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Sudbury Igneous Complex: Simulating phase equilibria and in situ differentiation for two proposed parental magmas

Alexey A. Ariskin
Vernadsky Institute, Kosygin St. 19, Moscow 117975, Russia; ariskin@geokhi.ru
Alexander Deutsch
Institut für Planetologie, Universität Münster, D-48149 Münster, Germany; deutsca@uni-muenster.de
Markus Ostermann*
Institut für Planetologie, Universität Münster, D-48149 Münster, Germany; markus.ostermann@irmm.jrc.be

ABSTRACT

One of the major problems in the geology of the 1.85-Ga Sudbury impact structure, Ontario, Canada, is the origin and the evolution of the Sudbury "Igneous" Complex. The 2.5-km-thick Main Mass of this complex consists of from bottom to top, mafic to felsic norites, a layer of oxide- and apatite-rich quartz-gabbro, and granophyres. Genetically related to these lithologies are fragment-laden breccias on top (Basal Member of the Onaping Formation), and below the complex (Sublayer). The Sudbury Complex is interpreted to represent either a differentiated impact melt sheet, a hybrid endogenic magma that intruded in several pulses, or an endogenic magma topped by impact-generated granophyres.

Using the COMAGMAT–3.5 phase equilibria model, equilibrium and fractional crystallization were computed at 1 atm with the two initial liquids SIC (granophyres and norites in the ratio 2:1) and QRN (quartz-rich norite from the South Range). The calculated liquidus temperatures are 1,120°C for the SIC, and 1,180°C for the QRN parental melts. The modeled crystallization sequence for the SIC parent is independent of f_{O2}: Opx → Opx + Pl → Opx + Pl + Aug → Opx + Pl + Aug + Mt. For QRN, we observed Ol → Ol + Pl → Opx + Pl → Opx + Pl + Aug → Opx + Pl + Aug + Ilm (followed by Mt at the QFM buffer), and Opx + Pl + Aug + Mt (at the NNO buffer). The calculated liquid lines of descent show that the SIC composition potentially can produce about 70% of a residual melt containing more than 67.5 wt% SiO_2. In contrast, the quartz-rich norite magma can generate only 30% of such a "granophyric" liquid. These results would imply that fractionation of either the SIC or the QRN parent can produce the huge observed mass of granophyres, currently constituting up to two-thirds of the Main Mass.

Dynamic calculations using the INTRUSION subroutine of COMAGMAT, however, yield a more realistic and different picture. We numerically simulated convective-cumulative in situ magma differentiation with regard to a silica-rich melt trapped in natural rocks as intercumulus material. Results of these computations indicate that, even in the case of the silica-enriched SIC starting composition, the total amount of "granophyres" does not exceed 12 vol% of the modeled Main Mass. In the case of the

*Present address: EC Joint Research Centre-IRMM, B-2440 Geel, Belgium.

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QRN liquid, the granophyres amount to only 1–3 vol%. These results indicate that, under the assumption of a closed melt system evolution of the Main Mass, *granophyres in their present volume did not originate by differentiation of the norites in their presently known volume*. The lower "mafic" part of the Main Mass, however, is modeled perfectly with the dynamic COMAGMAT calculations, using a ferroandesitic melt compositionally similar to QRN, as starting composition. The modeled series of cumulates exactly duplicates the natural sequence from mafic and quartz-rich norites to the quartz-gabbro as observed in drill core 70011 of the North Range. These findings substantiate the interpretation that the norites, the quartz-gabbro, and a small cap of granophyres are genetically linked by differentiation. On the other hand, the results contradict any interpretation of the quartz-gabbro as the product of mixing between a "granophyric" and a "noritic" magma.

INTRODUCTION

The 1.850-g.y.-old (Krogh et al., 1984) Sudbury Structure, Ontario, lies within a Proterozoic supracrustal sequence (Huronian Supergroup) in the South, and Archean basement rocks (Abitibi Subprovince) of the Superior Province in the North (Fig. 1) (Dressler, 1984). The structure covers an area of roughly 15,000 km^2 and includes brecciated country rocks, the Sudbury "Igneous" Complex, and the Sudbury Basin. The Sudbury Structure is now widely acknowledged as tectonized erosional remnant of a more than 200-km sized multi-ring impact basin, yet the origin and evolution of the >2.5-km-thick Igneous Complex in the central depression of the structure remains controversial (see, Deutsch et al., 1995, for review). Models interpreting the Igneous Complex as coherent impact melt sheet (e.g., Grieve et al., 1991; Masaitis, 1993; Deutsch et al., 1995) compete with mixed endogenic-exogenic views ("two-magma model") (e.g., Chai and Eckstrand, 1993, 1994; Dressler et al., 1996), and, at the other extreme, a purely endogenic magmatic origin of the Igneous Complex has also been proposed (e.g., Naldrett 1984; Dressler et al., 1987). The impact melt nature of the Sudbury Igneous Complex is supported by evidence including isotope systematics (e.g., Ding and Schwarcz, 1984; Faggart et al., 1985; Deutsch, 1994; Ostermann, 1996; Ostermann and Deutsch, 1998), constraints from impact mechanics (e.g., Lakomy, 1990; Grieve et al., 1991; Deutsch and Grieve, 1994), and geophysical data (e.g., Milkereit et al., 1992).

As shown in Figure 2, the Main Mass of the Igneous Complex includes three major units: the Lower Zone of mafic to felsic norites; the Middle, or Transition, Zone, consisting of an oxide-rich gabbro with high modal amounts of Ti-Fe oxides (up to 10%) and apatite (the so-called quartz-gabbro); and the grano-

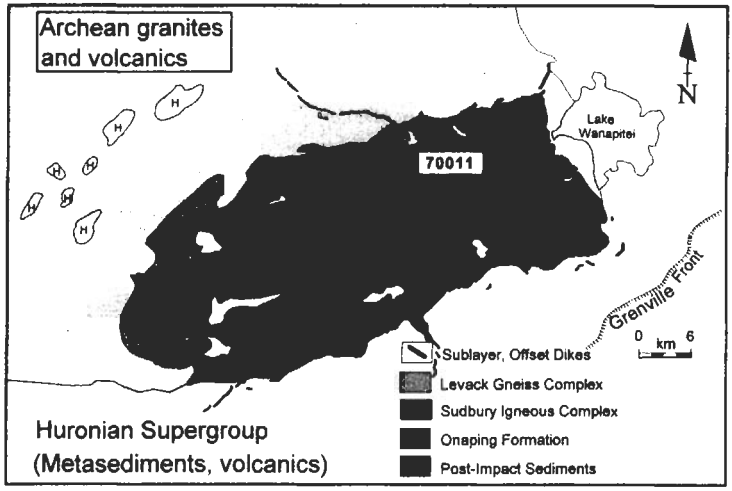

Figure 1. Sketch map of the inner part of the Sudbury multi-ring impact structure showing location of drill core 70011.

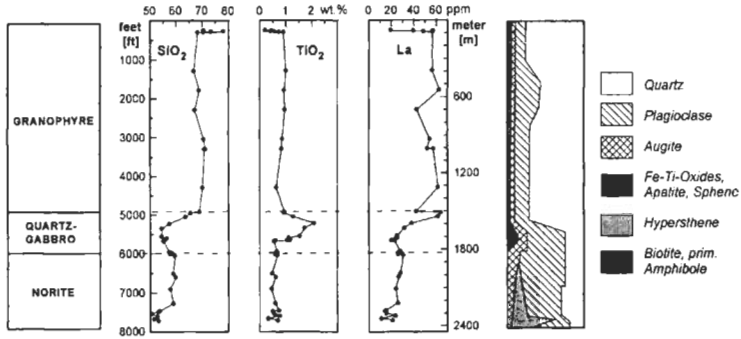

Figure 2. Variation of selected major elements and La over drill core 70011, North Range. To compare geochemical and mineralogic compositions, the simplified mineralogic composition of the Main Mass of the Sudbury melt system in the North Range is shown (after Naldrett and Hewins, 1984). Geochemical and mineralogic features are distinctly related between, for example, the noritic and quartz-gabbroic parts of the schematic stratigraphic column. Modified after Ostermann (1996).

phyric Upper Zone. Based on field evidence, Collins (1934) estimated a 1:2 ratio between norite and granophyre. Due to this odd volume ratio, the genetic relation between granophyres, the quartz-gabbro, and the norites still represents an unsolved problem, which is independent of the ongoing discussion of exogenic vs. endogenic origin.

A detailed geochemical study of the continuously sampled INCO core 70011 drilled in the North Range (Fig. 1) revealed for the first time rather smooth changes of elemental concentrations in the petrographically defined transitions from one to the other lithology of the Main Mass. Ostermann (1996), and Ostermann and Deutsch (1998) concluded that their geochemical data indicate a link of the three major units by differentiation. This interpretation prompted the present study to test whether petrologic modeling supports the proposed differentiation mechanism. Progress in theoretical igneous petrology over the past decades allows petrologists to study most of these effects numerically by means of numerical phase equilibria and dynamic models designed to simulate magma differentiation processes over a wide range of compositions and conditions.

Several different programs exist, which are based on data from melting experiments with igneous rocks. This empirical approach extends the available experimental data base to poorly studied natural systems and/or to a wider range of P-T-f_{O2} (oxygen fugacity) conditions (e.g., Nielsen and Dungan, 1983; Frenkel and Ariskin, 1984; Ghiorso, 1985; Ariskin et al., 1987, 1993; Weaver and Langmuir, 1990; Ghiorso and Sack, 1995). These models allow calculation of equilibrium and/or fractional crystallization in terrestrial basaltic to andesitic magmas, and they have been successfully applied to genetic interpretation of tholeiitic and calc-alkaline volcanic suites (Ghiorso and Carmichael, 1985; Nielsen, 1990; Ariskin et al., 1988, 1990, 1995). All these models except COMAGMAT (Ariskin et al., 1993) fail in the solution of thermal and dynamic problems, e.g., the movement of solidification fronts in magma chambers, effects of crystal settling on volumetric relations, as well as mineralogy and chemistry of rocks formed during differentiation (Frenkel et al., 1989).

In this chapter, we present the results of combined phase equilibria and dynamic calculations carried out with COMAGMAT software in order to simulate the proposed in situ differentiation of the impact melt layer (the so-called Sudbury Igneous Complex) in the central part of the Sudbury multi-ring impact structure (e.g., Grieve et al., 1991; Deutsch et al., 1995; Ostermann, 1996). The results of the simulation, which have been carried out for two different "initial" compositions of the Main Mass of the Sudbury Igneous Complex (Collins, 1934; Naldrett, 1984) set new constraints on the evolution of this controversely discussed silicate melt with an estimated total volume of about 12,500 –25,000 km^3 (Deutsch and Grieve, 1994).

See Table 1 for a list of abbreviations used in this chapter.

COMAGMAT PROGRAM

General description

The COMAGMAT software consists of a series of linked programs developed to simulate a variety of igneous processes including both simple crystallization of volcanic suites and in situ differentiation of tabular intrusions (Ariskin et al., 1993). COMAGMAT is designed for melts, ranging from basaltic to dacitic compositions. The modeled elements include Si, Ti, Al,

TABLE 1. LIST OF ABBREVIATIONS

Ab	albite
An	anorthite
Aug	cpx with an augitic composition
Cpx	clinopyroxene
En	enstatite
F_{crit}	maximal possible fraction of solid phases in a magma, which can accumulate to form a primary cumulate
F_{crys}	fraction of solid phases suspended in a magma
F_{int}	fraction of solid phases suspended in a magma directly after emplacement in the chamber
f_{O2}	oxygen fugacity
Fa	fayalite
Fo	forsterite
Fs	ferrosilite
Ilm	ilmenite
MGN	magnesium number (100xMg/(Mg+Fe))
Mt	magnetite
NNO	nickel-bunsenite oxygen buffer
Ol	olivine
Opx	orthopyroxene
P	pressure
Pl	plagioclase
QFM	quartz-fayalite-magnetite oxygen buffer
QRN	average chemical composition of the fine-grained Quartz-Rich Norites of the South Range according to Naldrett (1984)
SIC	average chemical composition of the Main Mass of the Sudbury "Igneous" Complex according to Collins (1934)
t	time
*t**	chilling duration
T	temperature
Ulv	ulvöspinel
Wo	wollastonite

Fe_{tot} (divided into Fe^{3+} and Fe^{2+}) ±Mn, Mg, Ca, Na, K, P, as well as 20 trace elements (see below). In the last version of COMAGMAT–3.5 used for this work (Ariskin, 1997[1]), the modeled minerals include olivine (Fo - Fa solution), plagioclase (An - Ab solution plus K), three pyroxenes (augite, pigeonite, and orthopyroxene: En - Fs - Wo solutions plus Al and Ti), ilmenite and magnetite (Fe^{2+} - Fe^{3+} - Ti - Al - Mg solutions). The program can be used at low to moderate pressures, approximately up to 12 kb, and allows calculations of open (12 oxygen buffers) and closed system differentiation with respect to oxygen (Ariskin, 1987, 1993).

Thermodynamic background

Mineral-melt geothermometers. The basic components of the COMAGMAT model are a system of empirically calibrated equations that describe mineral-melt equilibria as function of temperature and melt composition. These geothermometers have been calibrated using a data base, which consists of published results of melting experiments at 1 atm (Ariskin et al., 1987, 1996). For this calibration, the activities of the mineral components were assumed to equal the mole fractions of the cations in a single site (ideal solution). This model implies that the effects of nonideality on mineral-melt equilibria are attributed primarily to the liquid phase. Applying the calibrated geothermometers to liquid compositions of the initial data base, one can invert the calculations to estimate mineral-melt equilibria temperatures. Calculated and experimentally observed temperatures coincide with an accuracy of ±10°–15°C (Ariskin et al., 1987, 1993). A similar comparison of calculated and experimentally produced mineral compositions shows that Fo, An, En, and Wo contents can be predicted within 1–3 mol%. It is important to note that the best fit of calculated mineral-melt equlibria with experimental data is obtained for tholeiitic and transitional systems ranging from magnesian-basalts to dacites (45–60 wt% SiO_2, $Na_2O + K_2O < 5$ wt%).

Trace element partitioning. One of the major advantages of COMAGMAT is the linkage between major and trace element systematics. Computation of major element mineral-melt equilibria controlled parameters, such as temperature and fractionating mineral proportions, set constraints for the behavior of trace elements, based on empirically determined distribution coefficients. COMAGMAT calculates the distribution of Mn, Ni, Co, Cr, V, Sc, Sr, Ba, Rb, Cu, and 10 rare earth elements (REE) in an evolving melt system (Barmina et al., 1989b, 1992).

Algorithm to solve the equilibrium problem. To simulate the crystallization of multiple saturated magmas, an algorithm must be developed for the calculations of mineral-melt equilibrium at a given set of independent parameters of state, such as temperature and pressure. To address the problem, COMAGMAT takes advantage of numerical solutions of nonlinear empirical equations that describe mineral-melt equilibria and mass action law, coupled with the mass balance constraints for the whole system composition (Frenkel and Ariskin, 1984). This approach combines basic empirical and thermodynamic considerations into a hybrid algorithm. The simulation of the differentiation of natural magmas is thus performed step by step with increasing crystallization (Ariskin et al., 1993).

Dynamic background

To model dynamics of in situ differentiation of magmas, we have developed the INTRUSION subroutine. This part of the COMAGMAT program is placed in the crystallization algorithm so that after determination of the phase equilibria for a given crystallinity, the modeled magma composition can be modified by subtraction of the calculated equilibrium (cumulative) minerals and the melt, trapped in the cumulates (Frenkel et al., 1989). This enables the user to simulate a variety of igneous differentiation processes, accounting for changes in phase proportions and compositions during the system's evolution.

The INTRUSION subroutine simulates a number of physical processes taking place simultaneously during in situ magma differentiation. These processes include (1) loss of the heat of crys-

[1] The COMAGMAT program and its description are available on request from A. A. Ariskin.

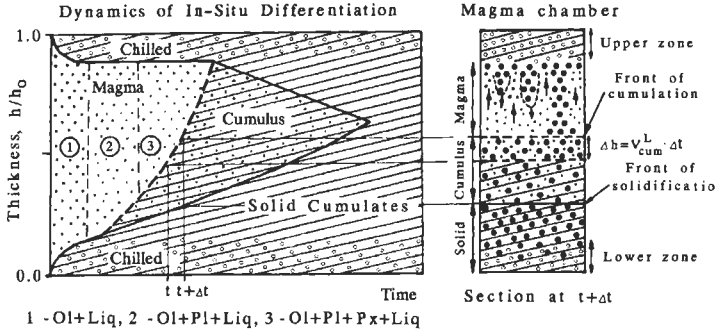

Figure 3. Dynamics of in situ magma differentiation based on the convective-cumulative model of Frenkel et al. (1989). High efficiency of vigorous convection is assumed to maintain uniform temperature and composition in the magma body up to the point where the magma chamber is filled with cumulates and the chemical differentiation is completed.

tallization through the upper and lower margins of a tabular magma chamber; (2) movement of solidification fronts into the magma body; (3) crystal settling, together with the formation of crystal-bonded (cumulus) and nonbonded (porphyric) crystal aggregates; and (4) the evolution of the primary mineral and the trapped liquid compositions. The basic framework for this model and its full mathematical description are given in Frenkel et al. (1989) and summarized in Ariskin et al.(1993).

Convective-cumulative model. 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 chosen for the responsible physical mechanisms. The convective-cumulative model used in COMAGMAT was originally designed for simulating the in situ differentiation of Siberian sills (Frenkel et al., 1989). This model is constrained by more than 20 yr of field work, petrographic and geochemical analysis, as well computer simulations.

Perhaps the most important result from this multi-disciplinary work is the obviously high efficiency of convection in 10^2–10^3-m-thick magma bodies. The convection yields a nearly uniform temperature distribution and quite homogeneous melt composition up to the point where the magma chamber becomes filled with cumulates. This will result in fractionation of the magma, but not perfect fractional crystallization due to effects caused by suspended crystals. These solid phases are assumed to form near the upper boundary of chamber, then descend through the convecting magma into cumulates at the base of the magma body. In this model, convection does not prevent settling of the suspended crystals. Figure 3 schematically illustrates the convective-cumulative model of magma evolution.

Frenkel et al. (1989) proposed a number of semi-empirical constraints that approximate the convective-cumulative process in order to link the dynamic equations with the basalt crystallization algorithm. Calculation of the equilibrium crystallization for a given initial magma composition always starts under the assumption of an entirely liquid system ($F_{crys} = 0$). This does not imply that the magma at the beginning of its evolution in the magma chamber indeed is free of crystals but simply that these calculations proceed incrementally up to the value $F_{crys} = F_{init}$, which is the assumed fraction of solid phases suspended in the magma at the time of emplacement. Beginning from F_{init}, the INTRUSION subroutine of COMAGMAT is used iteratively, after calculations of phase equilibria at each degree of crystallization.

Given the bulk composition and thickness H of a sheet-like magma body, the INTRUSION subroutine starts to compute the differentiation process at the initial time $t = 0$, with an assumed chilling duration t^*. This t^* defines the thickness of the upper and lower chilled zones (Frenkel et al., 1989). The formation of the chilled zones along the margins for the period $0 < t < t^*$, as well the formation of cumulates in the lower zone at $t > t^*$, results in a reduced volume of the model magma system for both the liquid (trapped melt) and the equilibrium solid (cumulative) phases. After correcting for this volume loss, the remaining melt is incrementally crystallized further in terms of ΔF. The phase equilibria at the new and higher crystallinity is then calculated. Each forthcoming iteration through the INTRUSION subroutine begins with the determination of the heat and crystal mass flux and the time interval corresponding to the given ΔF_{crys}.

In summary, the COMAGMAT algorithm simulates at the same time crystallization and the thermal history of the magma body, including the dynamics of crystal settling and the movement of the crystallization or accumulation fronts within the magma chamber. The simulation ends when the calculated fraction of solids suspended in the magma reaches the value of an assumed critical crystallinity F_{crit}. This F_{crit} is defined as the maximal possible fraction of minerals, which can be accumulated in the magma to form a primary cumulate. If the value of F_{crit} is

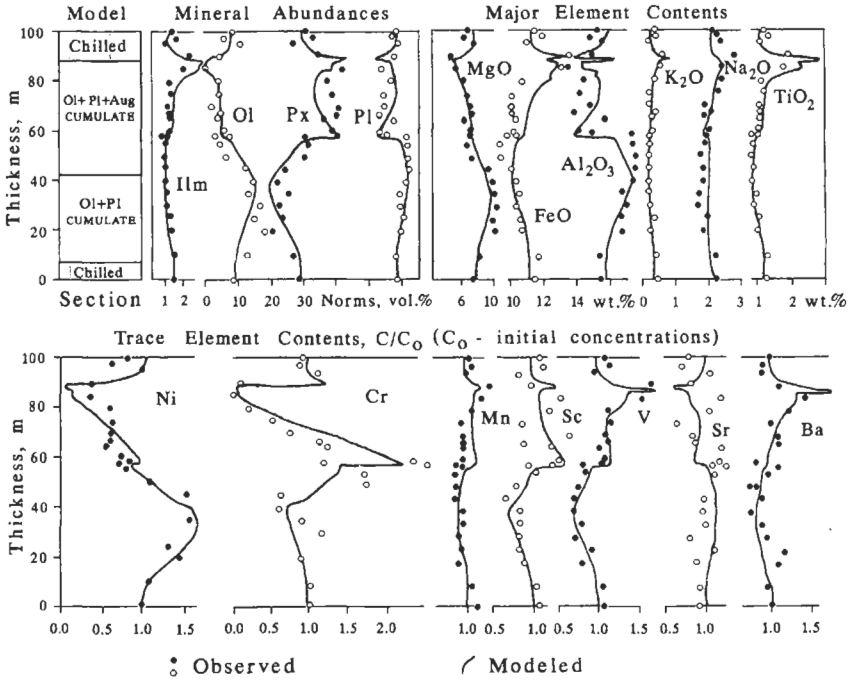

Figure 4. Comparison of observed data from Vavucan differentiated sill (eastern Siberia, Russia) with dynamic simulations using the COMAGMAT model. The phase boundary, which is separating Ol + Pl and Ol + Pl + Aug "cumulates" (porphyric rocks), predicted by the model, corresponds to boundary between poikilophitic and taxiophitic dolerites observed in nature (Frenkel et al., 1989; Ariskin et al., 1993).

not reached during these calculations, this modeling will proceed up to the point (height) where the upper crystallization front encounters the front of crystal accumulation.

Application of the convective-cumulative model to the natural case. The test of the proposed in situ differentiation mechanism is whether observed major and trace element distributions in tabular intrusions are quantitatively reproduced by the proposed model (Frenkel et al., 1989; Ariskin et al., 1993; Chalokwu et al., 1996). Figure 4 compares measured geochemical characteristics with results of the model calculations for one Siberian differentiated sill, the 100-m-thick Vavukan intrusion (Frenkel et al., 1989). Given the large number of data, particularly major and trace element analyses, and the relatively small number of variable parameters, the solution explaining all observational data is by no means overdetermined.

The successful application of the model to this sill indicates that the convective-cumulative mechanism represents a plausible physical explanation for the differentiation of sheet-like magma bodies, 10^2–10^3-m-thick. With this background, we applied the algorithm to the ~2,500-m-thick Main Mass of the Sudbury Igneous Complex in order to evaluate the evolution of this impact melt sheet. In principle, this silicate melt body cooled slowly enough (i.e., on the order of 0.5 Ma) to differentiate (Ivanov et al., 1997; Ivanov and Deutsch, this volume).

MODELING PHASE EQUILIBRIA FOR THE SUDBURY IGNEOUS COMPLEX

Defining parental melts

The principal problem in modeling a complex silicate melt system such as the Sudbury Igneous Complex lies in the definition of the parental melt (or starting) composition. There exist several approaches for this question. The classic petrologic-geologic approach uses bulk chemical analyses of fine-grained lithologies from the margins of layered intrusions, which are assumed to represent chilled initial liquids (Wager and Brown, 1967). This technique works only if thermal or chemical processes at the margin did not alter the composition of such rocks. The calculation of weighted average compositions from

TABLE 2. AVERAGE COMPOSITION OF THE MAIN ROCK TYPES OF THE SUDBURY "IGNEOUS" COMPLEX IN DRILL 70011 OF THE NORTH RANGE*

Rock Type	Granophyre	Quartz-gabbro	Norite	Sublayer	Calculated Average for the Main Mass	Analytical Error
Drillcore	70011	70011	70011	70011	70011	
% of drillcore	59.6	13.7	20.2	6.5	100	
(wt. %)						
SiO_2	69.5	55.2	57.3	51.7	63.9	±0.54
TiO_2	0.80	1.44	0.59	0.53	0.83	±0.01
Al_2O_3	12.6	14.7	15.4	9.00	13.22	±0.18
$Fe_2O_{3\,(tot)}$†	5.49	10.4	8.42	12.15	7.19	±0.21
MnO	0.08	0.14	0.13	0.21	0.11	±0.01
MgO	1.01	3.66	5.70	12.27	3.05	±0.15
CaO	2.24	7.25	6.39	10.17	4.28	±0.10
Na_2O	4.15	3.86	3.19	1.69	3.76	±0.14
K_2O	2.76	1.45	1.41	0.55	2.16	±0.05
P_2O_5	0.17	0.46	0.15	0.12	0.20	±0.02
Total	99.2	99.1	99.6	98.4	99.86	
LOI§	1.04	1.08	1.31	1.62	1.14	

*Ostermann, 1996.
†$Fe_2O_{3\,(tot)}$ = total iron.
§LOI = Loss on ignition.

well-documented vertical sections of tabular intrusion bodies, e.g., in differentiated traps, yields more accurate estimates of parental magma composition (Frenkel et al., 1989). This approach is less sensitive to processes at the contact. Such calculations, however, may result in an initial melt composition enriched in certain components that are suspended or accumulated in the magma as crystal phases.

A constructive way to escape both these problems is to combine calculated weighted average compositions with experimental studies or phase equilibria simulations. In this concept, known as geochemical thermometry (Frenkel et al., 1988), the equilibrium crystallization is calculated for an assumed parent melt up to the temperature corresponding to the estimated percentage of primary crystallization or crystal accumulation. This approach has been successfully applied to, for example, to the genetic interpretation of Siberian differentiated traps, hypabyssal bodies from eastern Kamchatka, and some mafic layered intrusions (Barmina et al., 1989a, b; Chalokwu et al., 1993, 1996).

Estimates of parental melt compositions for the Sudbury Igneous Complex

Application of the geochemical thermometry technique to the Sudbury Igneous Complex presents serious difficulties. The main problem rests in the fact that a successful approach requires strongly defined contacts to the country rocks, and correct estimates of major rock types in terms of volumetric proportions (thickness), geochemical composition, and density. In the case of the Sudbury Igneous Complex, two facts hinder a sound assessment of the parental melt by the geochemical thermometry technique. First the Sublayer rocks and melt breccias of the Basal Member (Onaping Formation) reliably belong to the impact melt body (Brockmeyer, 1990; Grieve et al., 1991; Deutsch and Grieve, 1994; Deutsch et al., 1995), and, hence, should be combined with the Main Mass for calculation of an weighted average composition of the whole Sudbury Igneous Complex. Volumetric proportions and geochemical composition of both formations, however, are not well constrained. Second, principal differences occur in the stratigraphic columns of the North and South Ranges of the Sudbury Igneous Complex, such as the diversity of norites, and different volumetric proportions between the three major lithologies, i.e., norites, quartz-gabbro, and granophyres (Naldrett and Hewins, 1984). Due to these difficulties, any estimated "bulk composition of the initial Sudbury melt" could represent only a first approximation of the true initial melt. Results of computer-based interpretations of the further evolution of such a melt, therefore, provide simply generalized conclusions on the possible evolution of the Sudbury Igneous Complex in nature.

In this study, two melt compositions have been used for phase equilibria calculations; they are assumed to be parental for the Main Mass of the Sudbury Igneous Complex. As proposed by Collins (1934) on the basis of field studies, the first average composition corresponds to a mix of granophyres and norites in the canonical ratio 2:1; for this initial melt, we use the abbreviation SIC. This average composition is close to the average composition of the Main Mass, calculated recently by Ostermann and Deutsch (1998) by weighting average compositions of the major lithologies in core 70011 (Table 2) drilled in the North Range

TABLE 3. PROPOSED PARENTAL SUDBURY MAGMAS USED IN COMAGMAT CALCULATIONS

Oxide	Average *SIC* (Collins, 1934)	Quartz-rich Norite *QRN* (Naldrett, 1984)
SiO_2	64.19	57.00
TiO_2	0.75	1.34
Al_2O_3	14.89	16.40
FeO_{tot}	5.57	7.33
MnO	0.08	0.13
MgO	2.90	6.40
CaO	4.10	7.28
Na_2O	3.35	2.41
K_2O	2.96	1.55
P_2O_5	0.23	0.16

Note: Normalized to water-free basis (100 wt. %).

(Fig. 1). The second parent used in our computations corresponds to the fine-grained Quartz-Rich Norites (QRN) of South Range; this lithology was proposed by Naldrett (1984) and Naldrett et al. (1986) as the initial, mantle-derived and contaminated magma for the Sudbury Igneous Complex. Table 3 lists these two assumed "parental" compositions.

Compared to the QRN composition, the SIC is high in SiO_2 (64 vs. 57 wt%) and alkalies yet depleted in the "mafic" and "plagioclase" components MgO (2.9 vs. 6.4 wt% for QRN), FeO, CaO (4.1 vs. 7.3 wt%), and Al_2O_3 (see Table 3). This significant compositional difference reflects the large proportion of exposed granophyre (Collins, 1934). It is noteworthy that drill core 70011 displays relative to the estimate of Collins (1934) a similar volumetric ratio between norite and granophyre (Ostermann, 1996; A. Therriault, personal communication). The SIC parental melt is "ferrodacitic" and the QRN is "ferroandesitic" composition. Using both given "initial" compositions, we applied COMAGMAT to study whether the three major lithologies of the Main Mass, i.e., norite, quartz-gabbro, and granophyre, are related by differentiation (e.g., Ostermann, 1996) or belong to separate silicate melt systems (e.g., Chai and Eckstrand, 1993, 1994). In this context, and as already pointed out by researchers including Kuo and Crocket (1979) and Naldrett (1984), we should emphasize that the odd ratio between silica-rich and mafic members of the Mass Mass represents a fundamental problem in all previously published models for the origin and evolution of the Sudbury Igneous Complex. This ratio contrasts with the observations on all true (i.e., endogenic) layered magmatic bodies.

Phase equilibria calculation for Sudbury parental melts

The COMAGMAT–3.5 program (Ariskin, 1997) was used for the modeling of equilibrium crystallization and fractional crystallization of the SIC and QRN parental magmas. Advantages of the new COMAGMAT version include equations describing mineral-melt equilibria for Ti-magnetite and ilmenite, which are significant components in the quartz-gabbro (Naldrett and Hewins, 1984) (see Fig. 2). In addition, a new orthopyroxene-melt model computes more accurately the orthopyroxene crystallization (Bolikhovskaya et al., 1996). Moreover, using the INFOREX experimental database (Ariskin et al., 1996), more realistic molar mineral-melt distribution coefficients for TiO_2 in clino- and orthopyroxenes, as well for K_2O in plagioclase, are calculated. These coefficients are also integrated in the COMAGMAT–3.5 software.

Crystallization sequence. The calculations of equilibrium and fractional crystallization were carried out at 1 atm total pressure and with a 1 mol% increment of solids from one step to the next. In addition, two different oxygen buffers were used, QFM (quartz-fayalite-magnetite) and NNO (nickel-bunsenite), in order to better constrain the f_{O2} conditions at which magnetite starts to crystallize on the calculated liquidus simultaneously with high-Ca clinopyroxene. This assemblage occurs in norites and the quartz-gabbro (Naldrett and Hewins, 1984). The maximum compositional range encountered is about 70 mol%, which corresponds to the final calculated temperatures of 1,025°C for SIC, and 1,050°C for QRN compositions, respectively.

Figure 5 illustrates the results for the simulated equilibrium crystallization of the two proposed parental magmas. As shown in these plots, the calculated liquidus temperatures are 1,120°C for the SIC and 1,180°C for the QRN composition, respectively. For the SIC parent, the modeled crystallization sequence is Opx (orthopyroxene) → Opx + Pl (plagioclase) → Opx + Pl + Cpx [Aug] (augitic clinopyroxene) → Opx + Pl + Aug + Mt (magnetite). This sequence is independent of f_{O2}. The main differences between calculations at QFM, and NNO buffers lie in the higher crystallization temperature for *Mt* at more oxidizing conditions.

For the QRN composition of the initial melt, calculated phase relations turned out to be more complex. The modeled crystallization sequence for silicate minerals is also independent of f_{O2}, whereas the appearence of iron-titanium oxides at the liquidus displays small, yet important, differences: Ol (olivine) → Ol + Pl → Opx + Pl → Opx + Pl + Aug → Opx + Pl + Aug + Ilm (ilmenite) → Opx + Pl + Aug + Ilm + Mt (at QFM); and Ol → Ol + Pl → Opx + Pl → Opx + Pl + Aug + Mt (at NNO). This variance in the onset crystallization temperatures for ilmenite and Ti-magnetite at QFM and NNO is in good agreement with available experimental data (Toplis and Carroll, 1995). In addition, we note that during progressive crystallization of QRN, olivine is completely dissolved after the first appearance of orthopyroxene. This orthopyroxene is partly dissolved with the onset of augite crystallization, implying peritectic (reaction) relations of these phases at the modeled range of temperatures and compositions.

The disappearance of *Ol* with commencement of Opx crystallization in the QRN system deserves a more detailed discussion. According to petrologic observations, olivine is absent in the norites of the Main Mass, even in the most magnesian norites of the North Range (Naldrett and Hewins, 1984). This observation might be considered as argument against the QRN composition representing the real parental melt. Yet, the phase equilibria calculations presented in Figure 5 demonstrate that such a con-

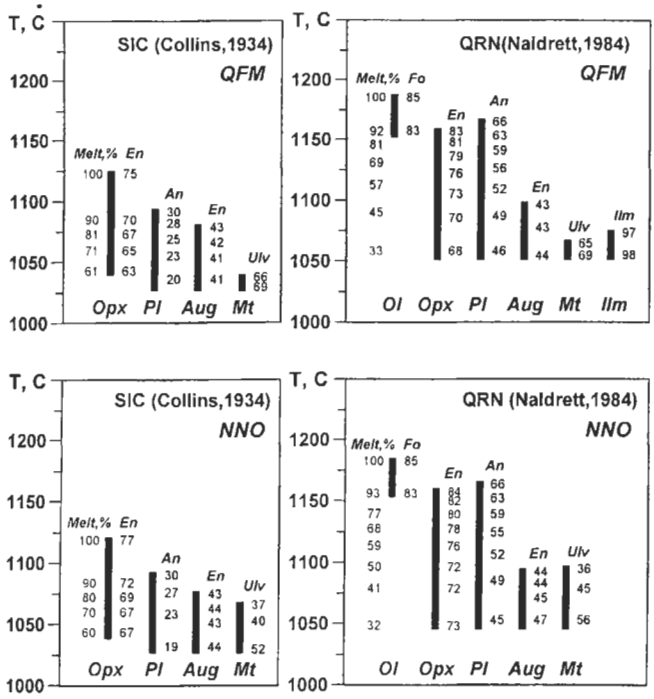

Figure 5. Mineral crystallization sequences calculated with the COMAGMAT model for the SIC and QRN parents at 1 atm and QFM to NNO oxygen buffer conditions. Values to the right of the magnetite and ilmenite lines represent the percent of ulvöspinel and ilmenite component in solid solutions, calculated using the equations of Stormer (1983).

clusion would be erroneous. After magma fractionation and complete accumulation of primary minerals, the first Ol crystals at the liquidus do not survive solidification of the crystal-trapped melt system, due to a highly efficient reaction of primary solids with the silica-enriched trapped liquid.

In general, both crystallization sequences, i.e., for the SIC or QRN initial melt, calculated at NNO conditions correspond well to observations in the Main Mass of the Sudbury Igneous Complex. Calculated mineral compositions provide additional genetic information.

Opx compositions. Naldrett and Hewins (1984) present data on the change in hypersthene and augite mineral chemistry in the norites of the South, and North Ranges. The most magnesian Opx crystals with the magnesium number MGN = 100 × Mg/(Mg + Fe) of 74–76 occur in mafic norites of the North Range; whereas, most of the felsic and quartz-rich norites contain Opx with MGN of 60–65. Comparing these natural Opx compositions with the calculated ones, shown in Figure 5, we conclude that the SIC composition crystallizes liquidus Opx with MGN = 75–77. This initial composition, hence, may accurately duplicate the parental melt. We want to emphasize, however, that the seemingly good accordance in Opx mineral chemistry could also be due to re-equilibration of primary more magnesian Opx crystals with a trapped liquid having a low MGN. Such postcrystallization processes occur generally both in differentiated sills (Barmina et al., 1989a), and mafic layered intrusions (Chalokwu et al., 1993).

Pl compositions. According to Naldrett and Hewins (1984), the anorthite content decreases upward from An_{61} at the base of the South Range norite to An_{50} halfway to the quartz-gabbro. Plagioclase in the quartz-gabbro and granophyres are altered to a high degree, so that only the bulk normative An content may be used to estimate the evolution of plagioclase compositions. The observed normative An content of Pl decreases abruptly from An_{50} in the quartz-gabbro to $An_{15\text{-}20}$ in the granophyres (Naldrett and Hewins, 1984). In this respect, the QRN composition matches observation better than the SIC starting liquid (Fig. 5).

Liquid lines of descent. Figure 6 illustrates the evolution of SiO_2 contents in the residual melts of the SIC and QRN starting compositions, calculated at NNO conditions for equilibrium, and fractional crystallization. Figure 6a was constructed in terms of degree of crystallization, Figure 6b gives silica contents as function of the modeled temperature. The liquid lines of descent for both parent melts exhibit only minor variations related to the type of crystallization process (equilibrium vs. fractional). The initial composition, SIC and QRN, however, causes significant differences in the respective trajectories.

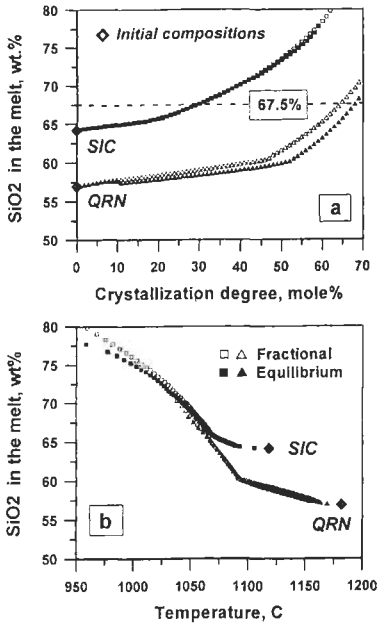

Figure 6. Liquid lines of descent during equilibrium and fractional crystallization of the SIC and QRN parents calculated at 1 atm and NNO oxygen buffer conditions. The SiO_2 contents in the melts are displayed as a function of the crystallization degree and the equilibrium temperature.

Figure 6a shows to what extent the SIC and QRN parents should be crystallized to produce differentiates with a silica content similar to that of the granophyre, i.e., >67.5 wt% (Collins, 1934). In the simulation, the SIC composition produces about 70 mol% of a residual melt with SiO_2 in excess of 67.5 wt%. In contrast, the QRN melt generates only 30 mol% of such a granophyric liquid. Figure 6b gives evidence that for both initial compositions, all calculated T-SiO_2 trajectories converge in the temperature range of 1,070°–1,025°C.

The results of our modeling indicate that, in principle, fractionation of the SIC parent could explain formation of enough granophyre to constitute two-thirds of the Main Mass in sections in the North Range. In contrast, differentiation of the QRN magma could result in the less thick granophyre horizon observed in the South Range (Naldrett and Hewins, 1984). Such a straightforward mass balance, however, seems to be of limited value for the natural differentiation process of the Sudbury melt body. In fact, due to the porosity of natural cumulates, a part of the silica-enriched liquid will be trapped as intercumulus material.

Although the norites of the Main Mass are not typical cumulates (Warren et al., 1996), they may contain a certain amount of trapped melt, which in turn results in a significant decrease of the total volume of granophyric melt that can be generated from the parents. In conclusion, both parental melts can yield, in principle, "granophyric" residuals. This fact strongly supports the concept that the Sudbury Igneous Complex represents a differentiated single melt body.

Constraints set by our phase equilibria calculations, however, do not define conditions of melt evolution in detail, and questions remain. For example, the structure of the lower zones of the Main Mass constitutes a serious problem. Any parental melt proposed for the Sudbury Igneous Complex must also generate differentiates compositionally similar to the quartz-rich and mafic norites observed in the lower zones of the Main Mass. The following gives a more quantitative treatment of this problem.

SIMULATING IN SITU MAGMA DIFFERENTIATION OF THE MAIN MASS

Using the INTRUSION subroutine of the COMAGMAT–3.5 software, we performed a set of calculations for the two proposed parental melts, SIC and QRN, simulating the convective-cumulative style of in situ differentiation as described above. The simulation technique for the Sudbury problem, which has been successfully applied to Siberian sills (Fig. 4), is a typical example of a forward model. Beginning with computer simulations to calculate the response of a modeled system to a set of assumed thermodynamic and dynamic parameters (initial and boundary conditions), the calculated results are then compared with observations of the natural case. The model may be used iteratively by modifying the parameters until a satisfactory fit is obtained. After defining a set of optimal parameters, this information is used to gain further insight into how crystallization will change other system parameters. They include the temperature path, changes in chemistry of liquidus phases, and changes in phase chemistry of the model cumulates and coexisting magma at every level in the body.

The detailed geochemical study of drill core 70011 (Ostermann, 1996) in the North Range (Fig. 1) served as natural data set to control and optimize parameters. The weighted average compositions for the three major lithologies of the Main Mass in the core samples are listed in Table 2.[2]

Modeling the whole Main Mass section

Initial and boundary conditions. Based on drill core 70011 (Fig. 2) (A. Therriault, personal communication), the thickness H of the magma body was set to 2,224 m. Initial crystallinity of the parental magmas was varied in the range $0 < F_{ini} < 10\%$, with the chilling duration t^* being 720 hr. Thermophysical parameters for country rocks, such as thermal conductivity, density, and heat capacity, were used from the Siberian sills simulations

[2] Detailed data are available by request from the authors, and as EXCEL file under <http://saturn.uni-muenster.de/>.

(Table 4), the initial temperature gradient at the upper crystallization front was assumed to be $\Delta T = 1{,}000°C$. The main variables include the critical crystallinity of modeled cumulates, which is $40 < F_{crit} < 80$ vol% (i.e., the portion of trapped melt F_m is 100% - F_{crit}). The *efficient* crystal settling velocities for the minerals Ol, Opx, Pl, Aug, and Mt varied in the range from 0.1 to 50 m a^{-1}. About 50 such simulations were performed. Figure 7 shows two typical results.

Main results. Figure 7 illustrates the distribution of SiO_2 and TiO_2 in the modeled sequence, which results from dynamic calculations of convective-cumulative differentiation of the Main Mass at $F_{crit} = 40\%$, and 60%; other parameters are listed in Table 4. The results for the SIC, and the QRN parent are displayed in Figure 7. Each of the two plots shown includes two curves. The solid one displays the evolution for $F_{crit} = 40\%$, the dotted one stands for $F_{crit} = 60\%$. We note that even in the case of the silica-enriched Collins' (1934) SIC composition, the total amount of "granophyres" generated does not exceed 4–12% of the total thickness. For the QRN starting composition, this amount is decreased to less than 3%. This is no surprise, as a part of the silica-enriched liquid is assumed to be trapped as intercumulus material.

These results indicate the following conclusion, which is independent on the initial melt composition, and boundary conditions. The convective-cumulative magma fractionation processes was neither able to produce the 60–70% of granophyre observed in the North Range nor the about 40% of granophyre occurring in the South Range. We assume this statement to be valid also for other magma fractionation mechanisms, such as directional crystallization from the bottom. In addition, neither

TABLE 4. PARAMETERS OF DYNAMIC CALCULATIONS SIMULATING THE FORMATION OF THE SUDBURY MAIN MASS BY THE CONVECTIVE-CUMULATIVE MODEL†

Initial conditions	
Parental magma compositions	*SIC* and *QRN*, see Table 2
Thickness of the Main Mass magma body, *H*	2224 m
Initial crystallinity of the parental magmas, F_{cr1}	5 vol. %
The chilling duration, t^*	720 hours
Boundary conditions	
Temperature gradient at the upper crystallization front, ΔT	1000°C
Density of country rocks	2.700 g/cm^3
Heat conduction of country rocks	0.006 cal/cm*sec*grad
Heat capacity of country rocks	0.250 cal/g*grad
Assumed dynamic parameters	
Critical primary crystallinity of modeled cumulates, F_{crit}	40 and 60 vol. %
Crystal settling velocities, m/year	
Olivine	20.0
Orthopyroxene	0.5
Plagioclase	0.5
Augite	6.0
Magnetite	1.0
Calculated	
Time needed to fill the magma chamber with cumulates, years	
F_{crit} = 40% (*SIC-QRN*)	(2.22–2.90) x 10^3
F_{crit} = 60% (*SIC-QRN*)	(3.68–5.72) x 10^3

†For the results shown in Figures 7, 8, and 9. For more details concerning the convective-cumulative model parameters, see Frenkel et al., 1989, and Ariskin et al., 1993.

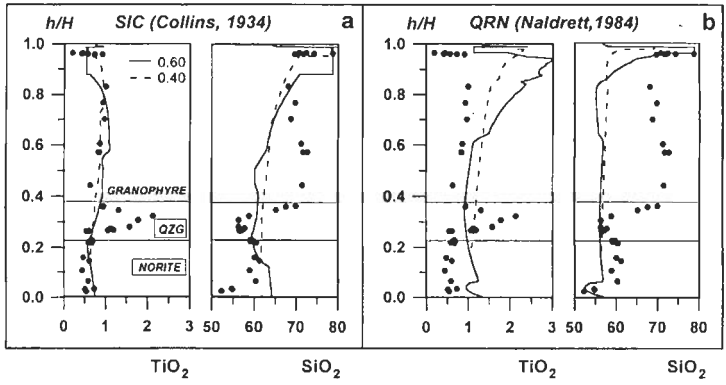

Figure 7. Results of dynamic calculations carried out with the SIC and QRN parent melts to study the effect of the convective-cumulative style of in situ magma differentiation on the composition of rocks, which could be formed in the Sudbury Main Mass as a result of crystal settling. The solid lines represent SiO_2, TiO_2, and other major element contents modeled at 1 atm and NNO oxygen buffer conditions using the INTRUSION subroutine of COMAGMAT (Frenkel et al., 1989; Ariskin et al., 1993). The assumed critical crystallinities are 40 and 60 vol%, respectively; for other main thermal and dynamic parameters, see Table 3. Natural data are from Ostermann and Deutsch (1998).

modeled parental melt can generate the sharp increase in TiO_2 occurring in the quartz-gabbro of the lower part of the Main Mass (Fig. 7; see also Table 2 and Fig. 2). This basic conclusion holds only in the case of closed system evolution, and under the assumption that the Main Mass indeed represents a complete section of the differentiated Sudbury melt body.

Formation of norites and the quartz-gabbro

The modeled results plotted in Figure 7b for TiO_2 and SiO_2 reproduce the titanium and silica distributions in the norites and quartz-gabbro of drill core 70011 in most details. The elemental distributions modeled for the lower zone appear to be "stretched" in the Main Mass along the vertical axis. The differentiation of a melt similar to the QRN parent could, therefore, be responsible for the formation of the lower part of the Main Mass including both norites and the quartz-gabbro. To test this hypothesis, we normalized the major element distributions, calculated for the whole Main Mass section at $F_{crit} = 60\%$, to the total relative thickness of both these "mafic" lithologies H = 823 m. The newly obtained modeled distributions are again compared with geochemical data for norites and gabbro of drill core 70011 in Figure 8.

Evolution of major element distributions. In the normalized height sections of Figure 8, the calculated concentrations of major element oxides match those in the natural rocks at the same height levels, except TiO_2, and Na_2O. The somewhat strange behavior of sodium could be related to the significant postimpact alteration, which is documented for the Main Mass by reopening of isotope systems (e.g., Deutsch, 1994), for example. But far more important are the calculated major element evolution trends in Figure 8, which are similar to those observed in the drill core. MgO reaches its maximum close to the contact with the Sublayer, whereas the highest FeO_{tot} and TiO_2 concentrations occur in the middle part of the quartz-gabbro. The decrease in CaO and Al_2O_3 is coupled with the increase in SiO_2 and K_2O toward the boundary with granophyres. Given the large number of geochemical analyses, and the relatively small number of variable parameters, this calculation reproduced the natural observations to a sufficient degree; this result is not a casual artifact of the model.

Calculated cumulative assemblages. An additional output of the COMAGMAT program allows the quantitative interpretation of the modeled major element distributions in terms of modal equlibrium phase occurrences. Figure 9 summarizes data for the calculated evolution of trapped melt temperature and volume, porosity F_m of the modeled cumulates, and the amount of "primarily accumulated" (Chalokwu et al., 1993) phases as result of efficient crystal settling.

Interpreting these data, the maximum MgO concentrations in the lower part of the modeled sequence are caused by accumulation of olivine crystals initially suspended in the parental QRN magma (Fig. 5; Table 4). Enrichment of FeO_{tot} and TiO_2 in the quartz-gabbro is correlated with the maximum of cumulative

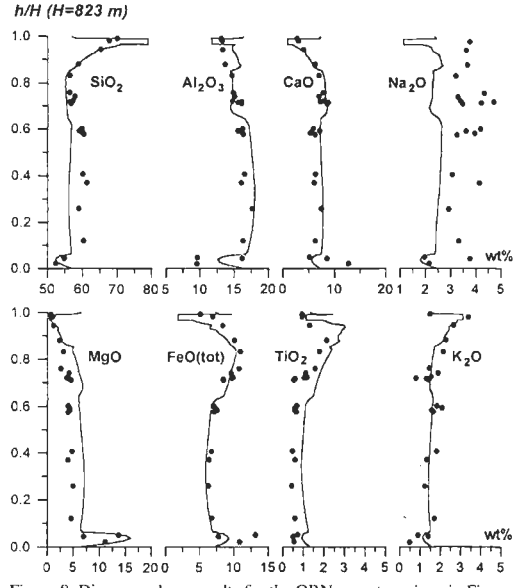

Figure 8. Diagrams show results for the QRN parent as given in Figure 7, but normalized to the total thickness of "mafic" rocks observed in the North Range (Ostermann and Deutsch, 1998). These plots demonstrate that the QRN parental magma is a plausible source for the observed upward sequence of rocks, from the mafic and quartz-rich norites to oxide gabbro.

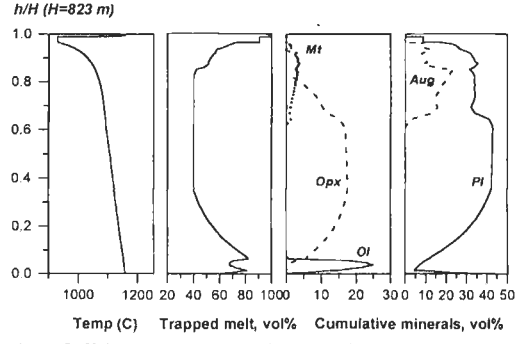

Figure 9. Height normalized distribution of the temperature of the trapped melt and "primarily accumulated" mineral phases (cumulates) in the rocks as result of crystal settling. Normalization for true thickness is for the North Range, drill core 70011, see text for further explanations. These data, coupled with the calculated liquid lines of descent, define all chemical features of modeled rocks shown in Figure 8 (Frenkel et al., 1989; Ariskin et al., 1993).

magnetite, a feature already described in detail (e.g., Naldrett and Hewins, 1984). The increase in CaO within the lowermost quartz-gabbro is due to the onset of high-Ca clinopyroxene crystallization. Cumulative plagioclase controls the behavior of Al_2O_3, whereas the increase in K_2O toward the boundary with the granophyre reflects the amount and composition of the trapped melt (Fig. 9). The behavior of SiO_2 is mainly controlled by primary phase proportions in the Opx + Pl and Aug + Mt + Pl cumulates. Enrichment in silica within the uppermost quartz-gabbro is caused by the abrupt decrease in the total amount of cumulative phases toward the boundary with the overlying granophyre (Fig. 9). The calculated compositions of the extreme differentiates duplicate the granophyre, which rest on the more "mafic" part of the Main Mass. Thus, the results shown in Figures 8 and 9 suggest the following:

1. A ferroandesitic melt compositionally similar to the QRN of Naldrett (1984) might be considered as the parent melt for the lower part of the Main Mass of the Sudbury melt system.

2. The convective-cumulative process (Frenkel et al., 1989) is a plausible physical mechanism to explain differentiation of this melt into the naturally observed sequence from mafic and quartz-rich norites to the quartz-gabbro with a small cap of silica-rich granophyres.

3. This lithologic sequence corresponds to the series of rocks consisting of accumulated crystals and trapped melt.

Undoubtedly, the quartz-gabbro belongs to the rock series, which differentiated from one single parent melt. The quartz-gabbro lithology, which certainly does not represent an "intermediate" magma, originated from mixing between impact-derived granophyres and endogenic norites (Chai and Eckstrand, 1993, 1994). The most important conclusion from points 1 to 3, however, is that differentiation of the ferroandesitic/QRN melt body cannot explain the huge mass of granophyres overlying the quartz-gabbro at present.

CONCLUSIONS

The results of modeling the Sudbury melt system with the COMAGMAT–3.5 program yield one important conclusion: If the Main Mass in its currently known (or estimated) volume evolved as a closed magmatic system, the observed volume ratio of 2:1 for granophyres to norites cannot be obtained by differentiation. This conclusion already has been drawn, based on petrologic-geologic (Masaitis, 1993; Warren et al., 1996) and geochemical data (Chai and Eckstrand, 1993, 1994). The latter authors, although based on a strongly biased data set, have argued for the existence of a batch of an "impact-triggered" endogenic magma overlain by a silica-rich impact melt, which finally resulted in formation of the Sudbury Main Mass. New detailed geochemical data for drill core 70011 (Ostermann, 1996), on the other hand, provide evidence for a continous evolution of trace element concentrations over the Main Mass (Fig. 10). The observed distribution patterns corresponds to those known for fractionally crystallized single parent melts

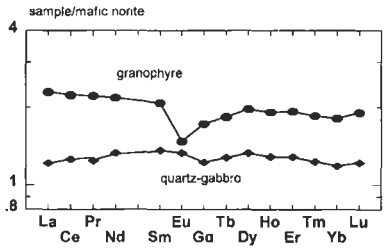

Figure 10. The average REE content of granophyre (black circles) and quartz-gabbro (black diamonds), normalized to the average content of mafic norite (data after Ostermann, 1996), indicate a close relation of the three major lithologies of the Main Mass.

(Ostermann and Deutsch, 1998). We purpose two different scenarios to solve this dilemma:

1. The ferroandesite QRN magma indeed represents the parent melt for the Main Mass, but the initial volume of the impact melt was much larger than the presently estimated volume of the Sudbury Igneous Complex. This postulate implies the existence of cumulative rocks enriched in mafic phases, such as olivine and orthopyroxene (Naldrett and Hewins, 1984), which are complementary to the observed volume of granophyres. Geophysical data do not totally exclude the presence of such cumulate layers at the bottom of the Sudbury melt system (B. Milkereit, personal communication).

2. The second, more speculative hypothesis focuses on the high initial temperature for the impact melt on the order of 2,000°C, and the high initial formation temperature of the overlying suevite layer, estimated at about 550°C (Ivanov et al., 1997; Ivanov and Deutsch, this volume). Due to these extreme conditions, melting of the already impact-melt rich breccias may have occurred. Such molten material could have been assimilated at a large scale by the underlying impact melt layer to form part of the granophyres. If such a process indeed took place, the smooth trends for all elements in the continuously analyzed drill core 70011 indicate a high efficiency in mixing between silica-rich differentiates of the impact melt body and the silica-rich melts, generated from the suevites during slow cooling of the underlying impact melt layer. In addition, we generally would not expect to see significant differences in trace element contents, as both the impact melt body and the breccias have, to a large degree, the same precursor lithologies.

Both scenarios deserve a careful study, and both may have contributed to this unique feature, which is known as the Sudbury melt system. Finally we observe that current understanding of the evolution of large-scale impact melts is still in its infancy. Moreover, kinetics and dynamics of assimilation and mixing at such high temperatures have not been studied in detail. We hope that thermophysical modeling (Ivanov et al., 1997; Ivanov and Deutsch, 1998) will provide more accurate

constraints to understand the evolution of the Sudbury impact melt in greater detail.

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