11. Referências bibliográficas.

ANTON, H; RORRES, C. **Elementary linear algebra**. New York: John Willey e Sons, 1994.

ATKINS, W. P. **Physical chemistry**. New York: W. H. Freeman and Company, 1994.

AVILLEZ, R. R.; ALTSTETTER, C. J. **Modeling oxygen activities in ternary solid solutions: niobium-vanadium-oxygen system**. Acta Metall., vol. 30, p. 1613-1617, 1992.

AZMOV, S. A., et. al., L. M. Izv. Akad. Nauk SSSR, Neorg. Mater., vol. 20, p. 469-471, 1984.

BAN-YA, S.; CHIBA, A.; HIKOSAKA, A., Tetsu-to-Hagané, vol. 66, p. 1484-1493, 1980.

BARIN, I. **Thermochemical data of pure substances**. Weinheim: VCH, 1989.

BARIN, I.; KNACKE, O.; KUBASCHEWSKI, O. **Thermochemical properties of inorganic substances**. Berlin: Springer-Verlag, 1977.

BERMAN, R. G.; BROWN, T. H. Contrib. Mineral. Petrol., vol. 89, p. 168-183, 1985.

BLANDER, M. e PELTON, A. D. **Thermodynamic analysis liquid silicates and prediction of ternary solution properties by modified quasi-chemical equations**. Geochimica et Cosmochimica Acta, vol. 51, p. 85-95, 1987.

BYUNG-CHUL, L.; DANNER, R. P. **Application of the group-contribution lattice-fluid equation of state to random copolymer-solvent systems**. Fluid Phase Equilibria, vol. 117, p. 33-39, 1996.

COUGHANOUR, L. W.; DEPROSSE, V. A., J. Research Natl. Bur. Standards, vol. 51, p. 87, 1953.

COUGHLIN, J. P. Bull. U. S. Bureau of Mines, vol. 542, 1954.

CHASE, M. W., et al. **JANAF thermochemical Tables, J. phys. chem. ref. data**. 3^{rd} ed., vol. 14, no.1, 1985.

CHASE, M. W. et al. **Thermodynamic models and data for pure elements and other end-members of solutions**. Calphad, vol. 19, no. 4, p. 437-447, 1995.

DARKEN, L. S.; GURRY, R. W. **Physical chemistry of metals**. New York: McGraw-Hill, 1953.

DEHOFFE, R. T. **Thermodynamics in materials science**. New York: McGraw-Hill, 1993.

ELLIOTT, J. F. Trans. AIME, vol. 203, p. 485, 1955.

ERICKSON, G.; PELTON, A. **Critical evaluation and optimization of the thermodynamics properties and phase diagrams of the systems MnO-TiO_2, MgO-TiO_2, FeO-TiO_2, Ti_2O_3-TiO_2, Na_2O-TiO_2 e K_2O-TiO_2**. Metall. Trans., vol. 24B, p. 795-805, 1992.

FORLAND, T. **Fused salts**. New York: McGraw-Hill, 1964.

FLOOD, H.; KNAPP, W. J. J. American Ceramic Society, vol. 46, p. 61, 1963.

GASKELL, D. R. **Thermodynamic models of liquid silicates**. Can. Metall. Quater., vol. 20, no.1, p. 3-19, 1981.

GAYE, H.; WELFRINGER, J. **Modeling the thermodynamic properties of complex metallurgical slags**. Second international symposion on metallurgical slags and Fluxes, Lake Tahoe, Nevada, p.357-375, 1984.

GAYE, H. et al. **Statistical Thermodynamics model of slags: applications to systems containing S, F, P_2O_5 and Cr_2O_3**, 4th International conference on molten slags and fluxes, Sendai, p.103-108, 1992.

GIBSON, G. E.; GIAUQUE, W. F. **The third law of thermodynamics: evidences from the specific heats of glycerol that the entropy of a glass exceeds that of a crystal at the absolute zero**. J. Am. Chem. Soc., vol. 45, p. 93-104, 1923.

GOKCEN, N. A. **Statistical thermodynamics of alloys**. New York: Plenum Press, 1986.

GOLDBERG, R.; WEIR, R. D. **Conversion of temperatures and thermodynamic properties to the basis of the international temperature scale of 1990**. Pure and Applied Chemistry, vol. 64, p. 1545-1562, 1992.

GOLDBERG, D., Rev. Int. Hautes Temper. et Refract., vol. 5, p. 181-194, 1968.

GÖPEL, W.; WIEMHÖFER H. **Statistische thermodynamik**. Berlin: Spektrum Akademischer Verlag, 2000.

GULAMOVA, D.; SARKISOVA, M. K. (A) Russian Metallurgy (Engl. Transl.), p. 671-676, 1989.

GULAMOVA, D.; SARKISOVA, M. K. (B) Izv. Akad. Nauk SSSR, Neorg. Mater., vol. 25, p. 789-794, 1989.

GUILL P. E.; MURRAY, W.; WRIGHT, M. H. **Practical optimization**. London: Academic Press Inc., 1981.

GRAETZEL, M; INFELTA, P. **The bases of chemical thermodynamics**. Parkland, Florida: Universal Publishers, 2000.

GRAU, A. E., Can. Metall. Quater., vol. 18, p. 313-322, 1979.

GRIEVE, J.; WHITE, J. **The system: FeO-TiO_2**. J. Roy. Techn. Coll., vol. 4, p. 441-448, 1939.

GRIEVE, J.; WHITE, J. **The Systems: MnO-TiO_2 and MnO-FeO-TiO_2**. J. Roy. Techn. Coll., vol. 4, p. 660-670, 1940.

GUGGENHEIM, E. A. **Mixtures**. London: Oxford University Press, 1952.

HILLERT, M. **Hardenability concepts with applications to steel: prediction of iron-based phase-diagrams.** AIME, p. 1-27, 1978.

HILLERT, M. **Empirical methods for representing thermodynamic properties of ternary solution phases**. Calphad, vol. 4, p. 1-12, 1980.

HILLERT, M. **Some Viewpoints on the use of a computer for calculating phase diagrams**. Physica, vol. 103B, p. 31-40, 1981.

HILLERT, M. **Phase equilibria, phase diagrams and phase transformations**. New York: Cambrige University Press, 1998.

KAPOOR, M. L.; FROHBERG, M. G. **Theoretical treatment of activities in silicate Melts**. Proceedings of a congress on chemical metallurgy of iron and steel, London, p. 17-12, 1971.

KAPOOR, M. L.; MEHROTA, G. M.; FROHBERG, M. G., Archiv. Eisenhutten, vol. 45, p. 663, 1974.

KATO, E.; DAIMON, K.; TAKAHASHI, T. J. Am. Ceram. Soc., vol. 63, p. 355-356, 1952.

KAUZMANN, W. **The nature of the glassy state and the behavior of liquids at low temperatures**. Chemical Reviews, vol. 48, p. 219-256, 1948.

KELLOG, H. H. **Applications of fundamental thermodynamics to metallurgical processes**. G. R. Fitterer (Ed.), Gordon and Breach, 1967.

KUBASCHEWSKI, O.; ÜNAL, H. High temperatures. high pressures, vol. 9, p. 361, 1977.

KUBASCHEWSKI, O.; ALCOCK, C. B. **Materials Thermochemistry**, 5th ed., Oxford: Pergamon Press, 1979.

LANG, S. M.; FILLIMORE, C. L.; MAXWELL, L. H. J. Res. Natl. Bureau Standards, vol. 48, p. 298-312, 1952.

LEJUS, A. M., GOLDBERG, D., REVCOLEVSCHI, C. R. Acad. Sci., Ser. C, vol. 263, p. 1223-1226, 1966.

LEUSMANN, D. **A new determination of phase relations in the join MnO-TiO_2 between 1200 e 1600°C**. Neues Jahr Miner. Monatish., vol. 6, p. 262-266, 1979.

LEVIN, E. M., ROBBINS, C. R., MCMURDIE, H. F. **Phase diagrams for ceramists**. The American Ceramic Society, Columbus, Ohio, 1964.

LIN, P. L.; PELTON, A. D. **A structural model for binary silicate systems**. Metallurgical Transactions, vol. 10B, p. 667-675, 1979.

LITTLETON, J. T. **Critical temperatures in silicate glasses**. Industrial Engineering Chemistry, vol. 25, p. 748-755, 1933.

MACCHESNEY, J. B.; MUAN, A. Am. Mineral., vol. 46, p. 572-582, 1961.

MASSARZA, F.; SIRCHIA, E. Chim. Ind., vol. 40, p. 378, 1958.

MASSON, C. R. **An approach to the problem of ionic distribution in liquid silicates**. Proc Roy Soc., vol. 287A, p. 201-221, 1965.

MASSON C. R.; SMITH, I. B.; WHITEWAY, S. G. **Activities and ionic distribution in liquid silicates: application of polymer theory**. Canadian Journal of Chemistry, vol. 48, p. 1456-1464, 1970.

MARTIN, E.; BELL, H. B. Trans. Inst. Min. Metall., vol. 83C, p. 193, 1974.

MERRIT, R. R.; TURNBULL, A. G. J. Solid State Chem., vol. 10, p. 252-259, 1974.

MEYER F. R.; LEHMANN, J. E; GAYE, H. **Thermodynamic analysis of inclusions in Ti-deoxidized steels**. Scandinavian Journal of Metallurgy, vol. 29, p. 206-212, 2000.

OTHA, M.; MORITHA, K. **Thermodynamics of the MnO-Al_2O_3-TiO_2 System**. ISIJ International, vol. 39, p. 1231-1238, 1999.

PELTON, A.; BLANDER, M. **Thermodynamic analysis of ordered liquids by a modified quasi-chemical approach: application to silicate slags**. Met. Trans., vol. 17B, p. 295-304, 1986.

PELTON, A.; BLANDER, M. **A least squares optimization method for the analysis of the thermodynamic data in ordered liquid**. Calphad, vol. 12, no. 1, p. 97-108, 1988.

PLOOY, H.; PISTORIUS, P. C. **Melting point determination of TiO_2-rich slag**. Meas. Sci. Technol., vol. 9, p. 1728-1736, 1998.

PRESTON-THOMAS, H. **The international practical temperature scale of 1968. Amended edition of 1975**. Metrologia, vol. 12, p. 7-17, 1968.

PRAUSNITZ, J. M.; LICHTENHALER, R. N.; AZEVEDO, E. G. **Molecular thermodynamics of fluid-Phase equilibria**, New Jersey: Prentice Hall PTR, 1999.

PRIGOGINE, I.; DEFAY, R. **Chemical thermodynamics**. New York: Longmans Green and Co., 1954.

RAO, B. K. D. P.; GASKEL, D. R. (A) **The thermodynamic activity of Mn in Pt-Mn alloys in the temperature range 1300^{o}C to 1600^{o}C**. Metallurgical Transactions, vol. 12B, p. 207-211, 1981.

RAO, B. K. D. P.; GASKEL, D. R. (B) **The thermodynamic properties of melts in the system MnO-SiO_2.** Metallurgical Transactions, vol. 12B, p. 311-317, 1981.

RAO, B. K. D. P.; GASKEL, D. R. (C) **The thermodynamic activity of MnO in melts containing SiO_2, B_2O_3 and TiO_2**. Metallurgical Transactions, vol. 12B, p. 469-477, 1981.

REISMAN, A. **Phase equilibria**. New York: Academic Press, 1970.

RICHARDSON, F. D.; DAVIES, M. W. **The non-stoichiometry of manganous oxide**. Trans. Farad. Soc., vol. 55, p. 604-610, 1959.

ROSENQVIST, T. **Principles of extractive Metallurgy**. New York: MacGraw-Hill, 1983.

ROUF, M. A.; COOPER, A. H.; BELL, H. B. Trans. Br. Ceram. Soc., vol. 68, p. 253-267, 1969.

ROY, S. K.; COBLE, R. I. J. Am. Ceram. Soc., vol. 51, 1968..

SANDLER, S. I. **From molecular theory to thermodynamic models – part 2: mixtures**. Chem. Eng. Education, vol. 24, p. 80-87, 1990.

SCHUMANN, R.; ENSIO, P. J. J. Met., vol. 3, p. 401, 1951.

SCHREIFELS, W.; MUAN, A. Geochim. Cosmochim. Acta, Suppl., Proc. Lunar Sci. Conf., 6^{th}, vol. 6, p. 973-985, 1975.

SEIFERT, H. J.; KUSSMAUL, A.; ALDINGER, F. **Phase equilibria and diffusion paths in the Ti-Al-O-N system**. J. Alloys and Compounds, vol. 317-318, p. 19-25, 2001.

SLEPETYS, R. A.; VAUGHAN, P. A. J. Phys. Chem., vol. 73, p. 2157-2162, 1969.

SLAG-ATLAS, Dusseldorf : VDEh, Verlag-Stahleisen, 1995.

SMITH, W. R.; MISSEN, R. W. **What is chemical stoichiometry?**. Chemical Engineering Education, vol. 13, no. 1, p. 26-32, 1979.

SOMMERVILLE, I. D.; BELL, H. B., Can. Metall. Q., vol. 21, p. 145-155, 1982.

SPENCER, P. J. **Estimation of thermodynamical data for metallurgical applications.** Thermochimica Acta, vol. 314, 1-21, 1998.

TAYLOR, C. R.; CHIPMAN, J. Trans. AIME, vol. 154, p. 228, 1943.

TESTER, W., J.; MODELL, M. **Thermodynamics and its applications**. New Jersey: Prentice Hall, 1997.

TOOP, G. W. e SAMIS, C. S. Trans. TMS-AIME, vol. 224, p. 878, 1962.

WECHSLER, B. A.; NAVROTSKY, A. **Thermodynamics and structural chemistry of compounds in the system MgO-TiO_2**. J. Solid State Chem., vol. 55, p. 165-180, 1984.

WINKLER, E. R.; SARVER; J. F., CUTLER, I., B., J. Am. Ceram. Soc., vol. 49, p. 634-637, 1966.

WOERMANN, E.; BRENZY, B.; MUAN, A., Am. J. Sci., vol. 267A, p. 463-464, 1969.

WOLVERTON, C., et al. **Incorporating first principles energetics in computational thermodynamics approaches**. Acta Materialia, vol. 50, p. 2187-2197, 2002.

WASEDA, Y., TOGURI, M., Metal. Trans., vol. 8B, p. 563, 1977.

12. Apêndices.

12.1. Macros construídas.

12.1.1. Al_2O_3-TiO_2.

```
@@ SETUP FILE WRITTEN  6- 3- 5
@@
GO GIBBS
ENT-EL  /- VA AL O TI
AM_EL_D /-  ELECTRON_GAS       0.0000E+00  0.0000E+00  0.0000E+00 1
AM_EL_D VA  VACUUM             0.0000E+00  0.0000E+00  0.0000E+00 1
AM_EL_D AL  FCC(A1)            2.6982E+01  0.0000E+00  6.7690E+00 2
AM_EL_D O   1/2_MOLE_O2(G)     1.5999E+01  0.0000E+00  2.4502E+01 2
AM_EL_D TI  HCP(A3)            4.7880E+01  0.0000E+00  7.3200E+00 2

ENTER-SPECIE A0_01_C00C08_23_AL2O3    AL2O3
ENTER-SPECIE A0_01_C00C03_12_TIO2     O2TI1
ENTER-SPECIE A0_01_C03C08_ALTI        AL4O12TI3
ENTER-SPECIE AL2O3                    AL2O3
ENTER-SPECIE AL2TIO5                  AL2O5TI1
ENTER-SPECIE O2                       O2
ENTER-SPECIE TIO2                     O2TI1

@@MODELOS DE G
ENT-SYM FUN F766T  2.9815E+02  -2677984.69+1146.00414*T
    -182.5479*T*LOG(T)-.0110876*T**2+2345132*T**(-1);  6.0000E+03  N
ENT-SYM FUN F13207T   2.9815E+02  -966837.628+381.983614*T
    -63.19571*T*LOG(T)-.005910235*T**2+3.25307833E-11*T**3
    +517357*T**(-1);  2.18500E+03  Y
    -1018565.34+675.854122*T-100*T*LOG(T); 5.00000E+03  N
ENT-SYM FUN GS_TIO2 2.9815E+02 +F13207T+66944-31.338*T; 6.0000E+03 N
ENT-SYM FUN F717T     2.98150E+02  -1707353.3+448.021205*T-67.48039*T*LOG(T)
    -.06746995*T**2+1.42054467E-05*T**3+938781*T**(-1);  6.00000E+02  Y
    -1724888.03+754.856079*T-116.2579*T*LOG(T)-.007225685*T**2
    +2.78531667E-07*T**3+2120702*T**(-1);  1.50000E+03  Y
    -1772165.64+1053.45681*T-156.0582*T*LOG(T)+.007091065*T**2
    -6.29401833E-07*T**3+12366670*T**(-1);  2.32700E+03  Y
    -1868789.09+1392.58608*T-192.464*T*LOG(T);  6.00000E+03  N
ENT-SYM FUN GS_AL2O3 2.9815E+02 +111085.2-47.7375161*T+F717T; 6.0000E+03 N
```

```
@@POSSIVEIS FASES PRESENTES
ENT-PHASE RUTILO,,1 TIO2; N N
ENT-PARAM G(RUTILO,TIO2) 2.9815E+02 +F13207T; 6.0000E+03 N

ENT-PHASE ALTI,, 1 AL2TIO5; N N
ENT-PARAM G(ALTI,AL2TIO5) 2.9815E+02 +F766T+v10+v11*T; 6.0000E+03  N

ENT-PHASE AL2O3_S,, 1 AL2O3; N N
ENT-PARAM G(AL2O3_S,AL2O3) 2.9815E+02 +F717T; 6.0000E+03 N

ENT-PHASE SLAG,,1
    A0_01_C00C08_23_AL2O3,A0_01_C00C03_12_TIO2,A0_01_C03C08_ALTI; N N

ENTER-PARAM G(SLAG,A0_01_C00C08_23_AL2O3) 2.9815E+02 +GS_AL2O3; 6.0000E+03 N
ENTER-PARAM G(SLAG,A0_01_C00C03_12_TIO2)  2.9815E+02 +GS_TIO2; 6.0000E+03 N
ENTER-PARAM G(SLAG,A0_01_C03C08_ALTI) 2.9815E+02 +2*GS_AL2O3
   +3*GS_TIO2+v20; 6.0000E+03 N
ENTER-PARAM G(SLAG,A0_01_C00C03_12_TIO2,A0_01_C00C08_23_AL2O3;0) 2.9815E+02
   +v22 ; 6.0000E+03 N

ENTER-PARAM G(SLAG,A0_01_C00C03_12_TIO2,A0_01_C00C08_23_AL2O3;1) 2.9815E+02
   +v24; 6.0000E+03 N

@@ENTER-PARAM G(SLAG,A0_01_C03C08_ALTI,A0_01_C00C03_12_TIO2;0) 2.9815E+02
@@    +v24; 6.0000E+03 N

@@ SET BIT XXXX8XXX
AMEND_PHASE_DESCRIPTION SLAG STAT 04208000,,,,,!

GO PAR
C-N-S-F AL2O3_TIO2.PAR
s-o-v 10    58293.239
s-o-v 11   -34.770
s-o-v 20   -53780.577
s-o-v 22    11799.900
s-o-v 24   -9090.610
SET-INTERACTIVE
```

12.1.2. MgO-TiO_2.

```
@@ Setup file written  5-3-9
@@
GO GIBBS
ENT-EL  /- VA MG O TI
AM_EL_D /-  ELECTRON_GAS         0.0000E+00  0.0000E+00  0.0000E+00 1
AM_EL_D VA  VACUUM               0.0000E+00  0.0000E+00  0.0000E+00 1
AM_EL_D MG  HCP(A3)              2.4305E+01  0.0000E+00  7.8140E+00 2
AM_EL_D O   1/2_MOLE_O2(G)       1.5999E+01  0.0000E+00  2.4502E+01 2
AM_EL_D TI  HCP(A3)              4.7880E+01  0.0000E+00  7.3200E+00 2


ENTER-SPECIE A0_01_C00C24_11_MGO      MG1O1
ENTER-SPECIE A0_01_C00C03_12_TIO2     O2TI1
ENTER_SPECIE A0_01_C03C24_TIMG        MG2O4TI1
ENTER-SPECIE MGO                      MG1O1
ENTER-SPECIE MG1O3TI1                 MG1O3TI1
ENTER-SPECIE MG1O5TI2                 MG1O5TI2
ENTER-SPECIE MG2O4TI1                 MG2O4TI1
ENTER-SPECIE O2                       O2
ENTER-SPECIE O2TI1                    O2TI1

@@MODELOS DE G:
ENT-SYM FUN CAL1     2.98150E+02  4.184;   6.00000E+03   N
ENT-SYM FUN Z6672T    2.98150E+02  -617678.793+441315.768*T**(-1)
    +271.461188*T-43.197708*T*LN(T)-.00731252324*T**2
    +9.77222013E-07*T**3; 9.00000E+02  Y
     -620730.383+741298.108*T**(-1)+311.970014*T-49.3381464*T*LN(T)
    -.0016771292*T**2+1.06486984E-09*T**3;  6.00000E+03  N
ENT-SYM FUN GI_MGO  2.98150E+02  -Z6672T ;   6.00000E+03   N
ENT-SYM FUN GS_MGO  2.98150E+02  +18500*CAL1 -5.98*CAL1 *T-GI_MGO ;
    6.00000E+03 N
ENT-SYM FUN F13207T   2.98140E+02  -966837.628+381.983614*T
    -63.19571*T*LN(T)-.005910235*T**2+3.25307833E-11*T**3
    +517357*T**(-1);  2.18500E+03  Y
    -1018565.34+675.854122*T-100*T*LN(T);  6.00000E+03  N
@@2137K = Tf
ENT-SYM FUN GS_TIO2 2.9815E+02  +F13207T +66944-31.338*T;
   6.00000E+03   N
ENT-SYM FUN F11755T   2.98140E+02  -1609150.22+582.848765*T
    -93.84126*T*LN(T)-.03450503*T**2+5.52438667E-06*T**3
    +870688.5*T**(-1);  7.00000E+02  Y
    -1620745.88+754.29494*T-120.2996*T*LN(T)-.00725085*T**2
    +1.97278333E-07*T**3+1841930.5*T**(-1);  1.30000E+03  Y
    -1628902.63+824.674969*T-130.1877*T*LN(T)-.001892302*T**2
    -3.49785833E-07*T**3+3112268.5*T**(-1);  1.95300E+03  Y
    -1677712.76+1095.40987*T-163.176*T*LN(T);  6.00000E+03  N
```

```
ENT-SYM FUN F11774T   2.98140E+02  -2570319.43+1000.77022*T
    -165.1387*T*LN(T)-.024174315*T**2+7.91536167E-07*T**3
    +1434451*T**(-1);  1.00000E+03  Y
    -2573849.3+1042.41948*T-171.316*T*LN(T)-.01928167*T**2
    +5.98558167E-08*T**3+1825379*T**(-1);  1.96300E+03  Y
    -2674805.52+1737.32682*T-261.0816*T*LN(T);  6.00000E+03  N

ENT-SYM FUN F11812T   2.98140E+02  -2218992.39+893.081142*T
    -146.3433*T*LN(T)-.02175387*T**2+5.76788167E-07*T**3
    +1352666.5*T**(-1); 2.01300E+03  Y
    -2304181.38+1518.87068*T-228.4464*T*LN(T);  6.00000E+03  N

@@FASES PRESENTES

ENT-PHASE MGO,,  1  MGO ;  N N
ENT-PARAM G(MGO,MGO;0)  2.98150E+02  -GI_MGO; 6.0000E+03 N

ENT-PHASE MG1O3TI1_S,,  1  MG1O3TI1 ;  N N
ENT-PARAM G(MG1O3TI1_S,MG1O3TI1;0)  2.98150E+02 +F11755T
   +v10+v11*T; 6.0000e+03 N

ENT-PHASE MG1O5TI2_S,,  1 MG1O5TI2 ;  N N
ENT-PARAM G(MG1O5TI2_S,MG1O5TI2;0)  2.98150E+02  +F11774T
    +v12;   6.00000E+03 N

ENT-PHASE MG2O4TI1_S,, 1  MG2O4TI1 ;  N N
ENT-PARAM G(MG2O4TI1_S,MG2O4TI1;0)  2.98150E+02  +F11812T
    +v14; 6.00000E+03 N

ENT-PHASE RUTILO,,  1  O2TI1 ;  N N
ENT-PARAM G(RUTILO,O2TI1;0)  2.98150E+02  +F13207T ;   6.00000E+03 N

@@MODELO DE KAPOR-GAYE-FROHBERG
ENTER-PHASE SLAG  ,  1
   A0_01_C00C03_12_TIO2,
   A0_01_C00C24_11_MGO, A0_01_C03C24_TIMG ;  N N

ENT-PARAM G(SLAG,A0_01_C00C03_12_TIO2;0) 2.98150E+02  +GS_TIO2 ;
   6.00000E+03  N
ENT-PARAM G(SLAG,A0_01_C00C24_11_MGO;0)  2.98150E+02  +GS_MGO ;
   6.00000E+03   N
ENT-PARAM G(SLAG,A0_01_C03C24_TIMG;0)  2.98150E+02  +V20+GS_TIO2
   +2*GS_MGO ;   6.00000E+03   N
ENT-PARAM G(SLAG,A0_01_C00C03_12_TIO2,A0_01_C00C24_11_MGO;0) 2.9815E+02
   +v22 ; 6.0000E+03 N
ENT-PARAM G(SLAG,A0_01_C00C03_12_TIO2,A0_01_C00C24_11_MGO;1) 2.9815E+02
   +v24 ; 6.0000E+03 N
@@ENT-PARAM G(SLAG,A0_01_C03C24_TIMG,A0_01_C00C03_12_TIO2;0) 2.9815E2
@@    +v24 ; 6.0000e+03 N

@@ SET BIT XXXX8XXX
```

```
AMEND_PHASE_DESCRIPTION SLAG STAT 04208000,,,,,!

GO PAR
C-N-S-F MGO_TIO2.PAR
s-o-v 10    12888.663
s-o-v 11   -3.672
s-o-v 12    8402.753
s-o-v 14    15164.848
s-o-v 20   -94856.3797
s-o-v 22    7749.361
s-o-v 24   -24999.497
SET_INTERACTIVE
```

12.1.3. MnO-TiO$_2$.

```
@@ SETUP FILE WRITTEN  5- 3-26
@@
GO GIBBS
ENT-EL  /- VA MN O TI
AM_EL_D /-  ELECTRON_GAS          0.0000E+00  0.0000E+00  0.0000E+00 1
AM_EL_D VA  VACUUM                0.0000E+00  0.0000E+00  0.0000E+00 1
AM_EL_D MN  BCC(A12)              5.4938E+01  0.0000E+00  7.6500E+00 2
AM_EL_D O   1/2_MOLE_O2(G)        1.5999E+01  0.0000E+00  2.4502E+01 2
AM_EL_D TI  HCP(A3)               4.7880E+01  0.0000E+00  7.3200E+00 2

ENTER-SPECIE MNO                          MN1O1
ENTER-SPECIE MN1O3TI1                     MN1O3TI1
ENTER-SPECIE MN2O4TI1                     MN2O4TI1
ENTER-SPECIE O2                           O2
ENTER-SPECIE TIO2                         O2TI1
ENTER-SPECIE A0_01_C00C03_12_TIO2         O2TI1
ENTER-SPECIE A0_01_C00C22_11_MN0          MN1O1
ENTER-SPECIE A0_01_C03C22_TIMN            MN2O4TI1
ENTER-SPECIE MNTIO3                       MN1O3TI1
ENTER-SPECIE MN2TIO4                      MN2O4TI1

@@MODELOS DE ENERGIA LIVRE DE GIBBS
ENT-SYM FUN F11856T   2.98140E+02  -400382.97+255.992739*T-46.48424*T*LOG(T)
   -.00405848*T**2+184096*T**(-1);  2.05810E+03  Y
    -412204.857+361.643065*T-60.668*T*LOG(T);  6.00000E+03  N
ENT-SYM FUN GI_MNO 2.9815E+02 +F11856T ; 6.0000E+03 N
ENT-SYM FUN GS_MNO 2.9815E+02 +GI_MNO+54392-26.4282591*T ; 6.0000E+03 N
ENT-SYM FUN F13207T   2.98140E+02  -966837.628+381.983614*T
   -63.19571*T*LOG(T)-.005910235*T**2+3.25307833E-11*T**3+517357*T**(-1);
   2.18500E+03  Y
   -1018565.34+675.854122*T-100*T*LOG(T); 6.0000E+03 N
ENT-SYM FUN GI_TIO2 2.9815E+02 +F13207T ; 6.0000E+03 N
```

```
ENT-SYM FUN GS_TIO2 2.9815E+02 +GI_TIO2+66944-31.338*T ; 6.0000E+03 N
ENT-SYM FUN F11874T   2.98140E+02  -1399644.33+724.123818*T
   -121.6707*T*LOG(T)-.00464424*T**2+1094116*T**(-1);  6.0000E+03  N
ENT-SYM FUN F11915T   2.98140E+02  -1812579.32+976.350959*T-168.155*T*LOG(T)
   -.00870272*T**2+1278212*T**(-1);  6.0000E+03  N
@@FASES PRESENTES

ENT-PHASE MN1O1_S  ,  1
   MNO ;  N N
ENT-PARAM G(MN1O1_S,MNO;0)  2.98150E+02  +F11856T ; 6.00000E+03 N

ENT-PHASE MN1O1_L  ,  1
   MNO ; N N
ENT-PARAM G(MN1O1_L,MNO;0) 2.9815E+02 +GI_MNO+54392-26.4282591*T ; 6.0000E+03 N

ENT-PHASE RUTILO  ,  1
   TIO2 ;  N N
ENT-PARAM G(RUTILO,TIO2;0)  2.98150E+02  +F13207T ;   6.00000E+03 N

ENT-PHASE MN1O3TI1_S  ,  1
   MNTIO3 ;  N N
ENT-PARAM G(MN1O3TI1_S,MNTIO3;0)  2.98150E+02 +F11874T+V10 ; 6.00000E+03 N

ENT-PHASE MN2O4TI1_S  ,  1
   MN2TIO4 ;  N N
ENT-PARAM G(MN2O4TI1_S,MN2TIO4;0)  2.98150E+02 +F11915T+V12 ; 6.00000E+03 N

ENT-PHASE SLAG  ,  1
   A0_01_C00C03_12_TIO2, A0_01_C00C22_11_MN0,
   A0_01_C03C22_TIMN ; N N

ENT-PARAM G(SLAG,A0_01_C00C03_12_TIO2) 2.9815E+02 +GS_TIO2 ; 6.0000E+03 N

ENT-PARAM G(SLAG,A0_01_C00C22_11_MN0) 2.9815E+02 +GS_MNO ; 6.0000E+03 N

ENT-PARAM G(SLAG,A0_01_C03C22_TIMN) 2.9815E+02 +GS_TIO2+2*GS_MNO
   +V20 ; 6.0000E+03 N

ENT-PARAM G(SLAG,A0_01_C00C03_12_TIO2,A0_01_C00C22_11_MN0;0) 2.9815E+02
   +V22 ; 6.0000E+03 N

ENT-PARAM G(SLAG,A0_01_C00C03_12_TIO2,A0_01_C00C22_11_MN0;1) 2.9815E+02
   +V24 ; 6.0000E+03 N

@@ENT-PARAM G(SLAG,A0_01_C03C22_TIMN,A0_01_C00C03_12_TIO2;0) 2.9815E+02
@@    +V26 ; 6.0000E+03 N

@@ SET BIT XXXX8XXX
AMEND_PHASE_DESCRIPTION SLAG STAT 04208000,,,,,!

GO PAR
```

```
C-N-S-F MNO_TIO2.PAR
S-O-V 10    -1504.817
S-O-V 12     10426.163
S-O-V 20    -59494.856
S-O-V 22    -7512.332
S-O-V 24    -14155.737
SET-INTERACTIVE
```

12.1.4. FeO-TiO_2.

```
@@ SETUP FILE WRITTEN  5- 3-31
@@
 GO GIBBS
 ENT-EL  /- VA FE O TI
 AM_EL_D /-  ELECTRON_GAS           0.0000E+00  0.0000E+00  0.0000E+00 1
 AM_EL_D VA  VACUUM                 0.0000E+00  0.0000E+00  0.0000E+00 1
 AM_EL_D FE  BCC(A2)                5.5847E+01  0.0000E+00  6.5200E+00 2
 AM_EL_D O   1/2_MOLE_O2(G)         1.5999E+01  0.0000E+00  2.4502E+01 2
 AM_EL_D TI  HCP(A3)                4.7880E+01  0.0000E+00  7.3200E+00 2

 ENTER-SPECIE A0_01_C00C03_12_TIO2      O2TI1
 ENTER-SPECIE A0_01_C00C16_11_FEO       FE1O1
 ENTER-SPECIE A0_01_C03C16_FETI         FE2O4TI1
 ENTER-SPECIE FE1O1                     FE1O1
 ENTER-SPECIE FE1O3TI1                  FE1O3TI1
 ENTER-SPECIE FE2O4TI1                  FE2O4TI1
 ENTER-SPECIE FEO                       FE1O1
 ENTER-SPECIE O2                        O2
 ENTER-SPECIE TIO2                      O2TI1
 ENTER-SPECIE FEO5TI2                   FE1O5TI2


 ENT-SYM FUN F9501T    2.9815E+02  -287925.353+278.651546*T
    -50.29712*T*LN(T)-.0017957875*T**2-1.3808525E-06*T**3+97306.85*T**(-1);
     6.00000E+02  Y
     -279727.454+154.251797*T-30.95955*T*LN(T)-.02301514*T**2
    +3.19654167E-06*T**3-579760*T**(-1);  9.00000E+02  Y
     -318246.729+562.931723*T-90.4949*T*LN(T)+.019062515*T**2
    -2.56551667E-06*T**3+4198916*T**(-1);  1.30000E+03  Y
     -390025.171+1032.92282*T-153.2256*T*LN(T)+.04081241*T**2
    -3.64372E-06*T**3+18660265*T**(-1);  1.65000E+03  Y
     -305488.803+416.042511*T-68.1992*T*LN(T);  6.0000E+03  N

 ENT-SYM FUN GS_FEO  2.98150E+02 +F9501T+24058-14.5806061*T
    +V16 ; 6.00000E+03 N
 ENT-SYM FUN GI_FEO 2.9815E+02 +F9501T ; 6.00000E+03 N

 ENT-SYM FUN F9519T    2.98140E+02  -1283022.82+691.850641*T
    -116.6081*T*LN(T)-.00912112*T**2+1002068*T**(-1);  1.68800E+03  Y
```

```
   -1395191.23+1356.71237*T-199.1584*T*LN(T);  6.0000E+03  N

ENT-SYM FUN F9604T    2.9815E+02  -1566451.76+797.078757*T
   -139.4946*T*LN(T)-.03154736*T**2+711280*T**(-1);  6.0000E+03  N

ENT-SYM FUN F13207T   2.98140E+02  -966837.628+381.983614*T
   -63.19571*T*LOG(T)-.005910235*T**2+3.25307833E-11*T**3+517357*T**(-1);
   2.18500E+03  Y
   -1018565.34+675.854122*T-100*T*LOG(T);  6.00000E+03  N

ENT-SYM FUN GI_TIO2 2.9815E+02  +F13207T ; 6.00000E+03 N
ENT-SYM FUN GS_TIO2 2.9815E+02  +F13207T+66944-31.338*T;  6.00000E+03  N

@@MODELO DE G OBTIDO DE PELTON (1993).A FAIXA DE VALIDADE, DEVIDO AO AJUSTE
@@DE CP É BASTANTE RESTRITA (1423K A 1728K)
ENT-SYM FUN FAUX 1.3E+02 0.5*LN(T); 6.000E+03 N.
ENT-SYM FUN F13003T 1.3E+02 -2203606.5+1617.223*T+22.5138E+05*T**(-1)
    -7.59193E+07*T**(-2)-247.154*T*LN(T)-4104.6*EXP(FAUX); 6.00000E+03 N

ENT-PHASE FE1O1_S,,  1   FEO ;  N N
ENT-PARAM G(FE1O1_S,FEO;0)  2.98150E+02  +F9501T ;   6.00000E+03 N

ENT-PHASE FE1O1_L,,  1   FEO ; N N
ENT-PARAM G(FE1O1_L,FEO;0) 2.9815E+02 +GS_FEO ; 6.00000E+03 N

ENT-PHASE FETI_S,, 1 FEO5TI2 ; N N
ENT-PARAM G(FETI_S,FEO5TI2;0) 1.3E+02 +F13003T+V10 ; 6.0000E+03 N

ENT-PHASE FE1O3TI1_S,,  1  FE1O3TI1 ;  N N
ENT-PARAM G(FE1O3TI1_S,FE1O3TI1;0)  2.98150E+02  +F9519T+V12 ; 6.00000E+03 N

ENT-PHASE FE2O4TI1_S,,  1  FE2O4TI1 ;  N N
ENT-PARAM G(FE2O4TI1_S,FE2O4TI1;0)  2.98150E+02  +F9604T
   +V14 ; 6.00000E+03 N

ENT-PHASE RUTILE,,  1  TIO2 ;  N N
ENT-PARAM G(RUTILE,TIO2;0)  2.98150E+02  +F13207T ;  6.00000E+03 N

ENT-PHASE SLAG  ,  1
   A0_01_C00C16_11_FEO,A0_01_C00C03_12_TIO2,A0_01_C03C16_FETI ;  N N

ENT-PARAM G(SLAG,A0_01_C00C03_12_TIO2;0)  2.98150E+02  +GS_TIO2 ;
   6.00000E+03  N
ENT-PARAM G(SLAG,A0_01_C00C16_11_FEO;0)  2.98150E+02  +GS_FEO ;
   6.00000E+03  N
ENT-PARAM G(SLAG,A0_01_C03C16_FETI;0)  2.98150E+02
   +V20+GS_TIO2+2*GS_FEO;  6.00000E+03   N
ENT-PARAM G(SLAG,A0_01_C00C03_12_TIO2,A0_01_C00C16_11_FEO;0) 2.9815E+02
   +V22 ; 6.00000E+03 N
ENT-PARAM G(SLAG,A0_01_C00C03_12_TIO2,A0_01_C00C16_11_FEO;1) 2.9815E+02
   +V24; 6.0000E+03 N
```

```
@@ENT-PARAM G(SLAG,A0_01_C03C16_FETI,A0_01_C00C03_12_TIO2;0) 2.9815E+02
@@    +V24 ; 6.0000E+03

@@ SET BIT XXXX8XXX
AMEND_PHASE_DESCRIPTION SLAG STAT 04208000,,,,,!

GO PAR
C-N-S-F FEO_TIO2
S-O-V 10    -4626.287
S-O-V 12    -4881.536
S-O-V 14    -18120.529
S-O-V 20    -32352.778
S-O-V 22    -579.694
S-O-V 24    -20125.675
SET-INTERACTIVE
```

12.2. Arquivos de experimentos.

12.2.1. Al_2O_3-TiO_2.

```
@@POP-FILE MODIFICADO EM 6/07/05

DEFINE_COMPONENT AL2O3 O2 TIO2

$FUSAO CONGRUENTE DO AL2TIO5
CREATE_NEW_EQUILIBRIUM 10,1
CHANGE-STATUS PHASE SLAG ALTI = FIX 1
SET_CONDITION P=1E5 X(O2)=0 X(SLAG,AL2O3)=0.5
S-S-V T=2139
EXPERIMENT T=2139:20

$EUTETICO SLAG-AL2O3_TIO2-TIO2
CREATE_NEW_EQUILIBRIUM 20,1
CHANGE_STATUS PHASE SLAG ALTI RUTILO = FIX 1
SET_CONDITION  P=1.013E5 X(O2)=0
SET_START_VALUE  T=1952 X(SLAG,AL2O3)=0.2
EXPERIMENT T=1952:20 X(SLAG,AL2O3)=0.2:0.05

$EUTETICO SLAG-AL2O3_TIO2-AL2O3
CREATE_NEW_EQUILIBRIUM 30,1
CHANGE_STATUS PHASE SLAG ALTI AL2O3_S = FIX 1
S-C P=1.013E5 X(O2)=0
S-S-V T=2080 X(SLAG,AL2O3)=0.62
EXPERIMENT T=2079:20 X(SLAG,AL2O3)=0.62:0.05

$REGIAO SLAG-AL2O3
```

```
TABLE_HEAD 500
CREATE_NEW_EQUILIBRIUM @@,1
CHANGE-STATUS PHASE SLAG AL2O3_S= FIX 1
SET_CONDITION P=1.013E5 X(SLAG,AL2O3)=@1:0.05 X(O2)=0
SET_START_VALUE T=@2
EXPERIMENT T=@2:20
TABLE_VALUES
$ X(SLAG,AL2O3) T(K)
0.66 2095
TABLE_END

$Região SLAG-TIO2
TABLE_HEAD 700
C-N-E @@,1
CH-ST P SLAG RUTILO = FIX 1
S-C P=1E5 X(O2)=0 X(SLAG,AL2O3)=@1:0.05
S-S-V T=@2
EXPERIMENT T=@2:20
TABLE_VALUES
0.11 2063.8
TABLE_END

$REGIAO SLAG-AL2O3_TIO2
TABLE_HEAD 600
CREATE_NEW_EQUILIBRIUM @@,1
CHANGE-STATUS PHASE SLAG ALTI= FIX 1
SET_CONDITION P=1.013E5 X(SLAG,AL2O3)=@1:0.05 X(O2)=0
SET_START_VALUE T=@2
EXPERIMENT T=@2:20
TABLE_VALUES
$ X(SLAG,AL2O3) T(K)
0.22 1945
0.24 1992
0.39 2077
0.44 2107
0.55 2105
TABLE_END

CREATE_NEW_EQUILIBRIUM 70,1
CH-ST P ALTI AL2O3_S RUTILO = FIX 1
S-C P=1.013E5 X(O2)=0
S-S-V T=1567
EXPERIMENT T=1567:20

SAVE_WORKSPACE
```

12.2.2. MgO-TiO_2.

D-C MGO O2 TIO2

$PERITETICO: SLAG-MGO-MG2TIO4
C-N-E 10,1
CH-ST P SLAG MG2O4TI1_S MGO = FIX 1
S-C X(O2)=0 P=1E5
S-S-V T=2028.4 X(SLAG,TIO2)=0.4
EXPERIMENT T=2028.4:10 X(SLAG,TIO2)=0.4:0.02

$PERITETICO: SLAG-MG2TIO4-MGTIO3
C-N-E 20,1
CH-ST P SLAG MG2O4TI1_S MG1O3TI1_S = FIX 1
S-C X(O2)=0 P=1E5
S-S-V T=1903 X(SLAG,TIO2)=0.52
EXPERIMENT T=1903:10 X(SLAG,TIO2)=0.52:0.02

$EUTETICO: SLAG-MGTIO3-MGTI2O5
C-N-E 30,1
CH-ST P SLAG MG1O3TI1_S MG1O5TI2_S = FIX 1
S-C X(O2)=0 P=1E5
S-S-V T=1893 X(SLAG,TIO2)=0.56
EXPERIMENT T=1893:10 X(SLAG,TIO2)=0.56:0.02

$FUSÃO CONGRUENTE DO MGTI2O5
C-N-E 40,1
CH-ST P SLAG MG1O5TI2_S = FIX 1
S-C X(O2)=0 P=1E5 X(SLAG,TIO2)=0.66667
S-S-V T = 1930
EXPERIMENT T =1930:10

$EUTETICO: SLAG-RUTILO-MGTI2O5
C-N-E 50,1
CH-ST P SLAG RUTILO MG1O5TI2_S = FIX 1
S-C X(O2)=0 P=1E5
S-S-V T=1905 X(SLAG,TIO2)=0.76
EXPERIMENT T=1905:10 X(SLAG,TIO2)=0.76:.02

$eutetoide: MgO-Mg2TiO4-MgTiO3
C-N-E 60,1
CH-ST P MGO MG1O3TI1_S MG2O4TI1_S = FIX 1
S-C X(O2)=0 P=1E5
S-S-V T=1273
EXPERIMENT T=1273:10

$eutetoide : Rutilo-MgTiO3-MgTi2O5
C-N-E 70,1
CH-ST P RUTILO MG1O5TI2_S MG1O3TI1_S = FIX 1

```
S-C X(O2)=0 P=1E5
S-S-V T=403
EXPERIMENT T=403:10

SAVE_WORKSPACE
```

12.2.3. $MnO-TiO_2$.

```
$Rao and Gaskel activities
TABLE_HEAD 100
C-N-E @@,1
S-R-S MNO MN1O1_S,,,,
CH-ST P SLAG = FIX 1
S-C P=1E5 X(O2)=0 T=1773 W(MNO)=@1:0.05
EXPERIMENT ACR(MNO)=@2:0.05
TABLE_VALUES
0.70  0.967
0.64  0.835
0.60  0.686
0.55  0.574
0.50  0.413
0.45  0.260
0.40  0.208
0.35  0.153
0.30  0.104
TABLE_END


TABLE_HEAD 400
C-N-E @@,1
S-R-S MNO MN1O1_S,,,,
CH-ST P SLAG = FIX 1
S-C P=1E5 X(O2)=0 T=1823 W(MNO)=@1:0.05
EXPERIMENT ACR(MNO)=@2:0.05
TABLE_VALUES
0.64 0.768
0.60 0.639
0.55 0.414
0.50 0.341
0.45 0.235
0.40 0.202
0.35 0.119
0.30 0.094
TABLE_END

$OTA e Morita activities
TABLE_HEAD 600
CREATE_NEW_EQUILIBRIUM @@,1
CHANGE_STATUS PHASE SLAG=FIX 1
```

```
SET-CONDITION T=1873,P=1E5,W(MNO)=@1:0.05,X(O2)=0
SET_REFERENCE_STATE MNO MN1O1_S,,,,
EXPERIMENT ACR(MNO)=@2:0.05
TABLE_VALUES
$  W(MNO)      ACR(MNO)
   59.7E-02    5.90E-01
   46.7E-02    3.00E-01
   38.6E-02    1.60E-01
   26.3E-02    1.10E-01
   23.8E-02    1.00E-01
TABLE_END

$MARTIN AND BELL ACTIVITIES
$
TABLE_HEAD 700
CREATE_NEW_EQUILIBRIUM @@,1
CHANGE_STATUS PHASE SLAG=FIX 1
SET-CONDITION T=1773,P=1E5,X(TIO2)=@1:0.05 X(O2)=0
SET_REFERENCE_STATE MNO MN1O1_S,,,,
EXPERIMENT ACR(MNO)=@2:0.05
TABLE_VALUES
$  X(TIO2)      ACR(MNO)
   47E-02    3.60E-01
   49E-02    3.40E-01
   59E-02    1.50E-01
TABLE_END


$FUSAO CONG.: SLAG-MNTIO3
C-N-E 40,1
CH-ST P SLAG MN1O3TI1_S = FIX 1
S-C P=1E5 X(O2)=0 X(TIO2)=0.5
S-S-V T=1683
EXPERIMENT T=1683:10

$EUTETICO: SLAG-RUTILO-MNTIO3
C-N-E 50,1
CH-ST P SLAG MN1O3TI1_S SLAG RUTILO = FIX 1
S-C P=1E5 X(O2)=0
S-S-V T=1640 x(SLAG,TIO2)=0.58
EXPERIMENT T=1640:10 x(SLAG,TIO2)=0.58:0.05

$EUTETICO: SLAG-MNO-MN2TIO4
C-N-E 10,1
CH-ST P SLAG MN2O4TI1_S MN1O1_S = FIX 1
S-C X(O2)=0 P=1E5
S-S-V T=1683 x(SLAG,TIO2)=0.28
EXPERIMENT T=1683:10 x(SLAG,TIO2)=0.28:0.02

$FUSAO CONG.: SLAG-MN2TIO4
C-N-E 20,1
```

```
CH-ST P SLAG MN2O4TI1_S = FIX 1
S-C P=1E5 X(O2)=0 X(TIO2)=0.3333333333
S-S-V T=1700
EXPERIMENT T=1693:10

$EUTETICO:MN2TIO4-SLAG-MNTIO3
C-N-E 30,1
CH-ST P SLAG MN2O4TI1_S MN1O3TI1_S = FIX 1
S-C P=1E5 X(O2)=0
S-S-V T=1656 x(SLAG,TIO2)=0.43
EXPERIMENT T=1656:10 x(SLAG,TIO2)=0.43:0.05


$LINHA LIQUIDUS!!!!
$RAO AND GASKELL LIQUIDUS
$
TABLE_HEAD 900
CREATE_NEW_EQUILIBRIUM @@,1
CHANGE_STATUS PHASE SLAG,MN1O1_S=FIX 1
SET-CONDITION P=1E5,X(O2)=0,T=@2:10
S-S-V X(SLAG,MNO)=@1
EXPERIMENT X(SLAG,MNO)=@1:0.05
TABLE_VALUES
$ MOL fraction MNO in SLAG     T/K
 0.71                       1773
TABLE_END

TABLE_HEAD 1000
CREATE_NEW_EQUILIBRIUM @@,1
CHANGE_STATUS PHASE SLAG,MN1O1_S=FIX 1
SET-CONDITION P=1E5,X(O2)=0,T=@2:10
S-S-V  x(SLAG,MNO)=@1
EXPERIMENT x(SLAG,MNO)=@1:0.05
TABLE_VALUES
$ MOL fraction MNO in SLAG     T/K
 0.77                       1823
TABLE_END

$OTHA E MORITHA LIQUIDUS
TABLE_HEAD 1200
CREATE_NEW_EQUILIBRIUM @@,1
CHANGE_STATUS PHASE SLAG,RUTILO=FIX 1
SET-CONDITION P=1E5,X(O2)=0,T=@2:10
S-S-V X(SLAG,MNO)=@1
EXPERIMENT X(SLAG,MNO)=@1:0.05
TABLE_VALUES
$ MOL fraction MNO in SLAG     T/K
    0.2                       1873
TABLE_END

TABLE_HEAD 1300
```

```
CREATE_NEW_EQUILIBRIUM @@,1
CHANGE_STATUS PHASE SLAG,MN1O1_S=FIX 1
SET-CONDITION P=1E5,X(O2)=0,T=@2:10
S-S-V X(SLAG,MNO)=@1
EXPERIMENT X(SLAG,MNO)=@1:0.05
TABLE_VALUES
$ MOL fraction MNO in SLAG     T/K
      0.83                     1873
TABLE_END

$Linha liquidus - Leusmann (1979):
$Região Mno-slag
TABLE_HEAD 1400
CREATE_NEW_EQUILIBRIUM @@,1
CHANGE_STATUS PHASE SLAG,MN1O1_S=FIX 1
SET-CONDITION P=1E5,X(O2)=0,T=@2:10
S-S-V x(SLAG,TIO2)=@1
EXPERIMENT x(SLAG,TIO2)=@1:0.05
TABLE_VALUES
0.26 1850
0.28 1693
TABLE_END


$Região SLAG-Mn2TiO4
TABLE_HEAD 1500
CREATE_NEW_EQUILIBRIUM @@,1
CHANGE_STATUS PHASE SLAG,MN2O4TI1_S=FIX 1
SET-CONDITION P=1E5,X(O2)=0,X(SLAG,TIO2)=@1:0.05
S-S-V T=@2
EXPERIMENT  T=@2:10
TABLE_VALUES
0.36 1687
0.38 1678
TABLE_END


$Região SLAG-MnTiO3:
TABLE_HEAD 1600
CREATE_NEW_EQUILIBRIUM @@,1
CHANGE_STATUS PHASE SLAG,MN1O3TI1_S=FIX 1
SET-CONDITION P=1E5,X(O2)=0,x(SLAG,TIO2)=@1:0.05
S-S-V T=@2
EXPERIMENT T=@2:10
TABLE_VALUES
0.45 1671
0.54 1671
TABLE_END

$Região SLAG-TiO2:
TABLE_HEAD 1700
```

```
CREATE_NEW_EQUILIBRIUM @@,1
CHANGE_STATUS PHASE SLAG,RUTILO=FIX 1
SET-CONDITION P=1E5,X(O2)=0,T=@2:10
S-S-V x(SLAG,TIO2)=@1
EXPERIMENT x(SLAG,TIO2)=@1:0.05
TABLE_VALUES
0.58 1662
0.59 1686
0.63 1824
TABLE_END

SAVE-WORKSPACE
```

12.2.4. FeO-TiO$_2$.

```
D-C FEO O2 TIO2

$ATIVIDADES DE BELL
TABLE_HEAD 100
C-N-E @@,1
CH-ST P SLAG = FIX 1
S-R-S FEO FE1O1_L,,,,
S-C P=1E5 T=1748 X(SLAG,TIO2)=@1:0.05 X(O2)=0
S-S-V ACR(FEO)=@2
EXPERIMENT ACR(FEO)=@2:0.05
TABLE_VALUES
7.6604e-02  9.0359e-01
1.6319e-01  8.0082e-01
2.5199e-01  7.0132e-01
3.2527e-01  6.0487e-01
3.8968e-01  5.0506e-01
4.4967e-01  4.0194e-01
TABLE_END

$ATIVIDADES DE BAN-YA.
TABLE_HEAD 200
C-N-E @@,1
CH-ST P SLAG = FIX 1
S-R-S FEO FE1O1_L,,,,
S-C P=1E5 T=1673 X(SLAG,TIO2)=@1:0.05 X(O2)=0
S-S-V ACR(FEO)=@2
EXPERIMENT ACR(FEO)=@2:0.05
TABLE_VALUES
3.9633e-01  5.0839e-01
4.1744e-01  4.6646e-01
4.2300e-01  4.5030e-01
TABLE_END

TABLE_HEAD 300
```

```
C-N-E @@,1
CH-ST P SLAG RUTILE = FIX 1
S-C P=1E5 X(O2)=0 X(SLAG,TIO2)=@1:0.05
S-S-V T=@2
EXPERIMENT T=@2:20
TABLE_VALUES
7.3e-01  1.8636e+03
6.9e-01  1.8146e+03
6.6e-01  1.7704e+03
TABLE_END

TABLE_HEAD 400
C-N-E @@,1
CH-ST P SLAG FETI_S = FIX 1
S-C X(O2)=0 X(SLAG,TIO2)=@1:0.05 P=1E5
S-S-V T=@2
EXPERIMENT T=@2:20
TABLE_VALUES
0.58  1707
0.50  1668
TABLE_END

C-N-E 10,1
CH-ST P FE1O3TI1_S FETI_S RUTILE = FIX 1
S-C X(O2)=0 P=1E5
S-S-V T=1423
EXPERIMENT T=1423:10

$PERITÉTICO MEDIDO POR GRAU
C-N-E 20,1
CH-ST P SLAG RUTILE FETI_S = FIX 1
S-C X(O2)=0 P=1E5
S-S-V T=1737 X(SLAG,TIO2)=0.63
EXPERIMENT T=1737:20 X(SLAG,TIO2)=0.63:0.05

$APENAS A TEMPERATURA DO PERITETICO É CONHECIDA
$A COMPOSIÇÃO FOI ESTIMADA ATRAVÉS DA MÉDIA ENTRE 0.47 E 0.5
$PERITÉTICO SLAG-FETIO3-FE2TIO5
C-N-E 60,1
CH-ST P SLAG FETI_S FE1O3TI1_S = FIX 1
S-C X(O2)=0 P=1E5
S-S-V X(SLAG,TIO2)=0.49 T=1653
EXPERIMENT T=1651:20 X(SLAG,TIO2)=0.49:0.05

$FUSÃO CONGRUENTE DE MUAN
C-N-E 40,1
CH-ST P SLAG FE2O4TI1_S = FIX 1
S-C P=1E5 X(TIO2)=0.3333333333 X(O2)=0
S-S-V T=1670
EXPERIMENT T=1670:10
```

```
$EUTÉTICO DE MUAN
C-N-E 30,1
CH-ST P SLAG FE1O3TI1_S FE2O4TI1_S = FIX 1
S-C P=1E5 X(O2)=0
S-S-V T=1638 X(SLAG,TIO2)=0.47
EXPERIMENT T=1638:20 X(SLAG,TIO2)=0.47:0.05

$EUTÉTICO DE MUAN
C-N-E 50,1
CH-ST P SLAG FE1O1_S FE2O4TI1_S = FIX 1
S-C P=1E5 X(O2)=0
S-S-V X(SLAG,TIO2)=0.09 T=1587
EXPERIMENT X(SLAG,TIO2)=0.09:0.05 T=1587:20
```

12.3. Dados de atividade química e linha liquidus.

12.3.1. Linha liquidus do sistema Al_2O_3-TiO_2:

T(K)	Fração molar de Al_2O_3
1945	0.22
1992	0.24
2077	0.39
2107	0.44
2105	0.55
2095	0.66
2063.8	0.11
2079	0.62
1926	0.2
2116	0.0735
2116	0.0735
2071	0.289
2155.1	0.751
2179.6	0.839
2204	0.939

Tabela 1: Linha liquidus de acordo com Gulamova e Sarkisova (1989a).

T(K)	Fração molar de Al_2O_3
1975	0.2

Tabela 2: Linha liquidus de acordo com Goldberg (1968).

12.3.2. Linha liquidus do sistema $MnO-TiO_2$.

T(K)	Fração molar de TiO_2
1850	0.26
1693	0.28
1687	0.36
1678	0.38
1671	0.45
1683	0.50
1671	0.54
1662	0.58
1686	0.59
1824	0.63

Tabela 3: Linha liquidus de acordo com Leusmann (1979).

T(K)	Fração molar de TiO_2
1773	0.29
1823	0.23

Tabela 4: Linha liquidus de acordo com Rao e Gaskel (1981c).

T(K)	Fração molar de TiO_2
0.80	1873
0.17	1873

Tabela 5: Linha liquidus de acordo com Otha e Moritha (1999).

12.3.3. Atividades químicas do sistema $MnO-TiO_2$.

Fração mássica da MnO	Atividade química do MnO
0.70	0.967
0.64	0.835
0.60	0.686
0.55	0.574
0.50	0.413
0.45	0.260
0.40	0.208
0.35	0.153
0.30	0.104
0.25	0.080
0.20	0.077
0.15	0.078
0.10	0.075

Tabela 6: Atividades químicas do MnO determinadas a 1773 K por Rao e Gaskel (1981c).

Fração mássica de MnO	Atividade química do MnO
0.80	0.993
0.74	0.983
0.70	0.996
0.64	0.768
0.60	0.639
0.55	0.414
0.50	0.341
0.45	0.235
0.40	0.202
0.35	0.119
0.30	0.094
0.25	0.070
0.20	0.064
0.15	0.063
0.10	0.064

Tabela 7: Atividades químicas do MnO determinadas a 1823 K por Rao e Gaskel (1981c).

Fração molar de MnO	Atividade química do MnO
0.47	0.36
0.49	0.34
0.59	0.15

Tabela 8: Atividades químicas do MnO determinadas a 1823 K por Martin e Bell (1974).

Fração mássica de MnO	Atividade química do MnO
0.59	0.590
0.467	0.300
0.386	0.160
0.263	0.110
0.238	0.100

Tabela 9: Atividades químicas do MnO determinadas a 1873 K por Otha e Moritha (1999).

12.3.4. Linha liquidus do sistema FeO-TiO_2.

T(K)	Fração molar de TiO_2
1896.2	0.79
1822.4	0.69
1814.6	0.69
1780.9	0.66
1770.4	0.66
1737.0	0.63
1707.0	0.58
1668.0	0.50
1651.0	0.49

Tabela 10: Linha liquidus determinada por Grau (1979).

12.3.5. Atividades químicas do sistema FeO-TiO_2.

Fração molar de TiO_2	Atividade química do FeO
0.08	0.90
0.16	0.80
0.25	0.70
0.33	0.61
0.39	0.51
0.45	0.40

Tabela 11: Atividades químicas do FeO determinadas a 1748 K por Sommerville e Bell (1982).

Fração molar de TiO_2	Atividade química do FeO
0.396	0.508
0.417	0.467
0.423	0.450

Tabela 12: Atividades químicas do FeO determinadas a 1643 K por Ban-Ya et al. (1980).