New computer program TecD for tectonomagmatic
discrimination from discriminant function diagrams for basic and
ultrabasic magmas and its application to ancient rocks

Nuevo programa informático TecD para la discriminación
tectonomagmática basada en diagramas de funciones discriminantes
para magmas básicos y ultrabásicos y su aplicación a rocas antiguas

S. P. Verma1*, M. A. Rivera-Gómez2

1Departamento de Sistemas Energéticos, Instituto de Energías Renovables, Universidad Nacional Autónoma de México, Privada Xochicalco s/no., Centro, Apartado Postal 34, Temixco, Mor., 62580, Mexico. spv@ier.unam.mx

2Posgrado en Ingeniería, Instituto de Energías Renovables, Universidad Nacional Autónoma de México, Privada Xochicalco s/no., Centro, Apartado Postal 34, Temixco, Mor., 62580, Mexico. marig@ier.unam.mx

*corresponding author

Received: 20/01/2011 / Accepted: 12/04/2013

Abstract

Due to the unavailability of suitable software, a new computer program TecD (Tectonomagmatic Discrimination) was written in Visual Basic for using four sets of new discriminant function based diagrams published during 2004-2011. This bilingual (both in English and Spanish) program evaluates igneous rock geochemistry data in 20 different multi-dimensional diagrams (4 sets of 5 diagrams each), automatically counts the number of samples plotting in different tectonic fields, computes success rates (%) for a given area or set of rock samples, provides scalable vector diagrams that can be opened and modified in different commercial software, and presents a synthesis of this application in a final report. Three examples are presented to highlight the use of TecD. Ocean island setting is inferred for ~56 Ma basic rocks from Faroe Islands (Atlantic Ocean), mid-ocean ridge for ~2700 Ma Archean Abitibi greenstone belt (Canada), and arc setting for ~2950 Ma Mallina basin (Australia). Additional criteria for the interpretation of these diagrams are also briefly discussed.

Keywords: tectonomagmatic discrimination diagrams, linear discriminant analysis, discordancy tests, arc, rift, ocean-island, mid-ocean ridge

Resumen

Devido a falta de software adecuado, se ha creado un nuevo programa informático TecD (Discriminación Tectonomagmática) en Visual Basic para usar cuatro conjuntos de nuevos diagramas basados en funciones discriminantes que han sido publicados entre 2004 y 2011. Este programa bilingüe (en inglés y español) evalúa los datos geoquímicos de rocas ígneas en 20 diagramas multidimensionales diferentes (4 conjuntos de 5 diagramas cada uno), cuenta automáticamente el número de muestras graficadas en diferentes campos tectónicos, calcula las tasas de éxito (%) para un área dada o para un conjunto de muestras de rocas, proporciona diagramas vectoriales escalables que pueden ser abiertos y modificados en muchos paquetes comerciales y presenta una síntesis de
1. Introduction

Tectonomagmatic discrimination diagrams have been in use in igneous petrology almost since the advent of plate tectonics theory (Rollinson, 1993; Verma, 2010). The first diagrams for igneous rocks were proposed by Pearce and Cann (1971, 1973) and since then there have been many proposals (e.g., Wood, 1980; Shervais, 1982; Pearce et al., 1984; Cabanis and Lecolle, 1989; Vasconcelos-F. et al., 1998, 2001). Recently, Verma (2010) extensively evaluated a large number of such diagrams and inferred that those proposed recently (during 2004-2011) show the highest success rates (%) that vary from 76% to 96% for Agrawal et al. (2004), 83% to 97% for Verma et al. (2006), 79% to 96% for Agrawal et al. (2008), and 78% to 93% for Verma and Agrawal (2011). Satisfactory functioning of these diagrams was also confirmed by Sheth (2008) and Verma et al. (2011). Except for the first set (Agrawal et al., 2004), which was obtained from linear discriminant analysis (LDA) of adjusted major-element concentrations from SINCLAS computer program (Verma et al., 2002), these diagrams are based on LDA of natural logarithm-transformed element ratios. Because of complex arithmetical calculations involved, their use is likely to be cumbersome and less frequent as compared to simple bivariate or ternary diagrams. All these simple diagrams are, however, plagued by incoherent statistical treatment of compositional data; besides, the tectonic field boundaries in them were drawn by eye (e.g., Aitchison, 1986; Agrawal, 1999; Aitchison et al., 2000; Thomas and Aitchison, 2005; Agrawal and Verma, 2007; Verma, 2010; Verma et al., 2010). Similarly, deficiencies in several existing discrimination diagrams for sedimentary rocks have also been documented (Armstrong-Altrin and Verma, 2005). From this discussion, it is clear that only the new discriminant function based, multi-dimensional diagrams obtained from LDA comply with all statistical requirements and provide satisfactory answers to the need of tectonic discrimination.

Nevertheless, for such newer diagrams, complex discriminant functions must be computed before the data can be plotted in these new sets of 20 diagrams (Agrawal et al., 2004, 2008; Verma et al., 2006; Verma and Agrawal, 2011), and tectonic inferences have to be achieved through tedious counting of samples plotting in different fields and later calculations of success rates in terms of “correctly” classified percentages. Therefore, a suitable computer program could be helpful for an efficient use of such discriminant function based diagrams.

We present a new program TecD (Tectonic Discrimination) that enabled us to apply all four sets of five new diagrams for each set (a total of 20 diagrams) to three areas (Faroe Islands in the Atlantic Ocean, Abitibi greenstone belt in Canada, and Mallina basin in Australia). This program will be available to any interested user from request to anyone of the authors (spv@ier.unam.mx or marig@ier.unam.mx).
2. Computer program

TecD was written in VisualBasic (VB.NET). A simplified flow diagram is shown in Figure 1. Basically, a series of options, such as the language, adjusted silica range, and all four sets, or only some sets of diagrams, must first be examined, and a proper selection should be made if the user does not want to process the samples under the default option. The data can be input in an Excel or Statistica file. The program validates the file for possible typographical and other types of errors such as missing variable names or incomplete data. An error-free file is obligatory for using the diagrams, although for a file with incomplete data a suitable selection of diagrams would help. The user can then process the file for different sets of discrimination diagrams (Fig. 1) and save the results as “res” file (all results) or “rep” file (synthesis of results including information on success rates), or both files. The user also has the option to process and save scalable graphics, which can be opened and edited in other conventional software. More details on the functioning and use of TecD in README document (in English as well as Spanish) will be available from the authors.

The rocks from four tectonic settings that can be discriminated from these new sets of diagrams are as follows: IAB (island arc basic rocks) numbered as group 1, CRB (continental rift basic rocks) as group 2, OIB (ocean-island basic rocks) as group 3, and MORB (mid-ocean ridge basic rocks) as group 4.

A total of 40 equations were programmed in TecD. These are presented according to the papers published in the time sequence from 2004 to 2011 (ADJ in these equations refers to the adjusted data from SINCLAS (Verma et al., 2002) or IgRoCS (Verma and Rivera-Gómez, 2013) computer program; the major oxide symbols refer to oxide concentrations in weight % or % m/m units, e.g., SiO$_2$ stands for SiO$_2$ concentration, i.e., general names, rather than the standardised chemical symbols, were used in these equations; the symbol * is used to show the multiplication operation; function ln stands for natural logarithm; the subscripts m1, m2, t1, and t2 refer, respectively, to the first and second sets of major-element and trace- or immobile element based diagrams).

For Agrawal et al. (2004) the equations are as follows. Note these equations use natural logarithm (ln)-transformed ratios of major oxides using SiO$_2$ as the common denominator for all ratios. Although adjusted data from SINCLAS (Verma et al., 2002) provide essentially the same results, they are certainly useful for ascertaining the basic or ultrabasic nature of magmas before their use in discrimination diagrams. We encourage people to use these (and more recent) diagrams only for such basic and ultrabasic magmas as those inferred from SINCLAS.

\[
\begin{align*}
DF_{1}(IAB-CRB-OIB)_{m1} &= (0.251*SiO2_{ADJ}) + (2.034*TiO2_{ADJ}) - (0.109*Al2O3_{ADJ}) + (0.573*FeO_{ADJ}) - (0.032*FeO_{ADJ}) - (2.877*Mno_{ADJ}) + (0.256*CaO_{ADJ}) + (0.322*Na2O_{ADJ}) - (0.229*K2O_{ADJ}) - 18.974 \\
DF_{2}(IAB-CRB-OIB)_{m2} &= (2.159*SiO2_{ADJ}) + (2.711*TiO2_{ADJ}) + (1.792*Al2O3_{ADJ}) + (2.295*FeO_{ADJ}) + (1.484*FeO_{ADJ}) + (8.594*Mno_{ADJ}) + (1.896*CaO_{ADJ}) + (2.158*Na2O_{ADJ}) + (1.201*Na2O_{ADJ}) + (1.763*K2O_{ADJ}) - 200.276 \\
DF_{1}(IAB-CRB-MORB)_{m1} &= (0.435*SiO2_{ADJ}) - (1.392*TiO2_{ADJ}) + (0.183*Al2O3_{ADJ}) + (0.184*FeO_{ADJ}) - (7.698*Mno_{ADJ}) + (0.021*Mgo_{ADJ}) + (0.389*CaO_{ADJ}) + (0.036*Na2O_{ADJ}) + (0.462*K2O_{ADJ}) - (1.192*P2O5_{ADJ}) - 29.435 \\
DF_{2}(IAB-CRB-MORB)_{m2} &= (0.601*SiO2_{ADJ}) - (0.335*TiO2_{ADJ}) + (1.332*Al2O3_{ADJ}) + (1.449*FeO_{ADJ}) + (0.756*Mno_{ADJ}) + (0.893*Mgo_{ADJ}) + (0.448*CaO_{ADJ}) + (0.525*Na2O_{ADJ}) + (1.734*K2O_{ADJ}) + (2.494*P2O5_{ADJ}) - 78.236 \\
DF_{1}(IAB-OIB-MORB)_{m1} &= (2.126*SiO2_{ADJ}) + (4.166*TiO2_{ADJ}) + (1.856*Al2O3_{ADJ}) + (3.522*FeO_{ADJ}) + (0.596*FeO_{ADJ}) - (3.930*Mno_{ADJ}) + (1.334*CaO_{ADJ}) + (1.085*CaO_{ADJ}) + (0.416*Na2O_{ADJ}) + (0.827*K2O_{ADJ}) - 119.050 \\
DF_{2}(IAB-OIB-MORB)_{m2} &= (1.384*SiO2_{ADJ}) + (1.091*TiO2_{ADJ}) + (0.908*Al2O3_{ADJ}) + (2.419*FeO_{ADJ}) + (0.363*FeO_{ADJ}) - (0.886*FeO_{ADJ}) + (5.281*Mno_{ADJ}) + (1.269*Mgo_{ADJ}) + (1.790*CaO_{ADJ}) + (2.572*Na2O_{ADJ}) + (1.138*K2O_{ADJ}) - 134.295 \\
DF_{1}(CRB-OIB-MORB)_{m1} &= (0.310*SiO2_{ADJ}) + (1.956*Al2O3_{ADJ}) + (0.341*Al2O3_{ADJ}) + (1.760*FeO_{ADJ}) + (0.351*FeO_{ADJ}) - (11.315*Na2O_{ADJ}) + (3.930*Na2O_{ADJ}) + (0.526*Mgo_{ADJ}) + (0.084*CaO_{ADJ}) + (0.312*K2O_{ADJ}) + (1.892*P2O5_{ADJ}) - 32.909 \\
DF_{2}(CRB-OIB-MORB)_{m2} &= (0.703*SiO2_{ADJ}) + (2.454*TiO2_{ADJ}) + (0.233*Al2O3_{ADJ}) + (1.943*FeO_{ADJ}) + (0.182*FeO_{ADJ}) - (2.421*Na2O_{ADJ}) + (0.618*Mgo_{ADJ}) + (0.712*CaO_{ADJ}) - (0.866*CaO_{ADJ}) - (1.180*P2O5_{ADJ}) - 56.455
\end{align*}
\]

For Verma et al. (2006) the equations are as follows. Note these equations use natural logarithm (ln)-transformed ratios of major oxides using SiO$_2$ as the common denominator for all ratios. Although adjusted data from SINCLAS (Verma et al., 2002) provide essentially the same results, they are certainly useful for ascertaining the basic or ultrabasic nature of magmas before their use in discrimination diagrams. We encourage people to use these (and more recent) diagrams only for such basic and ultrabasic magmas as those inferred from SINCLAS.

\[
\begin{align*}
DF_{1}(IAB-CRB-MORB)_{m1} &= 4.6761*ln(TiO2/SiO2) + 2.5330*ln(Al2O3/SiO2) - 0.3884*ln(FeO_{2}/SiO2) + 3.9988*ln(FeO_{2}/SiO2) + 0.8580*ln(MnO/SiO2) - 0.5852*ln(MgO/SiO2) - 0.2086*ln(CaO/SiO2) - 0.2704*ln(Na2O/SiO2) + 1.0810*ln(K2O/SiO2) + 0.1845*ln(P2O5/SiO2) - 1.5445 \\
DF_{2}(IAB-CRB-MORB)_{m2} &= 4.5059*ln(Al2O3/SiO2) + 2.0897*ln(FeO_{2}/SiO2) + 0.8514*ln(FeO_{2}/SiO2) - 0.4334*ln(MnO/SiO2) + 1.4832*ln(MgO/SiO2) + 2.3627*ln(CaO/SiO2) - 1.6558*ln(Na2O/SiO2) + 0.6757*ln(K2O/SiO2) + 0.4130*ln(P2O5/SiO2) + 13.1639 \\
DF_{1}(CRB-OIB-MORB)_{m1} &= 3.9998*ln(TiO2/SiO2) - 2.2385*ln(Al2O3/SiO2) + 0.8110*ln(FeO_{2}/SiO2) - 2.5865*ln(FeO_{2}/SiO2) - 1.2433*ln(MnO/SiO2) + 0.2897*ln(FeO_{2}/SiO2) + 1.046*ln(MgO/SiO2) + 1.0100*ln(CaO/SiO2) + 0.4802*ln(Na2O/SiO2) - 0.5269*ln(K2O/SiO2) + 0.1839*ln(P2O5/SiO2) - 0.6839
\end{align*}
\]
For Agrawal et al. (2008) the equations are as follows. Note these equations use natural logarithm (ln)-transformed ratios of relatively immobile trace elements using Th as the common denominator for all ratios. Therefore, in the data file to be processed TiO₂ must be input in wt. % as a major element. Also as in Agrawal et al. (2008), the first diagram in this set discriminates the combined setting of CRB and OIB from IAB and MORB. Greater precision is used in these coefficients, because for this set of diagrams the authors have also published probability calculations of individual samples, and the use of higher precision here helps to achieve greater accuracy in these probability estimates. Finally, the prior processing of data in SINCLAS computer program (Verma et al., 2002) is essential for ascertaining the basic or ultrabasic nature of magmas and converting the measured TiO₂ into TIO₂ADJ. Similarly, the log-transformed ratio variables must also be processed in DODESSYS program (Verma and Díaz-González, 2012; DODESSYS uses the precise and accurate critical values of Verma et al. (2008) for discordancy tests; Barnett and Lewis, 1994) to comply with the probability estimates. Finally, the prior processing of data in SINCLAS computer program (Verma et al., 2002) is essential for ascertaining the basic or ultrabasic nature of magmas before their use in discrimination diagrams.

DF1(IAB-CRB+OIB-MORB)ₜ₁ = -0.3518*ln(La/Th) + 0.6013*ln(Sm/Th) - 1.3450*ln(Yb/Th) + 2.1056*ln(Nb/Th) - 5.4763 (21)

DF2(IAB-CRB+OIB-MORB)ₜ₁ = -0.5035*ln(La/Th) - 1.1689*ln(Yb/Th) + 1.2267*ln(Nb/Th) - 0.9944 (22)

DF1(IAB-CRB-OIB-MORB)ₜ₂ = 0.5553*ln(La/Th) + 0.2173*ln(Sm/Th) - 0.9699*ln(Yb/Th) + 2.0454*ln(Nb/Th) - 5.6305 (23)

DF2(IAB-CRB-OIB-MORB)ₜ₂ = -2.4498*ln(La/Th) + 4.8562*ln(Sm/Th) - 2.1240*ln(Yb/Th) - 0.1567*ln(Nb/Th) + 0.94 (24)

DF1(IAB-CRB-MORB)ₜ₂ = -0.3305*ln(La/Th) + 0.3484*ln(Sm/Th) - 0.9562*ln(Yb/Th) + 2.0777*ln(Nb/Th) - 4.5628 (25)

DF2(IAB-CRB-MORB)ₜ₂ = -0.1928*ln(La/Th) - 1.1989*ln(Sm/Th) + 1.7531*ln(Yb/Th) + 0.6607*ln(Nb/Th) - 0.4384 (26)

DF1(IAB-OIB-MORB)ₜ₂ = -0.5558*ln(La/Th) + 1.4262*ln(Sm/Th) + 2.2935*ln(Yb/Th) - 0.689*ln(Nb/Th) + 4.1422 (27)

DF2(IAB-OIB-MORB)ₜ₂ = -0.9207*ln(La/Th) + 3.652*ln(Sm/Th) - 1.9866*ln(Yb/Th) + 1.0574*ln(Nb/Th) - 4.4283 (30)

DF1(CRB-OIB-MORB)ₜ₂ = -0.5183*ln(La/Th) + 4.9886*ln(Sm/Th) - 0.0111*ln(Yb/Th) + 1.9426*ln(Nb/Th) + 2.2204*ln(Yb/Th) + 5.0825*ln(Nb/Th) + 5.7755 (17)

DF2(CRB-OIB-MORB)ₜ₂ = -0.7655*ln(La/Th) + 2.7737*ln(Sm/Th) - 0.1341*ln(Yb/Th) + 0.6672*ln(Nb/Th) + 0.8889*ln(Nb/Th) + 0.2225*ln(Yb/Th) + 0.5056 (16)

DF1(IAB-OIB-MORB)ₜ₂ = -0.5509*ln(La/Th) + 0.9471*ln(Sm/Th) - 0.1082*ln(Yb/Th) + 0.9471*ln(Nb/Th) - 1.0182*ln(Yb/Th) - 5.4984 (18)

DF2(IAB-OIB-MORB)ₜ₂ = -0.5509*ln(La/Th) + 1.0464*ln(Sm/Th) - 3.4849*ln(Yb/Th) + 0.5528*ln(Nb/Th) + 0.2025*ln(Nb/Th) + 1.2104*ln(Yb/Th) - 5.0825*ln(Nb/Th) + 2.8877 (20)

Finally, for Verma and Agrawal (2011) diagrams, the equations are reported as follows. Note these equations also use natural logarithm (ln)-transformed ratios of relatively immobile major and trace elements using TIO₂ADJ (expressed in µg g⁻¹ units rather than wt. % or % m/m, but this change of units is internally executed in TecD) as the common denominator for all ratios. Therefore, in the data file to be processed TiO₂ must be input in wt. % as a major element. Also as in Agrawal et al. (2008), the first diagram in this set discriminates the combined setting of CRB and OIB from IAB and MORB.

DF1(IAB-CRB+MORB-MORB)ₜ₁ = -0.66107*ln(Nb/TIO₂ADJ) + 2.92926*ln(V/TIO₂ADJ) + 4.9886*ln(Sm/TIO₂ADJ) + 1.9426*ln(Nb/TIO₂ADJ) + 2.2204*ln(Yb/TIO₂ADJ) + 0.9471*ln(Nb/TIO₂ADJ) + 0.8889*ln(Yb/TIO₂ADJ) + 0.2225*ln(Nb/TIO₂ADJ) + 13.2625 (19)

DF2(IAB-CRB+MORB-MORB)ₜ₁ = 5.0059*ln(La/TIO₂ADJ) - 0.1082*ln(Yb/TIO₂ADJ) + 1.0182*ln(Yb/TIO₂ADJ) + 0.9471*ln(Nb/TIO₂ADJ) + 0.9471*ln(Nb/TIO₂ADJ) - 0.1082*ln(Yb/TIO₂ADJ) + 7.4984*ln(Nb/TIO₂ADJ) + 2.8877 (20)

DF1(IAB-CRB-MORB-MORB)ₜ₂ = -0.66107*ln(Nb/TIO₂ADJ) + 2.92926*ln(V/TIO₂ADJ) + 4.9886*ln(Sm/TIO₂ADJ) + 1.9426*ln(Nb/TIO₂ADJ) + 2.2204*ln(Yb/TIO₂ADJ) + 0.9471*ln(Nb/TIO₂ADJ) + 0.8889*ln(Yb/TIO₂ADJ) + 0.2225*ln(Nb/TIO₂ADJ) + 13.2625 (19)

DF2(IAB-CRB-MORB-MORB)ₜ₂ = 5.0059*ln(La/TIO₂ADJ) - 0.1082*ln(Yb/TIO₂ADJ) + 1.0182*ln(Yb/TIO₂ADJ) + 0.9471*ln(Nb/TIO₂ADJ) + 0.9471*ln(Nb/TIO₂ADJ) - 0.1082*ln(Yb/TIO₂ADJ) + 7.4984*ln(Nb/TIO₂ADJ) + 2.8877 (20)

DF1(IAB-OIB-MORB-MORB)ₜ₂ = -0.614599*ln(Nb/TIO₂ADJ) + 2.2935*ln(Yb/TIO₂ADJ) + 0.689*ln(Nb/TIO₂ADJ) + 4.1422 (29)

DF2(IAB-OIB-MORB-MORB)ₜ₂ = -0.9207*ln(La/Th) + 3.652*ln(Sm/Th) - 1.9866*ln(Yb/Th) + 1.0574*ln(Nb/Th) - 4.4283 (30)
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Table 2. Synthesis of inferred tectonic setting results for the three examples presented in this work.

Tabla 2. Síntesis de los resultados de los ambientes tectónicos inferidos para los tres ejemplos presentados en este trabajo.

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AGV2004—Agrawal et al. (2004); VGA2006—Verma et al. (2006); AGV2008—Agrawal et al. (2008); VA2011—Verma and Agrawal (2011); Figure code refers to TecD program. The tectonic groups are numbered as follows: IAB=1, CRB=2, OIB=3, MORB=4. For Faroe Islands and Abitibi greenstone belt, one discordant outlier was observed in each case as judged by DODESSYS computer program (Verma and Díaz-González, 2012), also note Verma and Agrawal (2011) diagrams require the log-transformed ratios be normally distributed. For Mallina basin (Australia), both basic and intermediate type of rocks (6 and 5 samples, respectively) provide consistent results and no discordant outliers were detected.
The coordinates of probability-based boundaries were provided in the original papers (Agrawal et al., 2004, 2008; Verma et al., 2006; Verma and Agrawal, 2011; also see Verma, 2010). To correctly locate the tectonic field in which a given “unknown” sample will plot, it became necessary to accurately calculate each of the boundary equations as done earlier by Verma et al. (2002) for classi-
Fig. 3.- The five major-element based diagrams of Verma et al. (2006) for the tectonic discrimination of basic and ultrabasic rocks from four tectonic settings (island arc–IAB; continental rift–CRB; ocean island–OIB; and mid-ocean ridge–MORB). The samples plotted are from the Faroe Islands (north Atlantic) and Mallina basin (Australia). DF1 and DF2 are the two discriminant functions obtained from linear discriminant analysis (LDA), and the subscript \(_{m2}\) refers to the second LDA diagram set based on major-element data. Symbols used are shown as an inset in the first diagram. For Mallina both basic and intermediate rocks were plotted. a) discrimination of IAB, CRB, OIB, and MORB; b) discrimination of IAB, CRB, and OIB; c) discrimination of IAB, CRB, and MORB; d) discrimination of IAB, OIB, and MORB; and e) discrimination of CRB, OIB, and MORB.

Fig. 3.- Los cinco diagramas de Verma et al. (2006) basados en elementos mayores, para la discriminación tectónica de rocas básicas y ultrabásicas provenientes de cuatro ambientes tectónicos (arco isla–IAB; rift continental–CRB; isla oceánica–OIB; y dorsal oceánica–MORB). Las muestras graficadas son de las Islas de Faroe (Atlántico norte) y la cuenca de Mallina (Australia). DF1 y DF2 son las dos funciones discriminantes obtenidas del análisis discriminante lineal (LDA), y el subíndice \(_{m2}\) se refiere al segundo conjunto de diagramas por LDA, basados en los datos de elementos mayores. Los símbolos usados se muestran en el primer diagrama. Para Mallina ambos tipos de rocas, tanto básicas como intermedias, fueron graficados. a) la discriminación de los cuatro ambientes de IAB, CRB, OIB y MORB; b) la discriminación de tres ambientes de IAB, CRB, OIB y MORB; c) la discriminación de tres ambientes de IAB, CRB y OIB; d) la discriminación de tres ambientes de IAB, OIB y MORB; la discriminación de tres ambientes de CRB, OIB y MORB.

Classifying samples in the TAS diagram. In the DF1-DF2 plots, the equations of the type \(DF2 = m \times DF1 + b\); where \(m\) is the slope, \(b\) is the intercept of the corresponding boundary line, and the symbol \(*\) stands for multiplication are summarised in Table 1 for all dividing boundaries.

For a given plot, TecD compares the coordinates of an unknown sample with these respective reference boundaries, and decides the exact field in which that sample would plot. Thus, for a given file and a given diagram, all “valid” samples are individually counted and a synthesis is prepared in a report file. TecD thus facilitates an efficient and unequivocal use of all 20 (or less depending on the option used) diagrams for a given geological area. A final report is prepared and provided to the user for helping with the interpretation.

3. Applications

Three application examples of TecD are presented for (i) basic rock samples from the Faroe Islands (Atlantic Ocean), (ii) basic and ultrabasic samples from the Abitibi greenstone belt (Canada), and (iii) basic and intermediate rocks from the Mallina basin (Australia).

The data are plotted in figures 2-5 and the results from TecD program are summarised in Table 2. We also clarify that although TecD always calculates the success rates in percent (% success rates), we recommend to report only the number of samples plotting in each field when the
total number of samples is small, arbitrarily less than 20
(or any other number that the user may decide).

3.1. Paleogene Faroe Islands plateau basalts

Søager and Holm (2009) presented new analytical data for 13 high-Ti basalts from the top of the lava pile that was formed presumably by the time of break-up of the North Atlantic about 56–55 Ma ago. These samples were from Faroe Islands located on the eastern continental margin of the Atlantic Ocean. Three of the four sets of tectonic discrimination diagrams (except Agrawal et al. (2008), for which complete data were not available) were applied through TecD for inferring tectonic setting of these lavas.

This application will be described in greater detail than the other two presented in this work. The first diagram (Fig. 1234m1 of AGV2004 in Table 2; Fig. 2a) of Agrawal et al. (2004) shows for this area that out of 13 samples of basic and ultrabasic rocks, 10 samples plot in the OIB field, 1 in CRB and 2 in MORB. This diagram, therefore, suggests an OIB setting for the Faroe Islands. The second diagram (Fig. 123m1 of AGV2004 in Table 2; Fig. 2b) confirms these results of OIB setting, because 11 out of 13 samples plot in this field. The third diagram (Fig. 124m1 of AGV2004 in Table 2; Fig. 2c) is suggested as “inapplicable” diagram, because the OIB field (field no. 3) is absent from it. The fourth diagram (Fig. 134m1 of AGV2004 in Table 2; Fig. 2d) shows once again that
a large number of samples (11 out of 13) plot in the OIB field. Finally, the fifth diagram (Fig_234m1 of AGV2004 in Table 2; Fig. 2e) also shows 10 out of 13 samples in the OIB field. Thus, all four applicable diagrams (remember one of the five diagrams will generally be inapplicable) show a consistent result, viz., most samples plot in the OIB field. Therefore, we conclude that Agrawal et al. (2004) diagrams suggest an OIB setting for the Faroe Islands.

TecD was also used for the application of Verma et al. (2006) major-element based diagrams, which also provided the same results, viz., most samples (12 or 13 out of 13) plot in the OIB field (Table 2 and Fig. 3a-e).

The set of diagrams by Agrawal et al. (2008) could not be used for Faroe Islands because of the lack of complete data set (see figure 4a-e, in which samples from Faroe Islands are absent).

The application of Verma and Agrawal (2011) diagrams (VA2011 in Table 2; Fig. 5a-e) also gave a consistent result. The first diagram discriminates combined field of CRB and OIB (called “within plate” by many authors; see Verma, 2010), in which an indication of CRB+OIB field was clearly observed. The other three applicable diagrams (Table 2 and Fig. 5b, d, e) also suggest an OIB setting.
The correct use of Verma and Agrawal (2011) diagrams requires that the log-transformed ratios be normally distributed. We achieved this through the use of DODESSYS (Verma and Diaz-González, 2012) by applying all single-outlier type tests (Barnett and Lewis, 1994; Verma, 1997, 2005; Verma et al., 2009) to log-transformed ratios used in LDA by Verma and Agrawal (2011). We emphasize that discordancy tests should be applied to log-ratios and not to crude compositional data; see Verma (2012) for geochromometric reasons. Only one discordant outlier was obtained, which is plotted by filled diamond symbol in figure 5a-e. This particular sample generally plotted in a field different from the remaining samples, the latter suggested an OIB setting for Faroe Islands.

Clearly, an OIB setting is obtained for Faroe Islands. In this case, all four sets of diagrams provided consistent results.

3.2. Archaean Abitibi greenstone belt, Canada

Lahaye et al. (1995) presented geochemical data on basic and ultrabasic rocks from the ca. 2700 Ma Abitibi greenstone belt of Ontario, Canada. Major-element data for these samples from Alexo and Texmont areas are incomplete with non-zero Na2O reported for only three samples from Alexo and Texmont areas are for these samples from Alexo and Texmont areas are incomplete with non-zero Na2O reported for only three samples from Alexo and Texmont areas are incomplete with non-zero Na2O reported for only three samples from Alexo and Texmont areas are incomplete with non-zero Na2O reported for only three samples from Alexo and Texmont areas are incomplete with non-zero Na2O reported for only three samples from Alexo and Texmont areas are incomplete with non-zero Na2O reported for only three samples from Alexo and Texmont areas are incomplete with non-zero Na2O reported for only three samples from Alexo and Texmont areas are incomplete with non-zero Na2O reported for only three samples from Alexo and Texmont areas are incomplete with non-zero Na2O reported for only three samples from Alexo and Texmont areas are incomplete with non-zero Na2O reported for only three samples from Alexo and Texmont areas are incomplete with non-zero Na2O reported for only three samples. Interestingly, none of these 18 samples proved to be boninite according to the IUGS (International Union of Geological Sciences) scheme of classification (see SINCLAS computer program by Verma et al., 2002). The immobile element based diagrams of Agrawal et al. (2008) also indicated MORB setting for 11 samples of basic and ultrabasic rocks of Kerrich et al. (1998), although the diagrams of Verma and Agrawal (2011) suggested an arc setting (plots not shown) for four basic and ultrabasic rock samples with complete major and trace element data.

3.3. Mallina basin, Australia

Smithies (2002) reported the so-called boninite-like rocks from the ca. 3010-2935 Ma Mallina basin in the central part of the Pilbara craton (ca. 3120-3115 Ma), northwest Australia. During this long time span (3120-2935 Ma), both arc and rift settings have been suggested for this area. Smithies (2002) reported major- and trace-element data for 6 boninite-like rocks and 5 melanogabbro rocks.

We used TecD to evaluate the tectonic setting of 11 analyses (6 basic and 5 intermediate rock samples, according to the TAS diagram) reported by Smithies (2002). All sets of diagrams (Figs. 2-5) based on major- or trace-elements give consistently an arc setting for these samples (Table 2). With the exception of Agrawal et al. (2004) in which 8-11 samples plot in the IAB field, all sets of diagrams show that all 11 samples (both basic and intermediate types) consistently plot in the IAB setting. No discordant outliers were detected for this dataset. The results remain exactly the same for Verma and Agrawal (2011) diagrams.

Therefore, an arc setting can be inferred for the Mallina basin.

4. Final considerations

Even though the older binary, ternary and discriminant function based diagrams were not included in TecD because of the deficient statistical handling of compositional data, the newer four sets of five diagrams for each set (a total of 20 diagrams) for basic and ultrabasic magmas (Agrawal et al., 2004, 2008; Verma et al., 2006; Verma and Agrawal, 2011) may be considered too many for ap-
application to any given area. Nevertheless, when the results of all four sets of diagrams are consistent, there is no problem in the tectonic interpretation based on discrimination diagrams. However, that all four sets provide consistent results might be an exception rather than the rule. We summarise here some guidelines for making decisions in the case of likely inconsistencies (see also Verma et al., 2010). More definitive recommendations for the use of TecD may have to await additional computational work based on Monte Carlo simulations (for more details on Monte Carlo, see Verma, 2012).

Sometimes, complete data may not be available for all sets of diagrams to be applied for a given study area. The interpretation in such cases will be limited to the applicable set(s) of diagrams. If one is dealing with relatively old or altered rocks, the two sets of immobile element based diagrams (Agrawal et al., 2008; Verma and Agrawal, 2011) will have to be preferred in comparison to the major-element based diagrams (Agrawal et al., 2004; Verma et al., 2006). On the other hand, for relatively fresh rocks, the diagrams based on major-elements (Agrawal et al., 2004; Verma et al., 2006) will probably be preferable because these elements can generally be determined with less analytical errors than the trace-elements. If the two sets of major-element based diagrams provide inconsistent results, the newer set by Verma et al. (2006) is then preferable, because these diagrams are based on the correct statistical treatment of compositional data. If, on the contrary, the immobile-element based diagrams are mutually inconsistent, there is no simple answer at present, although probably the newer (Verma and Agrawal, 2011) diagrams might be preferable because this set complies additionally with the LDA requirements of normally distributed log-transformed ratio variables used for constructing them. It is also important that this condition be also fulfilled for the application samples, which can be easily achieved from DODESSYS (Verma and Diaz-González, 2012) or UDASYS software (Verma et al., 2013).

Finally, newer diagrams currently under preparation for acid and intermediate magmas should also be applied whenever possible for reaching at the final conclusion from geochemical tectonomagmatic discrimination tools.

Acknowledgements

The second author (M.A. Rivera-Gómez) is grateful to Conacyt for the fellowship for Master’s studies under the guidance of the first author (S.P. Verma). K. Pandarinath and Sanjeeet K. Verma are thanked for using the preliminary versions of TecD and providing suggestions for its improvement. We are also thankful to Alfredo Quiroz-Ruiz for continuous support and maintenance of our computing facilities essential for the development of our work. We are also much grateful to Prof. Rajesh K. Srivastava and an anonymous reviewer, both of whom greatly appreciated our work and recommended the publication of earlier manuscript in its present form, although we still tried to further improve our presentation through minor corrections of our original manuscript.

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