SOFTWARE VALIDATION REPORT FOR THERMOCALC VERSION N AND DICTRA VERSION 21

Prepared for

U.S. Nuclear Regulatory Commission
Contract NRC–02–02–012

Prepared by

Yi-Ming Pan

Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas

Approved by:

Vijay Jain, Manager
Corrosion Science and Process Engineering

2/2/04
Date

TABLE OF CONTENTS

Section Page

FIGURES iii
TABLES iv

1 SCOPE OF THE VALIDATION 1

2 THERMODYNAMIC AND MOBILITY DATA USED IN TESTING 1

3 TEST CASES 1
3.1 Solvus Temperature of γ'-Phase in Nickel-Base Alloys 2
3.2 Amount of γ'-Phase in Nickel-Base Alloys 3
3.3 Composition of γ'-Phase in Nickel-Base Alloys 4
3.4 Phase Fractions versus Temperature for Udimet 700 5
3.5 Diffusion of Carbon in Austenite Steels 6
3.6 Cementite Dissolution in Austenite Steels 8
3.7 Carburization of Nickel-Base Alloys 9
3.8 Interdiffusion in a Ni-Al System 10

4 SUMMARY AND CONCLUSIONS 13

5 REFERENCES 13

FIGURES

Figure Page

1 Comparison of Calculated and Observed Solvus Temperature of γ'-Phase in Various Nickel-Base Alloys 4
2 Comparison of Calculated and Observed Amount of γ'-Phase in Various Nickel-Base Alloys 6
3 Comparison of Calculated and Observed Composition of γ'-Phase in Various Nickel-Base Alloys for Aluminum, Chromium, Molybdenum, Nickel, Titanium, and Tungsten Content 7
4 Comparison of Calculated and Observed Volume Fraction of γ'-Phase Versus Temperature for Udimet 700 Nickel-Base Alloy 8
5 Comparison of Calculated and Observed Carbon Concentration Profile in an Fe-Si-C Diffusion Couple Annealed at 1,050 °C [1,922 °F] for 13 Days 9
6 Comparison of Calculated and Observed Volume Fraction of Cementite as a Function of Time in Seconds after Dissolution at 910 °C [1,670 °F] in an Fe-Cr-C Steel 10
7 Comparison of Calculated and Observed Chromium Concentration Profiles in Austenite and Cementite after 10, 100, and 1,000 Second Dissolution at 910 °C [1,670 °F] in a Fe-Cr-C Steel 11
8 Comparison of Calculated and Observed Carbon Concentration versus Penetration Depth after Carburization of a Ni-Cr Alloy at 850 °C [1,562 °F] for 1,000 Hours 12
9 Comparison of Calculated and Observed Interdiffusion Coefficient at 1,200 °C [2,192 °F] in a Ni-Al Alloy as a Function of Aluminum Content 12

TABLES

Table | Table

1 Chemical Composition of Various Nickel-Base Alloys for Test Case 1 3
2 Chemical Composition of Various Nickel-Base Alloys for Test Cases 2 and 3 5

1 SCOPE OF THE VALIDATION

The purpose of this document is to report the results of validating the functionality of THERMOCALC Version N and DICTRA Version 21 following the Software Validation Test Plan (Pan, 2003). THERMOCALC Version N and DICTRA Version 21 software packages are products of Thermo-Calc Software AB located at Stockholm, Sweden. THERMOCALC Version N is a software for calculating multicomponent phase diagrams and thermodynamic property diagrams whereas DICTRA Version 21 is for the simulation of diffusion-controlled phase transformation. Direct coupling of these two programs has been successfully utilized to simulate various diffusion-controlled phase transformation process applications. The software packages are used by staff at the Center for Nuclear Waste Regulatory Analyses (CNWRA) to provide technical assistance to the U.S. Nuclear Regulatory Commission (NRC) in its high-level waste program.

This software validation report is intended to completely validate all functions of these software packages for use in calculations of phase stability and diffusion-controlled processes in multicomponent alloys as identified in the test cases described in Section 3. Validation of the software is based mainly on comparisons of calculated results with published data available in the literature in accordance with the Technical Operating Procedure (TOP–018) (CNWRA, 2003).

2 THERMODYNAMIC AND MOBILITY DATA USED IN TESTING

The simulations using THERMOCALC Version N and DICTRA Version 21 require thermodynamic and mobility databases. Both the Ni-DATA Version 5 database, a multicomponent thermodynamic database developed by Thermotech for nickel-base alloys, and the MOB2 database, a mobility database developed by Thermo-Calc Software AB for calculating diffusion coefficients of iron-base alloys, are used in the validation tests.

In the thermodynamic and kinetic modeling, the thermodynamic properties for each phase are defined on the basis of the CALPHAD method (CALculation of PHAse Diagrams). The CALPHAD method employs a variety of mathematical models to describe the thermodynamic descriptions of the various phases. The coefficients used by the models are held in the databases that can be accessed by the software packages such as THERMOCALC Version N and DICTRA Version 21 to retrieve the thermodynamic and mobility data for performing simulations. The comprehensive guide to the development and application of the method can be found in Saunders and Miodownik (1998) and Hack (1996). It is important to note that because the CALPHAD method is primarily based on the chosen thermodynamic models and available experimental data for the assessed systems, theoretical modeling can yield disparate results, particularly for multicomponent systems.

3 TEST CASES

This section provides the results of the eight test cases that have been identified previously (Pan, 2003). The first four test cases involve calculations of multicomponent phase diagrams and properties diagrams using THERMOCALC Version N. Test Cases 5 through 7 deal with diffusion-controlled processes in multicomponent alloys using DICTRA Version 21. The last test case evaluates the diffusion data in a Ni-Al system using both THERMOCALC Version N and DICTRA Version 21.

For THERMOCALC simulations, input thermodynamic data to be used are retrieved from the Ni-DATA Version 5 database. The alloy systems are defined based on their chemical compositions. The initial conditions for all equilibrium calculations are kept as constants at a pressure of 101,325 Pa [14.7 psi], and the total amount of material equals to 1 mole. All test cases are run by conducting a single equilibrium calculation at a specific temperature. In addition, a stepping calculation is performed for Test Cases 1 and 4 using temperature as an independent axis variable. The diffusion models for Test Cases 5 through 7 have been developed and implemented into the DICTRA software. The general calculation scheme consists of two steps, diffusion and equilibrium. The diffusion step is assumed to take place in a matrix phase, and after each diffusion step there is a change in the average composition of the matrix. The new equilibrium corresponding to the new average composition can be calculated at each gridpoint during the equilibrium step using the THERMOCALC software. The diffusion step is then repeated with the new composition profile in the matrix phase. In the DICTRA simulations, input thermodynamic and mobility data to be used are retrieved from the Ni-DATA Version 5 database and the MOB2 database, respectively. The input alloy composition and various simulation parameters for each test case are then defined. While the work space from the runs with THERMOCALC Version N are saved as files with a default extension of ".POLY-3," using the POLY module for equilibrium calculations, the work spaces from the runs with DICTRA Version 21 are saved as DIC files. The calculated results of the test cases are saved as either JPEG files or WordPerfect files. If necessary, EXP files that store experimental data are generated. The experimental information can then be appended on the calculated plots by the POST-processor module in the THERMOCALC and DICTRA software for comparison purposes. The acceptance criteria for the test cases that have been defined in the software validation test plan (Pan, 2003) on the basis of the typical accuracy for each experimental technique employed are ±10 percent difference between the calculated and observed values for the THERMOCALC calculations and a factor of two times for the DICTRA simulations. A large deviation is also anticipated in the DICTRA simulations because the kinetic data from MOB2 have large uncertainties.

Key model results are summarized in tables and/or figures for each of the test cases. All the input and output files are included in electronic form on the compact disc accompanying this validation report.

3.1 Test Case 1—Solvus Temperature of γ'-Phase in Nickel-Base Alloys

This test case determines the ability of THERMOCALC Version N to calculate the solvus temperature of γ'-phase in various nickel-base alloy systems through comparison with experimental data. This temperature is useful in determining heat treatment conditions and the maximum use temperature of these alloys. Twelve nickel-base alloys are selected from the work of Dharwadkar, et al. (1992) and Van Der Molen, et al. (1971), and their compositions are given in Table 1. The tests are run by conducting a single equilibrium calculation at 800 °C [1,472 °F] for each alloy composition, followed by extrapolating it in a stepping calculation using temperature as an independent axis variable.

The calculated initial equilibria from the runs are saved as POLY-3 files named Case1x.poly3 where an alphabetical letter is assigned to the "x" for each of the alloys. The filing system will be applied throughout the document thereafter. The final phase diagrams are saved as JPEG files named Case1x.jpg. From these diagrams, the solvus temperatures of γ'-phase in different alloy systems can be obtained. Figure 1 compares the calculated γ'-phase solvus temperatures

Table 1. Chemical Composition of Various Nickel-Base Alloys for Test Case 1 (Weight Percent)*										
Alloy	**Ni**	**Al**	**C**	**Co**	**Cr**	**Fe**	**Mo**	**Ta**	**Ti**	**W**
1	79.90	3.91	0.013	—	15.80	—	—	—	0.38	—
2	81.20	8.40	0.022	—	10.00	—	—	—	0.38	—
3	69.69	4.90	0.023	10.18	15.00	0.21	—	—	—	—
4	78.14	4.90	0.027	—	14.90	0.16	—	—	1.87	—
5	76.76	4.90	0.027	—	15.20	—	—	3.11	—	—
6	68.34	5.32	0.006	8.39	12.41	—	—	—	—	5.53
7	68.25	5.22	0.007	8.40	9.99	—	—	—	—	8.13
8	66.13	5.35	0.005	8.41	9.98	—	—	—	—	10.12
9	63.59	5.41	0.007	10.03	15.06	—	—	—	—	5.90
10	72.90	4.40	0.066	—	14.40	—	1.93	—	2.36	3.94
11	67.02	5.24	0.020	4.65	7.75	—	—	5.85	1.00	7.85
12	55.00	4.10	0.080	17.50	14.50	—	5.10	—	3.70	—

*NOTES: Ni — nickel; Al — aluminum; C — carbon; Co — cobalt; Cr — chromium; Fe — iron; Mo — molybdenum; Ta — tantalum; Ti — titanium; W — tungsten

with the experimental data given in Dharwadkar, et al. (1992) and Van Der Molen, et al. (1971). Based on the chosen criterion, the test results are considered acceptable with the differences between the calculated values and those observed experimentally less than 5 percent.

3.2 Test Case 2—Amount of γ'-Phase in Nickel-Base Alloys

This test case determines the ability of THERMOCALC Version N to calculate the amount of γ'-phase in various nickel-base alloy systems through comparison with experimental data. Twelve nickel-base alloys are selected from the work of Dreshfield and Wallace (1974) and Loomis, et al. (1972), and their compositions are given in Table 2. The tests are run by conducting single equilibrium calculations at 850 °C [1,562 °F] for Alloys 21 through 28 and at 927 °C [1,700 °F] for Alloys 29 through 32.

The calculated initial equilibria from the runs are saved as POLY-3 files named Case2x.poly3. The results of the initial equilibrium calculations are saved as WordPerfect files named Case2x.wpd. From these results, the amount of γ'-phase, in either volume percent or weight percent, at a specific temperature can be obtained. Figure 2 compares the calculated amount

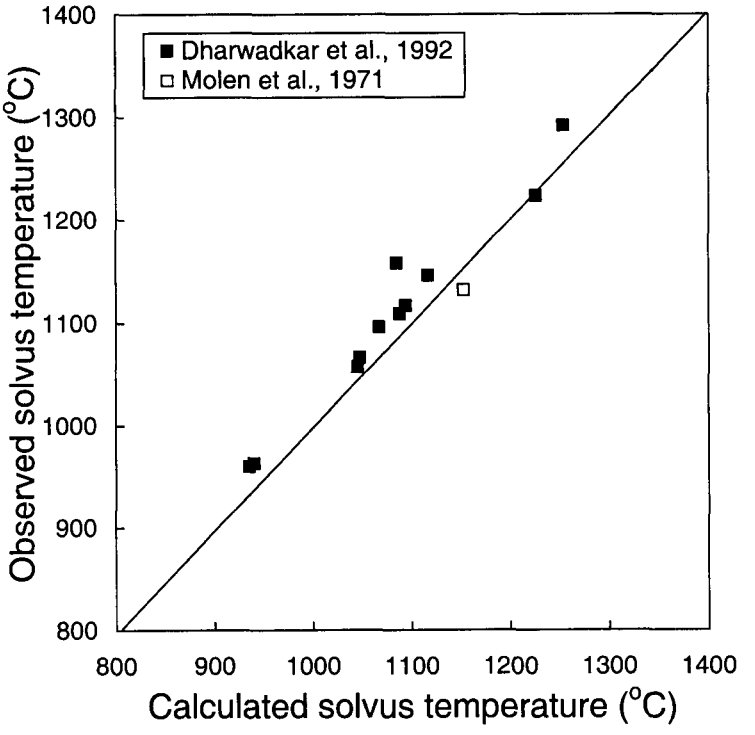

Figure 1. Comparison of Calculated and Observed Solvus Temperature of γ'-Phase in Various Nickel-Base Alloys

Note: Temperatures Provided in °C; for Conversion to °F use °F = 9/5 °C + 32.

of γ'-phase in weight percent with the experimental data given in Dreshfield and Wallace (1974) and Loomis, et al. (1972). The test results indicate that only five out of the twelve alloys are within ±10 percent of experimental data. In the simulations with the difference larger than 10 percent, the calculations tend to over-predict the amount of γ'-phase. The discrepancy is probably due to the kinetics of precipitation at these aging temperatures. In addition, as mentioned previously, the accuracy of the predictions derived from thermodynamic calculations depends critically on the database used. For instance, a revision of the thermodynamic database for nickel-base superalloys taking into account the crystallographic relation between the γ and γ' phases has been developed by Dupin and Sundman (2001). Available experimental data have also been used to modify the thermodynamic database of specific subsystems to yield better predictions.

3.3 Test Case 3—Composition of γ'-Phase in Nickel-Base Alloys

This test case determines the ability of THERMOCALC Version N to calculate the composition of γ'-phase in nickel-base alloys through comparison with experimental data. The twelve nickel-base alloys used in Test Case 2 are also evaluated in this test case. The calculated compositions of γ'-phase at a specific temperature can be found in the Case2x.wpd files. Figure 3 shows comparisons of the compositions of γ'-phase for aluminum, chromium, molybdenum, nickel, titanium, and tungsten content. Where the experimental data for Alloys 21

Table 2. Chemical Composition of Various Nickel-Base Alloys for Test Cases 2 and 3 (Weight Percent)*						
Alloy	**Ni**	**Al**	**Cr**	**Mo**	**Ti**	**W**
21	72.4	3.7	5.5	4.6	0.1	13.7
22	65.1	2.2	20.0	5.1	1.5	6.1
23	77.4	1.9	6.5	10.2	3.9	—
24	76.6	4.8	6.3	10.8	1.5	—
25	70.2	3.9	13.2	6.8	1.3	4.6
26	72.6	5.9	11.2	—	1.6	9.0
27	68.9	4.1	18.9	3.7	0.1	4.3
28	75.6	5.5	17.2	—	1.7	—
29	80.56	5.80	13.53	—	—	—
30	78.71	5.83	13.32	2.03	—	—
31	76.13	5.95	12.86	4.95	—	—
32	73.76	5.87	12.56	7.70	—	—
*NOTES: Ni — nickel; Al — aluminum; Cr — chromium; Mo — molybdenum; Ti — titanium; W — tungsten						

through 28 are given in Dreshfield and Wallace (1974) in atomic percent, they have been converted to weight percent to provide a consistent basis for comparison. The general tendency of distribution of the different elements in γ'-phase seems to be correctly predicted. Nevertheless, the agreement is not within 10 percent of experimental values in most cases. Because no systematic deviation exists, these discrepancies could partially be explained by experimental inaccuracy. The test case also indicated that additional assessment of the thermodynamic database is required to improve the model predictions.

3.4 Test Case 4—Phase Fractions Versus Temperature for Udimet 700

This test case determines the ability of THERMOCALC Version N to calculate the phase fraction of γ'-phase versus temperature for Udimet 700 nickel-base alloy through comparison with experimental data. The alloy composition given in Van Der Molen, et al. (1971) is 17.5Co-14.5Cr-5.1Mo-4.1Al-3.7Ti-0.08C-balance nickel in wight percent. The test is run by conducting a single equilibrium calculation at 800 °C [1,472 °F], followed by extrapolating it in a stepping calculation using temperature as an independent axis variable.

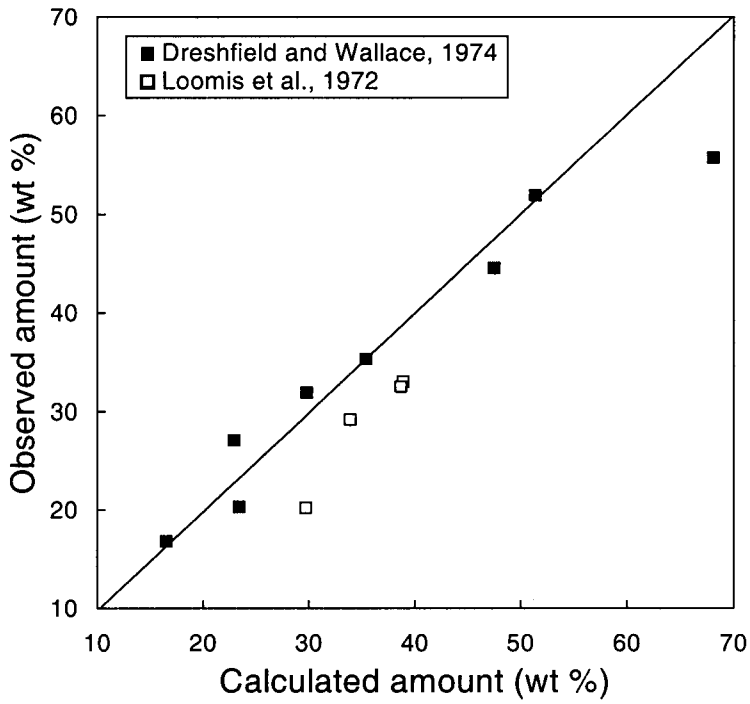

Figure 2. Comparison of Calculated and Observed Amount of γ'-Phase in Various Nickel-Base Alloys

The calculated initial equilibrium from the run with THERMOCALC Version N is saved as a POLY-3 file named Case4.poly3. The experimental data from the work of Van Der Molen, et al. (1971) are stored in an EXP file named Case4.exp. A comparison of the phase fraction of γ'-phase versus temperature for Udimet 700 can be made by appending the experimental data on the calculated plot. Figure 4 shows variation in the calculated and the observed volume fraction of γ'-phase. As seen in Figure 4, a small jump in the volume fraction of γ'-phase is observed at about 1,030 °C [1,886 °F], a temperature close to the solvus temperature of a carbide phase expected in Udimet 700. At this temperature, volume fraction of the carbide suddenly decreases to zero. The test results indicate that all the calculations over-predict the volume fraction of γ'-phase. The difference between the calculated and observed values, however, decreases with increasing temperature, with the exception of the calculation at 1,093 °C [1,999 °F]. The accuracy is within 5 percent in the cases of 1,038 and 1,066 °C [1,900 and 1,951 °F]. Since thermodynamic calculations predict equilibrium volume fraction, the low-volume fraction of γ'-phase measured at lower temperatures can be attributed the kinetics of precipitation.

3.5 Test Case 5—Diffusion of Carbon in Austenite Steels

This test case determines the ability of DICTRA Version 21 to calculate the diffusion of carbon in austenite steels. The test simulates the well-known Darken experiment (Darken 1949), in which two Fe-Si-C steels are joined and annealed at 1,050 °C [1,922 °F] in the austenite state. The input alloy compositions are defined to be 3.80Si-0.49C-balance iron and 0.05Si-0.45C-balance iron in wight percent. The input temperature is 1,050 °C [1,922 °F], and the simulation

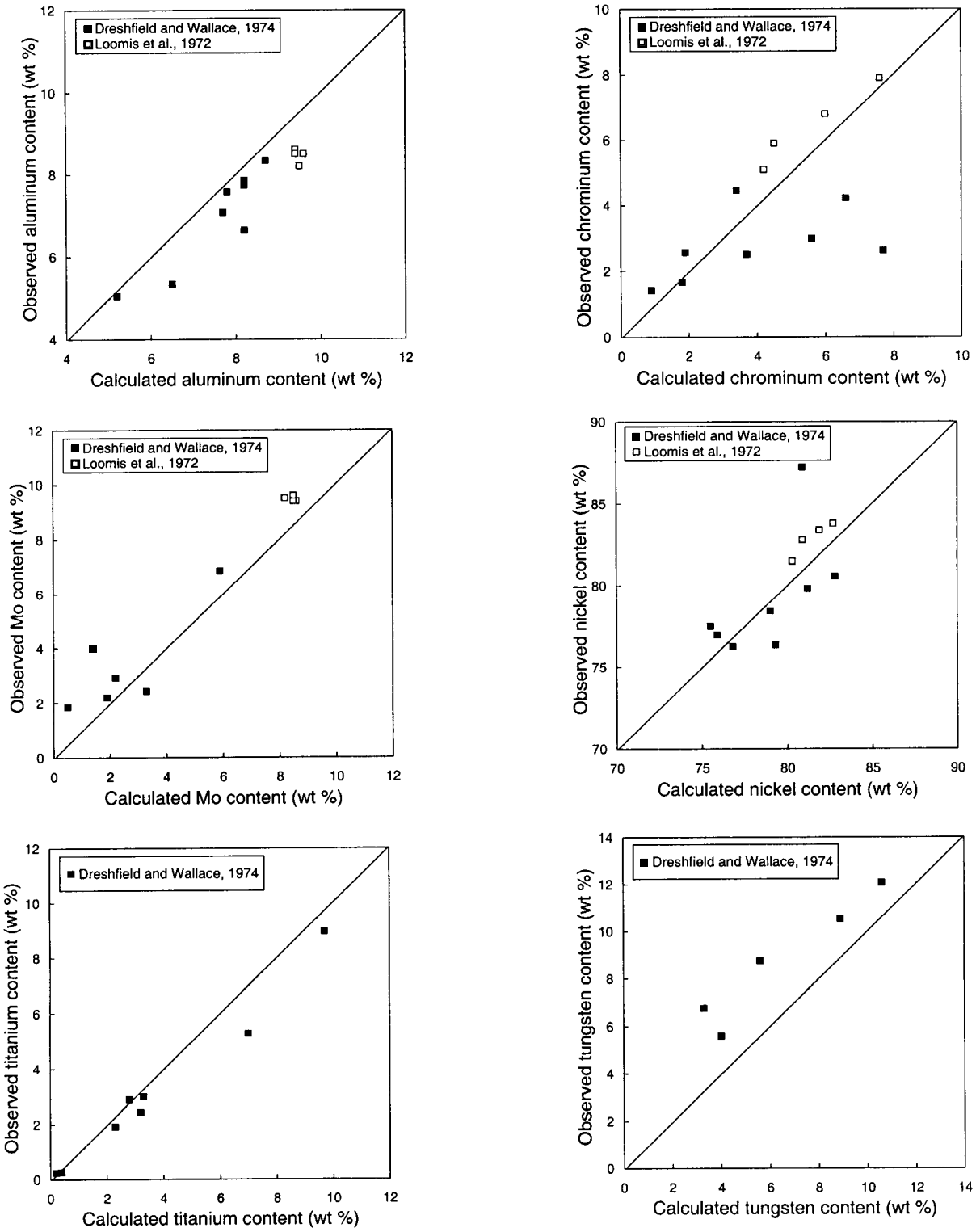

Figure 3. Comparison of Calculated and Observed Composition of γ'-Phase in Various Nickel-Base Alloys for Aluminum, Chromium, Molybdenum, Nickel, Titanium, and Tungsten Content

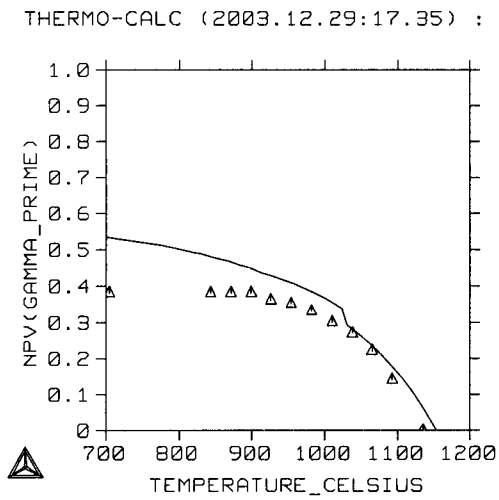

Figure 4. Comparison of Calculated and Observed Volume Fraction of γ'-Phase Versus Temperature for Udimet 700 Nickel-Base Alloy

Note: Temperature Provided in °C; for Conversion to °F Use °F = 9/5 °C + 32.

time is 13 days. The test is run by specifying the gridpoint type as a double geometrical grid calculation (i.e., a higher number of gridpoints at both ends of the austenite region).

The workspace from the run with DICTRA Version 21 is saved as a DIC file named Case5.dic. The experimental data from the work of Darken (1949) are stored in an EXP file named Case5.exp. In Figure 5, the experimentally measured carbon concentration profile stored in Case5.exp is appended and compared to the calculated one. As shown in Figure 5, the calculated carbon concentration profile is acceptable within less than 10 percent of the experimental data.

3.6 Test Case 6—Cementite Dissolution in Austenite Steels

This test case determines the ability of DICTRA Version 21 to calculate the cementite dissolution in austenite steels. The test simulates cementite dissolution during austenitization at 910 °C [1,670 °F] of a soft-annealed Fe-Cr-C alloy with a spherical cementite particle in an austenitic matrix. The input alloy composition given in Liu, et al. (1991) is 2.06Cr-3.91C-balance iron in atomic percent. The input dissolution temperature is 910 °C [1,670 °F], and the simulation times are 10, 100, and 1,000 seconds. The cementite particle is assumed spherical, and the initial particle size is set equal to the average particle size from the soft-annealed state. The test is run by specifying the gridpoint type as a geometrical grid calculation (i.e., a higher number of gridpoints at one end of the austenite and the cementite region).

The workspaces from the runs with DICTRA Version 21 is saved as a DIC file named Case6.dic. The experimental data from the work of Liu, et al. (1991) are stored in an EXP file

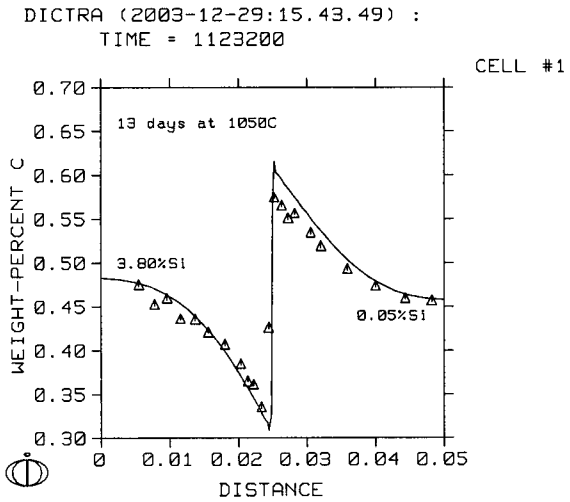

Figure 5. Comparison of Calculated and Observed Carbon Concentration Profile in an Fe-Si-C Diffusion Couple Annealed at 1,050 °C [1,922 °F] for 13 Days

Note: Distance Provided in Meters; for Conversion Use inch = m × 39.37.

named Case6.exp. Figures 6 and 7 show the comparisons for the volume fraction of cementite as a function of time and for the concentration profiles for chromium in austenite and cementite at various times by appending the experimental information stored in Case6.exp. It is evident that the agreement in general is acceptable between experiments and calculations. The discrepancy in the enrichment region at the interface where the chromium concentration profile is very sharp is the result of insufficient experimental measurements.

3.7 Test Case 7—Carburization of Nickel-Base Alloys

This test case determines the ability of DICTRA Version 21 to calculate carburization of nickel-base alloys. The test simulates carburization of a Ni-Cr alloy with dispersed spheroid carbide particles in a face-centered cubic matrix. This diffusion simulation case has been presented in detail by Engstrom, et al. (1994). The input alloy composition given in Engstrom, et al. (1994) is 75Ni-25Cr in weight percent. The input carburization temperature is 850 °C [1,562 °F], and the simulation time is 1,000 hours. The carbide particles are assumed as spheroid phases in a face-centered cubic matrix, and a constant surface carbon activity, $a_c = 1$ relative to graphite, is assumed. The test is run by specifying the gridpoint type as a geometrical grid calculation (i.e., a higher number of gridpoints at the lower end of the austenite region).

The workspace from the run with DICTRA Version 21 is saved as a DIC file named Case7.dic. The experimental data originally from the work of Bongartz, et al. (1986) as reported in Engstrom, et al. (1994) are stored in an EXP file named Case7.exp. The calculated carbon concentrations are compared with the experimental data by appending the experimental data stored in Case7.exp. As seen in Figure 8, significant difference exists between the calculated

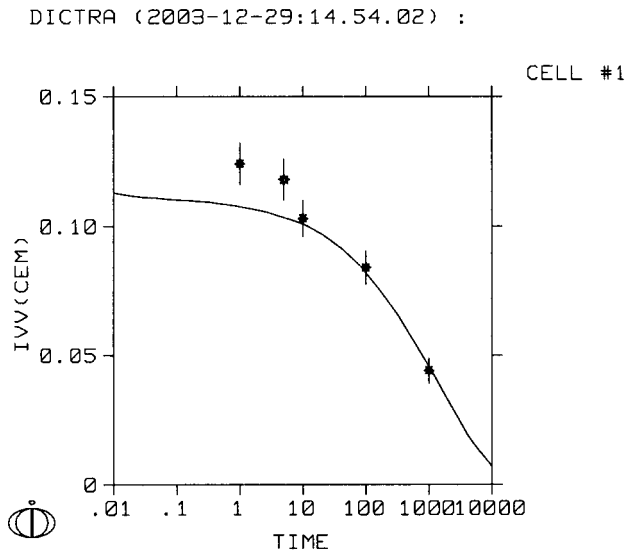

Figure 6. Comparison of Calculated and Observed Volume Fraction of Cementite as a Function of Time in Seconds after Dissolution at 910 °C [1,670 °F] in an Fe-Cr-C Steel

and observed carbon concentration and is partly attributed to the uncertainties of the kinetic data retrieved from the MOB2 database, originally developed from iron-base alloys. Nevertheless, the calculated carbon concentration versus penetration depth is in acceptable agreement with the one measured by Bongartz, et al. (1986).

3.8 Test Case 8—Interdiffusion in a Ni-Al System

This test case determines the accuracy of the assessed kinetic database for the Ni-Al alloy system. The initial alloy composition is assumed to be 90Ni-10Al in mole percent. The input diffusion temperature is 1,200 °C [2,192 °F], and the mobilities are assumed to be independent of concentration. The test is first set up with DICTRA Version 21 by specifying the diffusion coefficient matrix for the austenite phase at the given alloy composition. The diffusion coefficient as a function of composition is then calculated by a stepping calculation with THERMOCALC Version N using aluminum content as an independent axis variable.

The workspace from the setup with DICTRA Version 21 is saved as a DIC file named Case8.dic. The calculated initial equilibrium from the run with THERMOCALC Version N is saved as a POLY-3 file named Case8.poly3. The experimental data from the work of Yamamoto, et al. (1980) are stored in an EXP file named Case8.exp. The comparison of the experiments with the calculated interdiffusion coefficient as a function of aluminum content is made by appending the experimental data on the calculated plot in Figure 9. The agreement between calculation and experiments is acceptable.

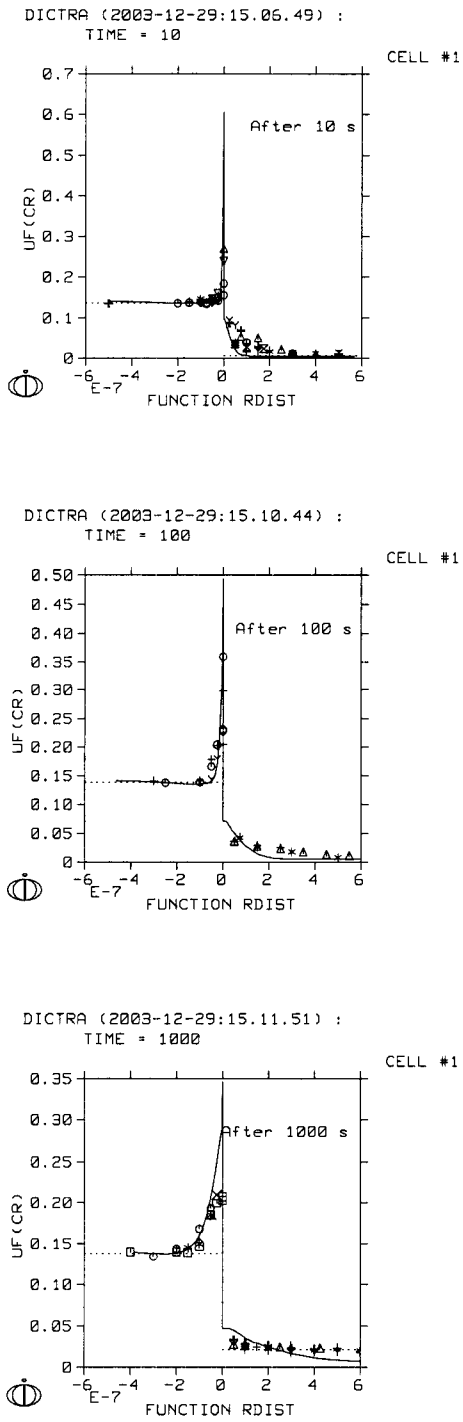

Figure 7. Comparison of Calculated and Observed Chromium Concentration Profiles in Austenite and Cementite after 10, 100, and 1,000 Second Dissolution at 910 °C [1,670 °F] in a Fe-Cr-C Steel

Note: Distance Provided in Meters; for Conversion Use inch = m × 39.37.

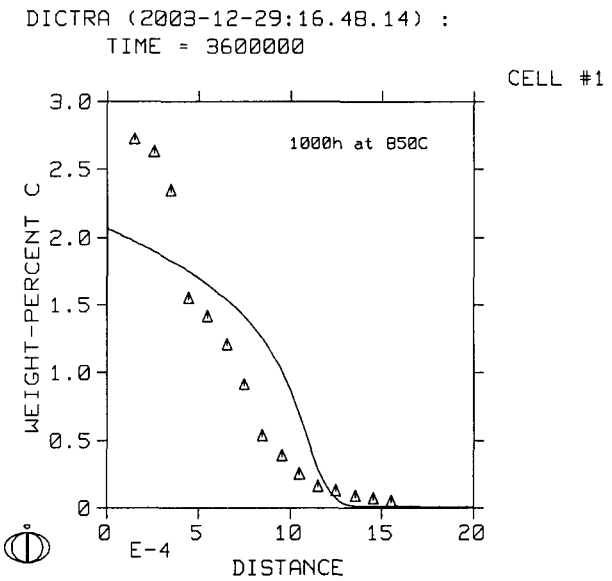

Figure 8. Comparison of Calculated and Observed Carbon Concentration Versus Penetration Depth after Carburization of a Ni-Cr Alloy at 850 °C [1,562 °F for 1,000 hours]

Note: Distance Provided in Meters; for Conversion Use inch = x 39.37.

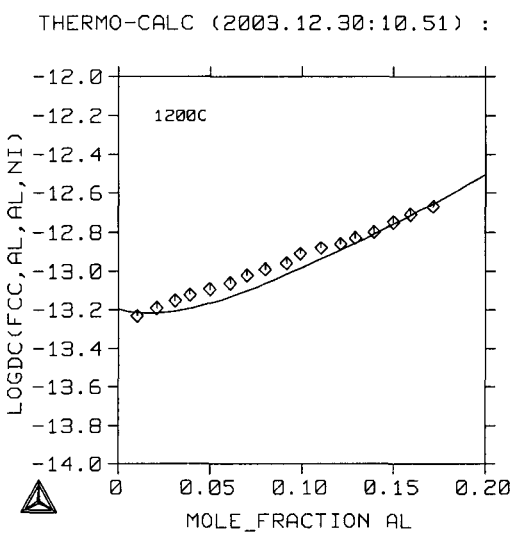

Figure 9. Comparison of Calculated and Observed Interdiffusion Coefficient at 1,200 °C [2,192 °F] in a Ni-Al Alloy as a Function of Aluminum Content

4 SUMMARY AND CONCLUSIONS

Thermodynamic and kinetic modeling has been applied to validate the functionality of the THERMOCALC Version N and DICTRA Version 21 software packages. Eight test cases are performed to completely validate all functions of the software for evaluating phase stability and diffusion-controlled processes in multicomponent alloy systems. Comparisons of the calculated results with the experimentally determined values indicate that the test results in general are considered acceptable in accordance with the criteria established in the Software Validation Test Plan. Significant deviations, however, still persist among the calculated and the observed values in a few validation test examples. The observed discrepancy can be attributed to the quality of the thermodynamic and mobility databases employed into the calculations and the uncertainties of the experimental data used for testing the predictions.

For the purpose of this validation, the discrepancy in the test results does not represent errors in the formalism of the thermodynamic and diffusion models but instead reflect that the databases may not have been fully assessed. In this regard, care needs to be exercised by the software user to interpret the results from model calculations, and experimental data are thus desirable for the validation of databases in predicting the relevant constituting phases in the alloy system of interest.

5 REFERENCES

Bongartz, K., R. Schulten, W.J. Quadakkers, and H. Nickel. "A Finite Difference Model Describing Carburization in High-Temperature Alloys." *Corrosion.* Vol. 42. pp. 390–397. 1986.

CNWRA. "Technical Operating Procedure (TOP-18): Development and Control of Scientific and Engineering Software, Revision 8, Change 2 (July 3, 2003)." San Antonio, Texas: CNWRA. 2003.

Darken, L.S. "Diffusion of Carbon in Austenite with a Discontinuity in Composition." *Transactions American Institute of Mining and Metallurgical Engineers.* Vol. 180. pp. 430–438. 1949.

Dharwadkar, S.R., K. Hilpert, F. Schubert, and V. Venugopal. "Determination of Solidus, Solvus, and Liquidus Temperatures for γ'-Hardened Nickel Base Alloys." *Zeitschrift fur Metallkunde.* Vol. 83. pp. 744–749. 1992.

Dreshfield, R.L. and J.F. Wallace. "The Gamma-Gamma Prime Region of the Ni-Al-Cr-Ti-W-Mo System at 850 °C." *Metallurgical Transactions.* Vol. 5. pp. 71–78. 1974.

Dupin, N. and B. Sundman. "A Thermodynamic Database for Ni-Base Superalloys." *Scandinavian Journal of Metallurgy.* Vol. 30. pp. 184–192. 2001.

Engstrom, A., L. Hoglund, and J. Agren. "Computer Simulation of Diffusion in Multiphase Systems." *Metallurgical and Materials Transactions.* Vol. 25A. pp. 1,127–1,134. 1994.

Hack, K. "The SGTE Casebook: Thermodynamics at Work." *Materials Modeling Series.* H.K.D.H. Bhadeshia, ed. London, United Kingdom: The Institute of Materials. 1996.

Liu, Z.-K., L. Hoglund, B. Jonsson, and J. Agren. "An Experimental and Theoretical Study of Cementite Dissolution in an Fe-Cr-C Alloy." *Metallurgical Transactions A.* Vol. 22A. pp. 1,745–1,752. 1991.

Loomis, W.T., J.W. Freeman, and D.L. Sponseller. "The Influence of Molybdenum on the γ' Phase in Experimental Nickel-Base Superalloys." *Metallurgical Transactions.* Vol. 3. pp. 989–1,000. 1972.

Pan, Y.-M. "Software Validation Test Plan for THERMOCALC Version N and DICTRA Version 21." San Antonio, Texas: CNWRA. 2003.

Saunders, N. and A.P. Miodownik. "CALPHAD (Calculation of Phase Diagrams): A Comprehensive Guide." Pergamon Materials Series. Vol. 1. R.W. Cahn, ed. New York City, New York: Elsevier Science. 1998.

Van Der Molen, E.H., J.M. Oblak, and O.H. Kriege. "Control of γ' Particle Size and Volume Fraction in the High Temperature Superalloy Udimet 700." *Metallurgical Transactions.* Vol. 2. pp. 1,627–1,633. 1971.

Yamamoto, T., T. Takashima, and K. Nishida. "Interdiffusion in the ζ-Solid Solution of a Ni-Al System." *Transactions Japan Institute of Metals.* Vol. 21. pp. 601–608. 1980.