From SOLGAS to FactSage 6.3
A tribute to Gunnar Eriksson

P.J.Spencer

Gunnar Eriksson Symposium, July 11, 2012

Eriksson, G.

Thermodynamic studies of high temperature equilibria. XII. SOLGASMIX, a computer program for calculation of equilibrium compositions in multi-phase systems.

Chem. Scr., Vol. 8, 1975, pp. 100-103

1976/77:

Erik Rosen brings a copy of Gunnar's thesis to Aachen – work begins on testing the potential use of SOLGASMIX for calculation of equilibria involving dilute metal solutions, which are being incorporated into the thermodynamic databank system under construction.

LEHRSTUHL FOR METALLURGIE OER KERNBRENNSTOFFE   51 AACHEN
UNO THEORETISCHE HOTTENKUNOE   Kopernikusstr. 16
Rheinlsch-Westf4l1sche Technlsche Hochschule Aachen   Telefon (0241) 80-5966
o. Prof. Dr. rer. nat. O. Knacke   Fernschreiber 832704

03.04.1979

Dear Professor Eriksson,

We have read with interest your papers dealing with the program SOLGASMIX and two members of our project have seen the program demonstrated by Dr. Rand, at Harwell, England, during a recent visit.

The program is of considerable interest to us in our work here, and we would like to ask if it is possible, in any way, to obtain a recent version of your program.

I see from the list of participants in the forthcoming CALPHAD meeting that you will also be present in Stockholm, and I would be very glad if it is possible to talk with you about this matter then.

With best wishes,

Yours sincerely,

Philip Spencert

Relevance to Charles Dickens

"Great Expectations"

Resulting publication

Aufbau und Nutzung einer thermochemischen Datenbank für anorganische Stoffe

I.Barin, B.Frassek, R.Gallagher & P.J.Spencer, Erzmetall **33** (1980) 226.

01.07.1980

Dear Gunnar,
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We would be delighted to support a visit by you in Aachen,
and have the opportunity to show you our work as well as
discuss your program in more detail. We would, in fact,
like to invite you to visit us in October or November of this
year, if this is convenient for you..................................

Relevance to Charles Dickens

"The Uncommercial Traveller"

Late 1980:

Link with dilute alloy solution database completed to allow calculation of complex equilibria involving both dilute alloy solutions and pure inorganic substances, e.g. melt-refractory interactions, carbide/nitride precipitation in steels

Resulting publication

The application of a thermochemical databank system to the solution of metallurgical problems
P..J.Spencer & R.Gallagher, Proc.2nd Australian Thermo.Conf., Melbourne, Feb.1981, p.62.

1983/4:

Link with data for concentrated alloys allowing full use of SOLGASMIX in complex metallurgical applications

Resulting publications

Calculation of Phase Equilibria in Multicomponent Alloy Systems Using a Specially Adapted Version of the Program SOLGASMIX
 G. Eriksson and K. Hack: *Calphad*, **8** (1984), 15

The application of a thermochemical databank system to the investigation of steelmaking problems
 R.Gallagher, K.Hack, M.Simons & P.J.Spencer, Steel Research **56** (1985) 7

10 Nov. 1985

....

I want to confirm that I intend to spend several months at Aachen next year, the period starting during the second half of January.

Here in Montreal I am dealing mainly with slag systems using the improved quasi-chemical model by Pelton and Blander. You might be interested to know that the activity coefficients of the slag components (so far MgO-CaO-FeO-$NaO_{0.5}$-SiO_2) are dependent on the number of different kinds of bonds in the melt.

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1988/89?:

Significantly extended and improved code – Gunnar instigates competition for new name – "Sage" is winner of champagne prize! Name modified to ChemSage because of other Sage software on the market.

Resulting publications

ChemSage - A Computer Program for the Calculation of Complex Chemical Equilibria
G.Eriksson, K.Hack, Metallurgical Transactions B , **21B** (1990)1013

The solution of materials problems using the thermochemical databank system THERDAS
P.J.Spencer & K.Hack, Swiss Materials **3a** (1990) 69

Publications continued

Application of a thermochemical databank system to the calculation of metastable phase formation during PVD of carbide, nitride and boride coatings
P.J.Spencer & H.Holleck, High Temp.Science 27 (1990) 295

Application of the thermochemical databank system THERDAS to the investigation and control of hazardous emissions during the thermal treatment of waste
P.J.Spencer, K.Hack, D.Neuschütz, Proc.BNF-Fulmer 8th Intl.Conf.on "Environmental Issues: Their Likely Impact on the Metals Processing & User Industries'' Amsterdam, May 1991, Paper 4.

Thermodynamic simulation of the cooling of waste gases from incineration furnaces including dioxin formation
P.J.Spencer, G.Eriksson, A.Buekens, D.Neuschütz, Proc.Coloquium on `Process Simulation', Helsinki, June 1994, p.127

The application of thermodynamics to the development of processes and materials
P.J.Spencer, G.Eriksson, A.von Richthofen, Proc.CODATA `94, Chambéry, France, Sept.1994.

1993/1994:

Origins of ChemApp – project in the direction of process simulation (N.B. The "Reactor Module" in earlier versions of the software had been used almost exclusively to simulate the commercial production of silicon).

Resulting publications

Some examples of use of a thermodynamic calculation interface (TQ) with ChemSage
G.Eriksson, P.Spencer, Proc.Coloquium on `Process Simulation', Helsinki, June 1994, p.105.

A general thermodynamic software interface
G.Eriksson, P.Spencer, H.Sippola, Proc.2nd.Colloquium on `Process Simulation', Helsinki, June 1995.

Comparison of thermochemically calculated and measured dioxin contents in the off-gas of a sinter plant
G.Eriksson, P.J.Spencer, D.Neuschütz, in "High Temperature Materials Chemistry 1X", ed.K.E.Spear, The Electrochemical Society, 1997, 278-287.

~2000 onwards:
Amalgamation of FACT and ChemSage software to produce FactSage

Resulting publications

FactSage thermochemical software and databases
C.W.Bale, P.Chartrand, S.A.Degterov, G.Eriksson, K.Hack, R. Ben Mahfoud, J. Melançon, A.D.Pelton, S.Petersen, CALPHAD **26** (2002) 189-228

FactSage thermochemical software and databases – recent developments
C.W.Bale, E.Bélisle, P.Chartrand, S.A.Decterov, G.Eriksson, K.Hack, I.-H.Jung, Y.B. Kang, J. Melançon, A.D.Pelton, C. Robelin, S.Petersen, CALPHAD 33 (2009) 295-311

Thermodynamic prediction of the formation and composition ranges of metastable coating structures in PVD processes
P.J.Spencer, in *Chemical Thermodynamics for Industry*, ed. T.M.Letcher, The Royal Society of Chemistry, Cambridge, 2004, pp. 197-208.

Relevance to Charles Dickens

"A Tale of Two Cities"

~1999 onwards: SimuSage

Resulting publications

A new tool for process modelling of metallurgical processes
M.Modigell, A.Traebert, P.Monheim, S.Petersen, U.Pickartz, Scandinavian Journal of Metallurgy, *28* (1999), 285

SimuSage– The Component Library for Rapid Process Modelling
K. Hack, T. Jantzen, A. Ruh, M. Spiegel, K. Pentillä, U. Krupp and V. Braz da Trindade, CALPHAD XXXIV, Maastricht, 2005.

Some companies for which thermochemical calculations were carried out using ChemSage or its predecessors

BASF, BBC, Balzus, Bedra, Benteler, Berzelius, BIRO, BMW,

Daimler-Benz, Degussa, Diehl, DLR, Dolomitwerk, Dornier,

ELINO, Energie Onderzoekzentrum (NL), Foseco, Genmin (S.Africa), Gesellschaft für Elektrometallurgie, Goldschmidt, Gonterman-Peipers, GST,

Heraeus, Hoesch, Hamburger Stahlwerk, Interatom, Junkers, KFA Jülich, KHD, Klöckner, KMC/Sumitomo (Japan), Krupp, KWU,

Lonza, Lurgi, Mahler, Mannesman, MBB/ERNO Raumfahrttechnik, MELCO (Japan), Messer-Griesheim, Metallwerk Plansee (Austria), MMC (Japan), MTU,

Ovako, Petten Laboratory (NL), Philips,

RADEX (Austria), Ruhr-Zink, Saarstahl, Schott, Shell (NL), Siemens, SKW, Sulzer, Teves-Thompson, Thyssen, VAW, Wacker Chemie, Xycarb, Zollern.

Some application topics

Energy

- Simulation of combustion processes

Environment

- Destruction of high chlorine content substances in a molten iron bath
- Prediction of process parameters leading to dioxin formation in
  metallurgical and waste incineration processes

Metastable coatings for machine tools

- Prediction of different stable and metastable ceramic and hard metal
  coating structures as a function of process parameters in CVD and PVD
  processes

Lead production

- Simulation of the QSL-reactor for lead production

Application topics continued

Undesirable solute reduction and removal

- Removal of iron from platinum and platinum/rhodium alloys by treatment with chlorine
- Desulphurisation for different steel/slag combinations

Spacelab

- Consideration of CO formation in carbon-containing nickel alloys with a Y_2O_3 dispersion

Glass production

- Behaviour of sulphates in a special lead-containing glass

Nuclear reactor failure simulations

- - Theoretical investigation of potential reactions occuring during a reactor core melt-down

Materials compatibility

- - Investigation of suitable new crucible materials for highly reactive alloys

Research contracts relying on use of ChemSage at RWTH Aachen

COST 507 - *Measurement and evaluation of thermochemical and thermophysical properties to provide a database for the development of new light alloys*

Approx. 30 to 40 individual projects in 14 participating countries with a total support funding of approximately $15 million over a 6 year period

CAPS - *The development of combined thermodynamic and kinetic models for the simulation of materials processing*

Institutes in 3 countries participating with total EU support funding of approximately $1 million over a 2 year period

FENICROS - *Thermochemical evaluation of the high-temperature equilibria of Fe-Ni-Cr alloys with oxygen and sulphur*

Total support funding of approximately $250,000 from the German Research Council over a 4 year period

Research contracts continued

SFB 370 - *Integrated Materials Modelling - subprojects Casting and Heat Treatment* **(DFG special research area)**

Total support funding of approximately $200000 from the German Research Council over a 3 year period

SFB 289 - *Thixoforming - subprojects Vormaterial and Prozessfenster* **(DFG special research area)**

Total support funding of approximately $200000 from the German Research Council over a 3 year period