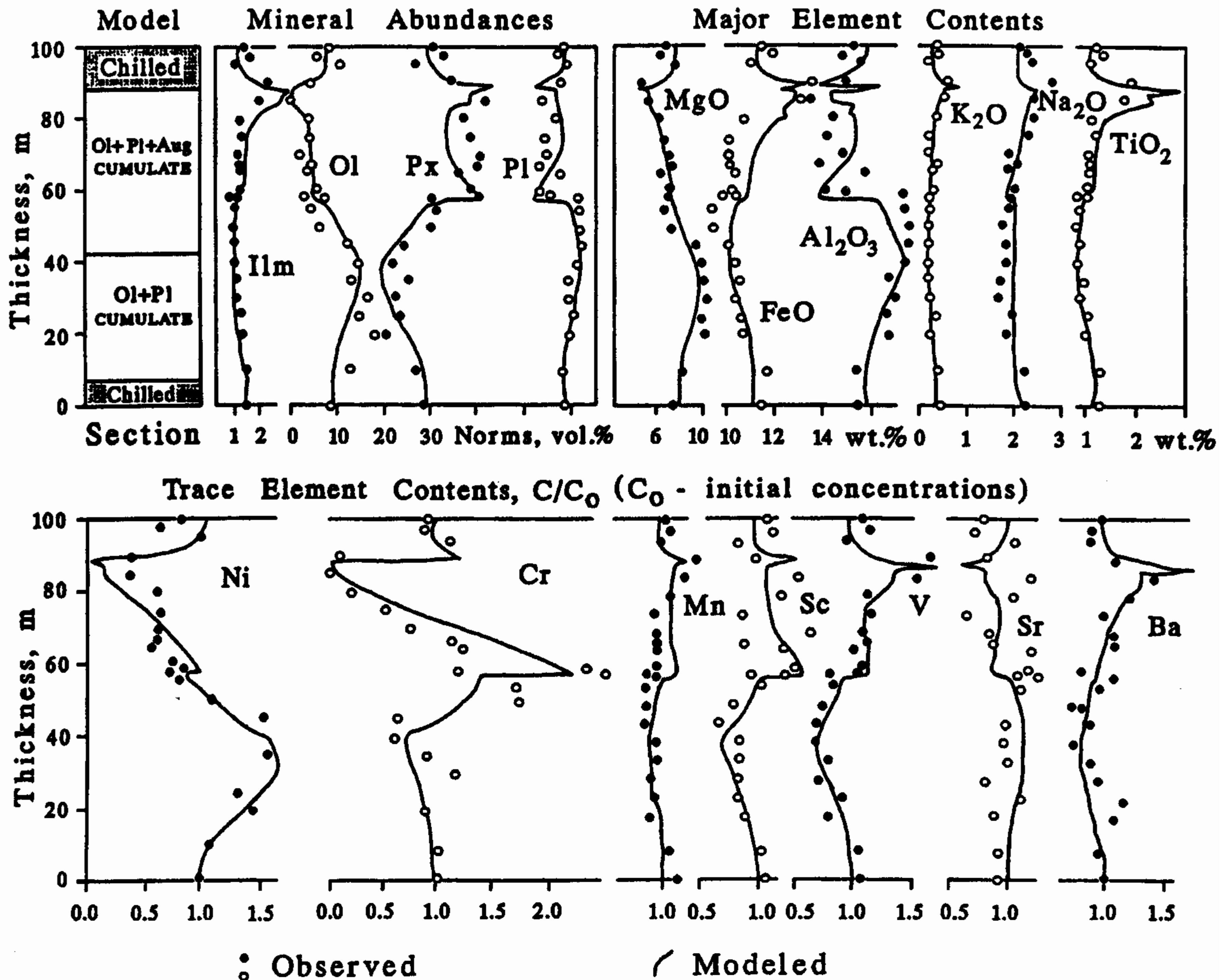


Figure 5. Comparison of observed data from Vavukan differentiated sill (eastern Siberia) with COMAGMAT simulation. Phase boundary predicted by model separating Ol + Pl from Ol + Pl + Aug cumulates (porphyritic rocks) corresponds to observed boundary between poikilophitic and taxitophitic rocks.

shift in the bulk model magma composition before the next increment of crystallization is calculated.

In summary, this algorithm makes it possible to simultaneously simulate crystallization, the thermal history of the magma body, the dynamics of crystal settling, and the movement of the crystallization or accumulation fronts within the magma chamber. The simulation is designed to end at the point where  $f'_{\text{mag}} = 1 - F_{\text{CR}}$ , when the total crystal fraction in magma is equal to the model cumulus critical crystallinity, and the point where the upper crystallization and lower accumulation fronts meet.

#### Forward modeling in situ differentiation

The simulation as discussed is a typical example of a forward model that involves a computer simulation that calculates the response of a modeled system to a set of assumed parameters, and then compares the calculated data with natural observations. Such a model may be used in an iterative way by modifying the parameters until a satisfactory fit is obtained.

The assumed parameters used in the COMAGMAT program are given in the file "intrus.dat" (see Appendix). Apart from a fixed thickness sheet body

(Hmod), the most important parameters include the fraction of intratelluric phases ( $F_{\text{in}}$ ), the duration of chilling (Sut), heat flux ratio ( $\alpha_L/\alpha_U$ ), and the critical crystallinity of model cumulates within the upper (Fcr1) and lower (Fcr2) zones. The final results of the simulation process are dependent most strongly on the crystal settling velocities. Those should be determined for each mineral and may be postulated as constant or assumed to be dependent on the extent of crystallization  $F$  (see abbreviation fi in "intrus.dat").

The INTRUSION subroutine of the COMAGMAT system has been applied to the major- and trace-element geochemistry of three differentiated sills from the Siberian Platform (Frenkel and others, 1989) to determine values of the dynamic parameters that will reproduce the geochemical features observed. Towards that end, a set of 40–50 calculations were made with differing parameter values. The result of the optimized model is presented in Figure 5. This simulation successfully reproduces the observed characteristics of the 100 m thick Vavukan intrusion (Frenkel and others, 1989). Given the large number of natural observations (particularly major- and trace-element analyses), and the relatively small number



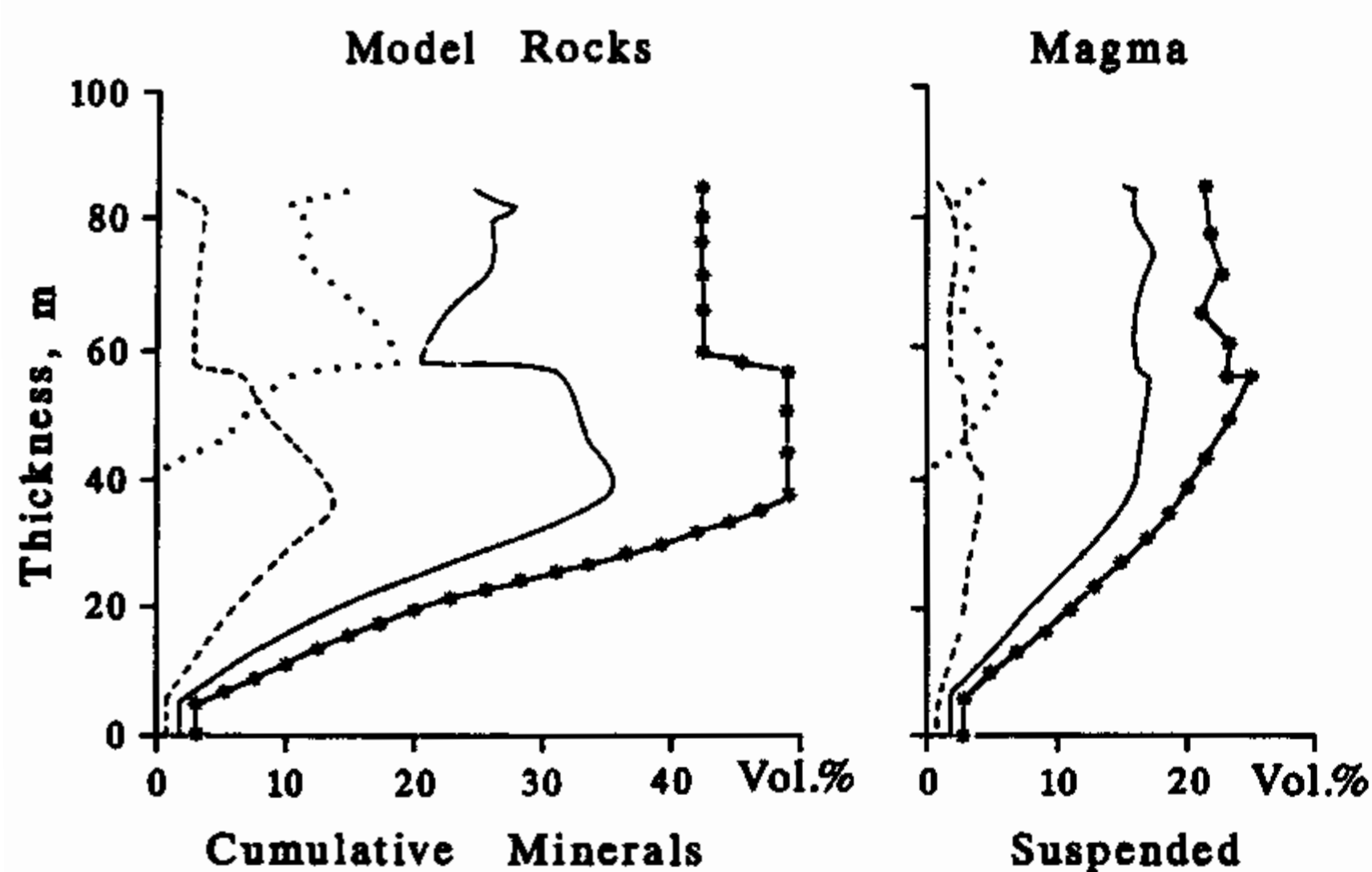


Figure 6. Model generated variations in percentage of cumulative and suspended minerals during evolution of Vavukan magma body (in both situations "Total" indicates bulk crystallinity). (\*—\*) Total; (—) Plag; (---) Oliv; (.....) Aug.

of variable parameters, the solution that explains all the data is not over-determined. The similarity of results to the natural suite suggest that the convective-cumulative model represents one possible physical mechanism that could be responsible for the generation of that observed suite.

If we define a set of optimal dynamic parameters, we can use that information to gain further insight into how crystallization will change other system parameters. This includes the path that temperature and phase chemistry will follow (Barmina and others, 1989) during solidification of the magma body, and changes in phase chemistry of the model cumulates and coexisting magma at every level in the body. The calculated mineral proportions in the cumulates and the suspended mineral percentage for the Vavukan intrusion rocks are shown in Figure 6. As interpreted from the model data, critical crystallinity of the primary cumulates did not exceed 50% whereas the total magma crystallinity did not exceed 20–25% during the differentiation process.

### CONCLUSIONS

Using a set of thermodynamic constraints we have developed an algorithm for the purpose of calculating phase equilibria of a wide range of magmatic systems. This algorithm is the theoretical basis for COMAGMAT, designed to model the crystallization of natural composition mafic magmas. The program can simulate the effects of pressure (up to 12 kbar) for systems that are either open or closed with respect to oxygen. The constraints that make up the model are calibrated to a general database, however, if experimental data exist on a specific system, the constraints can be modified to be consistent with those data. The COMAGMAT program makes it possible to calculate the equilibrium state of crystallizing silicate systems for a specific crystallinity. In order to simulate the dynamics of in situ differentiation, a subroutine containing physical constraints (DYNAM), has been added to the main COMAGMAT program.

This version of COMAGMAT 3.0 may be utilized to forward model the chemical differentiation of volcanic suites as well as tabular intrusions.

The input and output of COMAGMAT is designed to be user friendly, with the goal of making it useful for beginners and dabblers. This program is available on disc from any of the authors for US \$90 (\$50 for students).

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## APPENDIX

### *Examples of Data Files used in COMAGMAT Program*

#### MAINMENU.DAT:

Simulating Equilibrium Crystallization	
COMAGMAT software, ver.3.0 (1992) designed by A.A.Ariskin, Moscow	Isobaric crystallization
Oliv Plag Aug Pig Ilm Magn	Total pressure (P,kbar) 3.5 Maxim pressure(Pm,kbar) 10.0
N= 1 - number of start compositions	Open system (O2 buffers>Const)
Solving equilibrium problem at given Crystal increment 2 % up to 80 %	Main oxygen buffer : NNO Given lgfO2 - shifting: 0.00
◆◆◆ Simulating trace elements: 1. Mn,Ni,Co,Cr,Sc,V ,Sr,Ba,Rb,Cu ▶ 2. La,Ce,Nd,Sm,Eu,Gd,Dy,Er,Yb,Lu	◆◆◆ Precision of calculations: Temperature convergence,C 1.0 Phase compositions, mol.% 0.1
H2O content in model system, wt.% 0.0	Date : 11/25/92

#### COMMAJ.DAT:

SiO2	TiO2	Al2O3	FeO	MnO	MgO	CaO	Na2O	K2O	P2O5	Cr2O3	LOI	Sample
46.58	1.85	15.16	11.77	.17	10.09	10.22	2.94	.42	.14	.00	.30	Example



COMTRA.DAT:

Example

Ni	161.00
Co	68.00
Cr	249.00
Sc	8.40
V	0.00
Sr	319.00
Ba	141.00
Rb	8.00
Cu	93.00
La	6.47
Ce	14.60
Nd	7.50
Sm	1.67
Eu	1.62
Gd	0.00
Dy	0.00
Er	0.00
Yb	0.75
Lu	0.12

DICOEF.DAT:

	Oliv	Plag	Aug	Pig	Ilm	Magn
MnO	.	.030	.	1.000	1.000	2.000
Ni	.	.030	6.000	3.000	10.000	29.000
Co	.	.030	3.000	1.600	5.000	7.400
Cr	.900	.030	10.000	3.000	10.000	50.000
Sc	.370	.030	2.500	1.000	.500	2.500
V	.004	.030	1.500	1.000	10.000	26.000
Sr	.004	.	.220	.020	.010	.010
Ba	.004	.	.100	.010	.010	.010
Rb	.004	.200	.100	.010	.010	.010
Cu	.050	.030	.050	.050	1.000	1.000
La	.	.	.	.	.	.
Ce	.	.	.	.	.	.
Nd	.	.	.	.	.	.
Sm	.	.	.	.	.	.
Eu	.	.	.	.	.	.
Gd	.	.	.	.	.	.
Dy	.	.	.	.	.	.
Er	.	.	.	.	.	.
Yb	.	.	.	.	.	.
Lu	.	.	.	.	.	.

MINERS.DAT:

Olivine		Plagioclase		HCa Px (Augite)			LCa Px(Pigeonite)			LCa Px(Orthopyr)		
Fo	Fa	An	Ab	En	Fs	Wo	En	Fs	Wo	En	Fs	Wo
5543	6457	10641	11683	8521	13535	2408	8502	5865	4371	8870	5698	3409
-2.32	-4.22	-1.32	-6.16	-5.16	-9.87	-1.24	-4.74	-4.04	-4.02	-4.90	-3.93	-3.69
1.20	1.20	2.00	4.00	2.80	2.80	2.80	2.40	2.40	2.40	3.60	3.60	3.60

CORREC.DAT:

Miner	[Shift]	SiO2	TiO2	Al2O3	"FeO"	MgO	CaO	Na2O	K2O	[ H2O ]
Oliv	3.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-20.00
Plag	-20.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-120.00
Aug	.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-35.00
Pig	8.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-50.00
Ilm	.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-30.00
Magn	-15.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-30.00

OXYBUF.DAT:

PARAMETERS OF OXYGEN BUFFERS

Buffer	lgfO2 = a0 + a1/TK + a2*(P,bar-1)/TK			References
	a0	a1	a2	
1 IW	6.471	-26834.7	0.055	Myers, Eugster, 1983
2 WM	16.092	-36951.3	0.083	Myers, Eugster, 1983
3 IM	8.990	-29260.0	0.061	Huebner J.S., 1971
4 MH	13.480	-23847.6	0.019	Myers, Eugster, 1983
5 QFM	8.290	-24441.9	0.092	Myers, Eugster, 1983
6 IQF	6.396	-27517.5	0.050	Myers, Eugster, 1983
7 NNO	9.360	-24930.0	0.046	Huebner J.S., 1971
8 CCO	7.936	-25070.0	0.055 *	Myers, Gunter, 1979
9 COC>5	2.740	-19559.0	0.130	Woermann et al., 1977
10 COC<5	-0.044	-20586.0	-0.028	French B.H., 1966
11 GRS	4.620	-22324.0	0.189 #	Ulmer, Luth, 1991
12 ARB	-12.000	0.0	0.0	Arbitrary Buffer

\* Postulated    # ...-1.41\*[(P,kbar)\*\*2]/TK



