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The thermochemistry library ChemApp and its applications

Dedicated to Dr. Gunnar Eriksson on the occasion of his 65th birthday

ChemApp is a thermochemical software library which enables the user to perform thermochemical calculations across a wide spectrum of applications by providing an easily programmable interface to complex equilibrium calculation techniques for multicomponent, multiphase chemical systems. ChemApp is described, and an overview of selected application examples from areas such as metallurgy, gas phase and aqueous chemistry, combustion technology, corrosion, geochemistry, and more is given.

Keywords: Thermochemistry; Gibbs energy minimization; Process simulation; Computer aided process engineering; Databases

1. Introduction

During Gunnar Eriksson's stay at the former Lehrstuhl für Theoretische Hüttenkunde und Metallurgie der Kernbrennstoffe (LTH) at RWTH Aachen University, his original software code SOLGASMIX was further developed into ChemSage [1], which became a widely used program for the calculation of complex chemical equilibria. As a powerful analytical tool for research and industry, it quickly gained world-wide usage with the help of GTT-Technologies (Gesellschaft für Technische Thermochemie und -physik mbH), a spin-off founded by members of LTH.

From the beginning ChemSage had an excellent reputation for fast, reliable convergence of equilibrium calculations. A particular feature important to users was the fact that ChemSage never required them to specify initial estimates for phase compositions or starting points for the Gibbs energy minimization (GEM) process. This later became an essential point in the applicability and versatility of ChemApp.

It did not take long for users of ChemSage to ask the developers whether and how the equilibrium calculation capabilities of ChemSage could also be integrated into programs of their own. For this purpose, they preferred to have a software module with an application programming interface (API) to the core calculational routines of ChemSage.

In addition, scientists, engineers, and software developers from other fields of research and application who started to discover the potential of computational thermochemistry for their projects, realized that their software would benefit from the ability to calculate chemical equilibria. However, substantial know-how in the field of computational thermochemistry is necessary to design the required Gibbs energy minimization code, even for modest problems. As soon as multicomponent, multiphase complex equilibrium calculations are required, the need for a highly specialized, modular third-party code became obvious.

To fill this need, a thermodynamic software interface consisting of a library of FORTRAN subroutines was developed within the framework of a European Science project [2, 3], and subsequently given the name ChemApp when it was made available by GTT-Technologies. It was based on improved equilibrium routines of ChemSage, enhanced by a set of interface routines to permit their easy integration into existing programs [4]. This was facilitated by providing language bindings for several other programming languages and creating ChemApp distributions for a wide range of compilers and hardware platforms.

Since 1996, ChemApp has been available as a product from GTT-Technologies [5]. It is not only used as a module for custom program development in research and industry, but also as an add-on to third-party software, and furthermore became the basis for several commercial software products. The wide range of application areas is supported by the amount of thermochemical data available for ChemApp. In particular, all thermochemical data accessible through FactSage [6] can be used with ChemApp by exporting a subset of the data for a particular chemical system from one or more databases to a data-file. In addition to these standard databases (Table 1), all data entered into "private databases" in FactSage can be used as well. Thermochemical data-files can also be set up manually, or maintained and edited by specialized software available from GTT-Technologies.

Although ChemApp is primarily used to perform equilibrium calculations, not only perfect equilibrium processes may be considered. The modeling of thermodynamic properties also includes extrapolations into metastable states, thus driving forces for transformations, for instance, can be calculated. Another method to model a process that cannot be described by a single, overall equilibrium state is by conceptually dividing the process into a number of localized equilibrium "cells" or "reactors", and modeling the exchange of matter and energy by appropriate mechanisms. This way very complex processes can be modeled, for instance fluid flow applications in gaseous or liquid media, corrosion in solid alloys involving diffusion, or metallurgical processes where the reactor volume is divided into a small number of "localized reactors" connected by streams which are modeled according to experimental observation and analysis. A third option is to set kinetic controls for complex equilibrium calculations through the calculation of constrained equilibria with ChemApp [10, 11]. This

Table 1. Standard databases available for FactSage.

Source	Databases
CRCT [7]	Pure substance database Oxide database for slags, glasses, ceramics, refractories Salt database Hall aluminum database Aqueous database (ideal solution, Pitzer, Helgeson) Miscellaneous databases for sulfides, liquid alloys, etc. Pulp and paper database
Cooperative development (CRCT – Spencer Group [8] – GTT-Technologies)	Copper alloy database Lead alloy database Light metal database Steel database Ultrapure silicon database
SGTE [9]	Pure substance database General alloy database Noble metal database Nuclear database
Other	Thermodata nuclear database

technique is also described in a separate article elsewhere in this volume [12].

The remainder of the article is split into two parts. The first part describes ChemApp, its basic use and set of subroutines that form its API, while the second part introduces a number of projects for which ChemApp has been used, illustrating the wide range of practical applicability of ChemApp and Gibbs energy minimization in general.

2. Description of ChemApp

2.1. The thermochemical system

ChemApp employs the same concept of a thermochemical system as ChemSage and its successor FactSage. Such a system consists on the one hand of a number of chemical components and on the other hand of a number of phases, where some may have a composition expressed as amounts of a number of phase constituents, and others can have an invariant composition. Phases are divided into three groups in ChemApp – the gaseous phase, condensed mixtures, and condensed stoichiometric phases. For convenience, a condensed stoichiometric phase is considered to consist of a single phase constituent only. Phases and phase constituents always have thermochemical properties (activities, chemical potentials, enthalpies, volumes, etc.). Phase constituents have compositions expressed as amounts of a number of components. A component is a system-wide entity. This is often stressed by calling it a system component. Components are usually the chemical elements, but they may also be composed of elements in any combination. In the latter case the stoichiometric formulas of the components must be linearly independent. At complete equilibrium, the absolute activities (chemical potentials) of the components are the same in the entire system. At present, ChemApp can handle chemical systems consisting of up to 48 system components, 44 mixture phases, 1600 constituents (the sum of all phase constituents and stoichiometric phases/pure compounds), and 4800 Gibbs energy/heat capacity equations.

2.2. Thermochemical data

All thermochemical data that ChemApp needs for its calculations are loaded at run-time from a data-file, which contains the thermochemical data for a more or less complex chemical system. The concept of comprehensive thermochemical data-files, i.e. extracts of thermochemical databases which contain an internally consistent set of data for a particular chemical system, provides a level of application-oriented customization that supports users and programmers in their goal to develop application-specific software. It is also a prerequisite for the creation of a marketable end product which is built on ChemApp and which can be distributed to end users with only the data included that are actually required for the application. A significant feature of ChemApp, and one that it shares with FactSage, is that it includes a very comprehensive library of excess Gibbs energy models for various types of non-ideal solution phases. A list of these models with typical areas for their application are summarized in Table 2. Additional "customer-specified" models can be added upon request.

Another feature of ChemApp particularly relevant to researchers in the area of solution model development is that a special version of ChemApp is available that allows for the addition of user-defined solution models. The thermochemical data-files for ChemApp can come from a variety of sources. Typically they are created using FactSage, and each contains an extract of the thermochemical data managed by its database back-end.

2.3. Supported compilers and hardware platforms

While ChemApp is written in FORTRAN, interface libraries with language bindings for several other programming languages are available, for instance for C/C++, Visual Basic®, and Borland Delphi®. Special distributions, for instance for use with AspenTech's AspenPlus® process simulation package, are also available. Table 3 gives an overview of the currently supported distributions of ChemApp.

For most of these distributions, a special version of ChemApp is available for download from the ChemApp web site [5]. This non-commercial version, called ChemApp "light", is freely available and meant to provide developers interested in ChemApp with an opportunity to test the usability of ChemApp in their own software environment. It differs from the regular version in the size of the thermochemical system it supports and in the type of target calculations it permits.

ChemSheet [41], an add-in for Microsoft Excel, contains a special version of ChemApp for Visual Basic. SimuSage is a visual component library for flowsheeting tasks based on ChemApp for Borland Delphi, and is described in a separate article elsewhere in this volume [42].

Table 2. List of available solution models in ChemApp. Magnetic contributions are not permitted for phase models marked with an asterisk (*).

Solution model	Application area
Redlich-Kister-Muggianu [13] Kohler-Toop [14] Hoch-Arpshofen [15–17]	For general use with substitutional or associated solution phases
Compound energy formalism [18–20] Two-sublattice order/disorder formalism [21] Species chemical potential/bond energy formalism* [22]	Solid phases with sublattice descriptions
Two-sublattice ionic formalism* [23]	Ionic liquids
Two-sublattice equivalent fraction formalism [14] Two-sublattice equivalent fraction formalism as a polynomial [24] Guts formalism [25]	Molten salts
Gaye-Kapoor-Frohberg cell model* [26] Modified quasichemical model in the pair approximation* [27–29]	Ionic oxidic mixtures with or without non-oxidic solutes
Modified quasichemical model in the quadruplet approximation [30, 31]	Condensed non-aqueous solutions
Binary defect formalism* [32]	Binary condensed phases with a narrow stoichiometry range
Wagner [33]	Metallic dilute solutions
Davies formalism* [34] Helgeson-Tanger-Shock formalism (ideal)* [35] Helgeson-Tanger-Shock formalism (Debye-Hückel)* [35] Helgeson-Tanger-Shock formalism (Davies)* [35]	Dilute aqueous solutions
Pitzer formalism* [36] Pitzer formalism without E-theta and E-theta* [36] Specific ion-interaction formalism* [37] Helgeson-Tanger-Shock formalism (Pitzer)* [35]	Concentrated aqueous solutions
Revised Helgeson-Kirkham-Flowers (HKF) model* [38]	Aqueous solutions up to 5 kbar and 1300 K
C–H–O–S–N–Ar multicomponent fluid model* [39]	Fluid mixtures up to 1 Mbar and 6000 K; important for many geological and environmental systems
Virial equation with Tsonopoulos' second virial coefficient correlation* [40]	Non-ideal gas phases

Table 3. Available ChemApp distributions.

Microsoft Windows®	Unix® and Unix-like systems
Aspen Plus (V11.1 SP1 and later) Microsoft Visual Basic (Win32) Microsoft Visual C++ (Win32) Microsoft PowerStation FORTRAN 4.0 Borland Delphi (V5 and later, Win32) Borland C++ Builder (Win32) Digital/Compaq Visual FORTRAN (V6.0 and later) Lahey FORTRAN LF95 (V5.0 and later) Intel Visual Fortran (IA32, V8.0 and later)	PC, Linux (×86), g77/gcc PC, Linux (×86), Intel Visual Fortran (IA32, V8.0 and later) DEC Alpha, DigitalUNIX V4.0 SGI, IRIX64 IBM RS/6000, AIX HP9000 PA-RISC, HP-UX Sun Sparc, Solaris AMD Opteron, Linux

2.4. Programming steps

Essentially only three stages of simple programming are necessary to proceed from the initialization of ChemApp to the collection of results:

1. Initializing the interface, reading a thermochemical data-file, adjusting the chemical system.
2. Setting initial conditions for the equilibrium calculation.
3. Performing the calculation and collecting results.

In the simplest cases, each programming step requires calling only a few of the ChemApp interface routines. For more complicated applications, the number of routines called in each step increases; however, the demands on programming capabilities are never particularly difficult.

2.4.1. Initializing the interface, reading a thermochemical data-file, adjusting the chemical system

This first step of each program entails initializing ChemApp, reading a thermochemical data-file into the program, and changing default units for temperature, pressure, volume, energy, and amount, if necessary. This step involves calling ChemApp subroutines shown in Table 4.

A further series of subroutines enables the chemical system to be identified and adjusted to match the requirements of the subsequent calculation.

Identification of phases, phase constituents, and system components

Phases, phase constituents, and system components in a thermochemical data-file are automatically indexed and numbered sequentially when loaded by ChemApp. Phases are numbered in the order gas, condensed mixtures, and finally stoichiometric condensed phases. Phase constituents are numbered starting from one for each phase.

Internally, ChemApp handles phases, phase constituents, and system components using these index numbers. For this purpose, ChemApp provides a number of subroutines in order to determine the index number associated with a name, and vice versa. Most routines in this group (see Table 5) fall into this category.

Table 4. Selected ChemApp subroutines for the initialization stage.

Subroutine	Function
TQINI	Initializes ChemApp
TQVERS	Gets the ChemApp version number
TQLITE	Checks whether ChemApp "light" is used
TQGTID/TQGTNM	Gets the user ID/user name of the license holder of ChemApp
TQGTED	Gets the expiration date of the ChemApp license
TQSIZE	Gets the internal array dimensions of ChemApp
TQUSED	Gets the dimensions of the currently loaded thermochemical system
TQGIO/TQCIO	Gets/changes the value of an output option
TQRFIL/TQRBIN/TQRCST	Reads a thermochemical data-file in various formats
TQGTRH	Retrieves information stored in the header of a data-file in transparent format
TQGSU/TQCSU	Gets/changes a system unit

Table 5. Selected ChemApp subroutines for the identification of system data.

Subroutine	Function
TQINSC/TQINP/TQINPC/TQINLC	Gets the index number for a system component/phase/phase constituent/sublattice constituent
TQGNSC/TQGNP/TQGNPC/TQGNLC	Gets the name for a system component/phase/phase constituent/sublattice constituent
TQCNSC	Changes the name of a system component
TQNOSC/TQNOP/TQNOPC/TQNOSL/TQNOLC	Gets the number of system components/phases/phase constituents/sublattices/ sublattice constituents
TQSTSC	Gets the stoichiometry of a system component
TQCSC	Changes the set of system components
TQMODL	Gets the model name for a phase
TQSTPC	Gets the stoichiometry of a phase constituent
TQCHAR	Gets the charge of a phase constituent

Table 6. ChemApp subroutines for status changes of phases and phase constituents.

Subroutine	Function
TQGSP/TQCSP	Gets/changes the status of a phase
TQGSPC/TQCSPC	Gets/changes the status of a phase constituent

Deletion or activation of phases and/or phase constituents from a calculation

This group of subroutines enables the change of the status of phases and phase constituents once the chemical system is read from the data-file. Other than the standard status ENTERED, ChemApp knows the status DORMANT and ELIMINATED which are set using the subroutines shown in Table 6:

- DORMANT: The phase or phase constituent is considered in the Gibbs energy minimization process, and its thermochemical properties for the equilibrium state are calculated, but it is excluded from the mass balance and thus always has an equilibrium amount of zero. This status thus for instance enables otherwise stable phases to be suppressed in order to calculate metastable conditions.
- ELIMINATED: The phase or phase constituent is excluded entirely from the equilibrium calculation, as if it were not present in the thermochemical data-file. By elimination of phases and/or constituents which are known not to be stable under the chosen conditions, considerable increase in computation speed can be gained.

2.4.2. Setting initial conditions for the equilibrium calculation

ChemApp offers considerable flexibility in defining initial conditions for a chemical equilibrium calculation, the subroutines for this group are listed in Table 7. Two different methods are available that will cover most cases experienced in practice.

- By defining the global conditions of a system
  Using this method, it is merely needed to set single conditions for pressure and temperature, and enter incoming species to define the composition of the system. For example, if the thermochemical equilibrium for the system SiO_2–CaO is to be calculated, using a thermochemical data-file that contains the elements Ca, Si, and O, it is only required to define the temperature and pressure of the system, and the total amounts of SiO_2 and CaO present.
- By defining streams
  A stream is considered to be a medium for transferring non-reacted matter to a reaction zone. It has constant temperature and pressure, and contains one or more phases of given composition. Hence, when using this method, the conditions for the three variables – composition, temperature and pressure – need to be defined for one or more input streams. For instance, one stream entering a reaction zone can consist of O_2(g), preheated to a temperature of 1500 K, while the other consists of CO(g) at room temperature. This method must be used when extensive properties of reactions are to be calculated; for example, those involving the heat balance or the adiabatic temperature of a combustion process.

Instead of temperature and pressure, other variables of state can also be chosen. This is supported by ChemApp's ability to perform "target calculations" in the form of "extensive property target calculations" (defined by the value of an extensive property change) and "phase target calculations" (defined by the search for a particular phase). When performing an extensive property target calculation with ChemApp, one of the following five extensive properties of the system can be selected as target: Heat capacity, enthalpy, entropy, Gibbs energy, or volume. A phase target calculation enables conditions to be determined when a selected phase is present at equilibrium (formation phase target), or when an unspecified phase is precipitated from a specified solution phase (precipitation phase target).

2.4.3. Performing the calculation and collecting results

In the simplest case, only one subroutine (TQCE) needs to be called to execute phase equilibrium calculations defined by pressure, temperature, and input composition (see Table 8). TQCEL also outputs a 'ChemSage-Table' of the equilibrium state for a quick overview. The EQUILIB module of FactSage also permits the output of an equilibrium state in this format, thus allowing for an easy comparison of results between the two programs. Other versions of these two subroutines, TQCEN and TQCENL, omit the standard ChemApp-internal estimation routine used to find an initial guess for the set of stable phases, and results from the previous equilibrium calculation are used as initial estimates instead. This will result in a noticeable increase in the computational efficiency, especially when the current settings of global conditions or streams are close to those of the previous calculation, and the set of stable phases does not change between the two calculations. If, in the previous step, a target was defined, the necessary additional information about the target variable is supplied when calling the equilibrium calculation routine. Most of the results from a phase equilibrium calculation are retrieved by using only a single subroutine, TQGETR. For the following variables results can be obtained:

- Total pressure, total volume, temperature,
- Equilibrium amounts of phases, phase constituents, and system components,
- Chemical potential and activity of phases, phase constituents, and system components,
- Heat capacity, enthalpy, entropy, and Gibbs energy of the equilibrium state,
- Mass or mole fraction of a system component in the system or in a phase, equilibrium amount of a system component in a phase

Table 7. ChemApp subroutines for the definition of equilibrium calculations.

Subroutine	Function
TQSETC/TQREMC	Sets/removes an equilibrium condition
TQSTTP	Sets name, temperature, and pressure for a stream
TQSTCA	Sets constituent amounts for a stream
TQSTEC	Sets an equilibrium condition with input conditions defined by streams
TQSTRM	Removes a stream

Table 8. ChemApp subroutines for the execution of equilibrium calculations and the retrieval of results.

Subroutine	Function
TQCE/TQCEL	Calculates the chemical equilibrium/outputs a result table
TQCEN/TQCENL	Calculates the chemical equilibrium, taking results from the previous equilibrium calculation as initial estimates/outputs a result table
TQMAP/TQMAPL	Calculates a one-dimensional phase map/outputs a result table
TQCLIM	Changes limits of target variables
TQSHOW	Shows present settings (initial condition, streams, targets)
TQGETR	Gets calculated equilibrium results
TQGDPC/TQSTXP	Gets thermodynamic data for a phase constituent/for a stream
TQGTLC	Gets the calculated equilibrium sublattice site fraction
TQBOND	Gets a calculated quadruplet or pair fraction

ChemApp also calculates the thermodynamic properties *Cp*, *H*, *S*, and *G* of a phase and its constituents, the thermodynamic properties of streams, and various quantities specific to particular solution models, such as bond fractions for the quasichemical models, and sublattice site fractions for the sublattice model. In addition to individual equilibrium calculations, ChemApp can also be used to perform one-dimensional phase mapping, which is used to search for all phase transitions within a given interval of a search variable. The search variable can be either total pressure, temperature, or incoming amount.

3. Applications of ChemApp

Since its first release, ChemApp has been used in a multitude of projects in universities, corporate research and development departments, as well as government laboratories. The application range is only limited by the availability of suitable thermochemical data. The following is a list of selected projects that have resulted in publications.

3.1. Software products

ChemApp is used as the basis or add-on module for a variety of other software.

VTT Process Chemistry developed ChemSheet [41], an add-on for Microsoft Excel based on ChemApp. ChemSheet allows its users to set up thermochemical calculation and process models within their spreadsheets, linking individual cells of the spreadsheet to the input and output of ChemApp. ChemSheet has been used for a wide variety of projects from the areas of aqueous and process chemistry, metallurgy, combustion technology, constitutional thermochemistry, and more. SimuSage, which is described in detail in a separate article elsewhere in this volume [42], combines the rigorous Gibbs energy thermochemistry with the rapid application development (RAD) environment and visual programming concept of Borland Delphi® in order to allow for the fast and completely customizable creation of process simulation applications. Both software products are available through GTT-Technologies [43, 44].

KilnSimu [45], also developed at VTT Process Chemistry, uses ChemApp to simulate the multi-phase chemistry in counter-current and co-current rotary kilns, which are in widespread use as separation reactors in the mineral processing, metallurgical, and chemical industries. KilnSimu, which is available as a separate software product, has already been used to model such processes as the calcination of TiO_2 (pigment production), $CaCO_3$ (lime kiln used in the pulp industry), and coke; cement production; reduction of ilmenite; zinc oxide fuming (Waelz kiln used in zinc production); industrial waste incineration and the carburization of organic waste.

BALAS® [46], another VTT product, is a steady-state simulation package for pulp and paper mills with an extensive selection of unit operation modules for mechanical pulping, heat recovery, utilities, wastewater treatment, and more. It permits applications of site-wide material and energy balances, heat recovery and heat integration analyses, modeling of dissolved and colloidal substances, as well as process optimization and the fitting of the process model to measured data. However, it has been lacking the capability to handle the very complex chemistry of fiber suspensions. This problem has been solved by the integration of ChemApp into BALAS, allowing for instance for the calculation of the constrained equilibrium between two aqueous phases (Donnan equilibrium) [47].

The Åbo Advisor [48] is a program intended to provide information about the high temperature ash and flue gas chemistry in black liquor recovery boilers of kraft pulp mills. The program can be used for predictions of a variety of furnace and flue gas phenomena, such as fireside fouling of the heat exchanger surfaces caused by the flue gas particulate matter, emissions of SO_2(g), HCl(g) and NO_x(g) with the flue gas, and more.

ChemApp is also a significant component of ASSET [49, 50], a PC-based tool available from Shell Global Solutions, designed to help engineers assess the probable corrosion of commercial alloys used in process equipment containing complex, hot corrosive gases. ASSET is a joint industry project which brings together many industrial companies, several research institutions and testing facilities, as well as experts in the fields of corrosion, thermochemistry, and software development. It can currently predict corrosion product formation and corrosion for wide ranges of conditions for four corrosion mechanisms: oxidation, sulfidation, carburization, and sulfidation/oxidation. Corrosion product stability assessments for nitridation are also possible.

Users of CFD (computational fluid dynamics) programs were among the first who added ChemApp as a module to existing commercial software, enabling the setup of combined fluid-flow thermochemistry simulations which provide a new method of investigating complex thermochemical issues as part of a fluid flow simulation. CFD programs to which ChemApp has been successfully linked include Phoenics®, CFX®, FIDAP®, and FLUENT®. In particular

the FLUENT-ChemApp link is frequently used, which also encouraged the developers of this CFD software to investigate possibilities to further optimize the calculational efficiency of the combined fluid-flow thermochemistry approach [51, 52].

For users of AspenPlus®, ChemApp is available as a module which enables them to use most of the thermochemical data available in FactSage in their flowsheets. This AspenPlus-FactSage-ChemApp interface has already been used to model a number of processes, for instance in the area of metallurgy and cement production. PRO/II® is another process simulation program to which ChemApp has already been successfully linked.

3.2. Metallurgy

For their research on clean steel production and inclusion engineering Hassall et al. of Corus Research performed two- and three-dimensional mathematical modeling of the fluid flow and the temperature and concentration gradients within a steel ladle during tapping, alloy addition, and stirring operations to predict the composition of inclusions within the steel [53]. For this purpose they linked ChemApp to the CFD program CFX to model the time-dependent interactions of the inclusions with steel, refractories, slag, and atmosphere. In further work the behavior of ladle glaze under pilot plant conditions was investigated and the results incorporated into the combined fluid flow-thermochemistry model [54]. Treadgold [55] developed a three-dimensional combined fluid flow-thermochemistry model of the recirculation degassing process for Si–Mn deoxidized steels which includes the effects of slag glaze on the formation of slags and inclusions. Within the framework of a European research project on the improved control of inclusion chemistry and steel cleanness in the ladle furnace [56] ChemApp was used together with the Aspen Custom Modeler® to simulate ladle arc furnace processing.

At the Department of Metallurgy and Materials Engineering, Katholieke Universiteit Leuven, ChemApp has been in use since 2003 for a number of projects, some of which also make additional use of FactSage. Verhaeghe et al. [57, 58] used it to create a combined flow and thermodynamic model of a lead blast furnace, which was tested against a simplified blast furnace charge. ChemApp was used to calculate the equilibrium in the hearth and bosh stages of the model, where the temperature was considered to be high enough to assume thermochemical equilibrium. Arnout et al. [59, 60] developed a time-dependent model for the electric arc furnace (EAF) process for stainless steel production. The time-dependency is implemented by a stepwise input of energy and matter into an equilibrium reactor modeled with ChemApp. In order to treat zinc leach residues, EAF dusts, and other zinc-containing waste materials, two new pyrometallurgial processes, a high temperature submerged plasma zinc fuming process and a reductive roast followed by the oxidative ISASMELT process have been developed. ChemApp was used to model both processes, where one aspect was the investigation of the behavior of the freeze lining [61–63]. The use of ChemApp to study freeze lining was continued for the development of a water-cooled submerged probe, where the results from equilibrium calculations were compared to the solidification microstructure gained from experiments [64, 65]. ChemApp is also applied in a project that uses thermochemical calculations to supplement in-situ investigations into the conditions under which $MgAl_2O_4$ is formed when magnesia particles are dissolved in $CaO-Al_2O_3-SiO_2$-based slags [66].

At Helsinki University of Technology, ChemApp is used in a study on the formation and transformation of liquid and solid inclusions in steel containing oxidic and sulfidic components, where it was linked with the interdendritic solidification model IDS to calculate, interactively and stepwise, steel solidification and inclusion formation/transformation in the residual liquid fraction [67].

3.3. Gas phase chemistry

Early on in the development of ChemApp Sippola et al. [68] linked it to the commercial CFD package Phoenics® to simulate SO_2 oxidation in a waste heat boiler. Given the complex gas phase chemistry in the waste gas of a copper flash smelting furnace, which includes heavy metal oxides and sulfur oxides, ChemApp was used to investigate the formation of sulfates condensing from the gas both on the walls and on the cooling tubes.

Tan et al. investigated the distribution of dioxins and furans in industrial combustion processes [69, 70]. ChemApp was applied to compare the results of constrained equilibrium calculations using three different databases of dioxins and furans with experimental values from selected industrial processes.

3.4. Combustion technology

The Combustion and Materials Chemistry Research Group at Åbo Akademi has used ChemApp for a variety of combustion-related projects apart from the Åbo Advisor software program mentioned above. In particular, Mueller et al. investigated the fly ash deposition behavior in biomass fired boilers based on advanced fuel analysis combined with CFD calculations [71, 72]. Experimental investigations of the fuel provided the composition of the ash-forming elements in the fuel, which in turn was used as input for an advanced thermodynamic equilibrium analysis leading to a detailed description of the temperature-dependent melting behavior of the ash. The results obtained on the thermochemical properties of the ash particles were combined with an advanced CFD-based ash deposition model that allows for the quantitative prediction of the transport of fly ash particles near furnace walls and heat exchanger surfaces.

Liebetruth [73] coupled FLUENT and ChemApp in order to track the path and investigate the composition of ash particles in combustion chambers of coal fired power plants. Whether the particles form deposits when colliding with the chamber walls depends among other things on their liquid fraction. Due to the complex chemical makeup of such particles, which includes a variety of condensed mixture phases, ChemApp was used to update the chemical composition along their entire trajectory. Once the CFD code predicted a collision with a wall, the sticking probability calculated with the help of ChemApp was used to determine the buildup of deposits.

Combined gas and steam turbine processes based on direct coal firing show a high thermal efficiency. At the Insti-

tute of Heat and Mass Transfer, RWTH Aachen University, an experimental test furnace to investigate the pressurized pulverized coal combustion (PPCC) was designed and assembled. Different mathematical models were developed and combined with FLUENT to predict the behavior of slagging films at the furnace walls. Again, ChemApp was used to estimate the sticking probability and melting point of the mineral components [74, 75].

Apart from being involved in the modeling of the zinc fuming process mentioned above, the Pyrometallurgy Research Centre (PYROSEARCH) at the University of Queensland, Australia, is also active in the modeling of the behavior of coal ash slags in the operation of entrained flow slagging gasifiers [76]. Using ChemApp and new viscosity models (see below), it is possible to predict the behavior of complex slag systems relevant to various coal-based power generation technologies.

At the Central Research Institute of Electric Power Industry (CRIEPI) in Japan, ChemApp was used in a three-staged simulation approach to model a coal combustion process in a gasifier [77]. In particular it was employed to calculate the amount of recycle char, which, when combined with the calculation of coal particle residence times yields a three-dimensional model of the gas-particle two-phase flow in the gasifier.

At the Austrian Bioenergy Centre, Graz, ChemApp has also been coupled with FLUENT to develop a process model that describes and predicts the formation of ash deposits in biomass fired combustion plants [78–80]. Changes in the flue gas composition due to chemical reactions are considered by performing thermodynamic equilibrium calculations in order to determine the gas phase composition. The build-up of the deposit layer depending on wall temperature, deposit porosity and chemical composition was also taken into account.

Weghaus et al. [81] coupled ChemApp and CFX to create a combined fluid flow-thermochemistry model of a large combustion plant. Their goal was the investigation of the distribution of minority species in the flue gas (alkali and heavy metals in various compounds) because of their relevance in the corrosion of the heat exchangers.

3.5. Cement making

At Tokuyama Corporation and Invensys Systems, Japan, ChemApp was linked to PRO/II to model the calcination in the cement making process [82]. The predicted heat and mass balance data as well as the clinker composition were compared with the actual operational results.

The industrial cement clinker burning process was simulated by Ube Industries, Japan, using the AspenPlus-FactSage-ChemApp interface [83]. Apart from modeling the cement clinker phase formation, the circulation phenomena of chloride and sulfate in the process were also investigated. This relates in particular to the "Chloride Bypass System", which avoids accumulation of chloride in the bottom cyclone.

3.6. Corrosion

At the University of Siegen, ChemApp has been used to simulate the high-temperature corrosion of steels and Ni-base alloys. After performing experimental research on the corrosion of low-Cr steels, austenitic steels, and Ni-base superalloys [84], a computer simulation was developed in order to predict the corrosion rate depending on their chemical composition and microstructure, the type of gas atmosphere, and the temperature [85–88]. The kinetic part of the program models the grain-boundary and bulk diffusion of the reacting species. Due to the large number of equilibrium calculations performed by the thermochemical part of the program, the individual calculations were distributed among parallel processing units.

Similar simulation techniques were also used within the framework of the European-funded materials research project OPTICORR [89, 90], whose objective was the optimization of in-service performance of boiler steels by modeling high-temperature corrosion and the development of a life-cycle approach for the materials in energy production, particularly for the steels used in waste incinerators and co-fired boiler plants. While ChemSheet was used to model salt-induced high temperature corrosion, ChemApp was employed to simulate high temperature corrosion processes under near-service conditions, modeling in particular internal oxidation and corrosion as a diffusion controlled process.

3.7. Aqueous chemistry

Königsberger and Eriksson [91] applied ChemApp together with thermochemical data for concentrated aqueous solutions assessed using the Pitzer formalism to simulate various single- and multistage modifications of the industrial conversion process $Na_2SO_4 + 2\ KCl \rightarrow K_2SO_4 + 2\,NaCl$. Königsberger et al. also used ChemApp in the development of a Pitzer model representing the thermodynamic properties of synthetic Bayer liquor solutions [92], which are supersaturated alkaline aluminate solutions resulting from the leaching of bauxite with a solution of hot sodium hydroxide. For this work, the capability of ChemApp to support user-defined solution model development was employed.

At the VTT Technical Research Centre, Manninen et al. have linked ChemApp with FLUENT to simulate the pH neutralization process in a stirred water tank, where acid is added to a basic solution through a nozzle located in the center of the tank [93]. The combined fluid flow-thermochemistry approach allows for the simultaneous calculation of the flow pattern and the pH distribution.

3.8. Geochemistry

At the Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) in Germany and cooperating institutions, ChemApp is used in several projects dealing with geochemical modeling. To assess the performance of an underground disposal site for radioactive waste, the mass transport of geogene solutes in general and of dissolved radionuclides in particular is modeled. Recently, ChemApp has been coupled to two transport codes, one for 1-D transport in a clayey barrier, the other one for a number of interconnected caverns in salt rock [94]. Mass transport in salt rock poses the challenge that solute activities cannot be computed with Debye–Hückel-type approaches. Instead, the Pitzer formalism was used. More than 200 solute species were considered including hydroxo-, carbonato-, chloro-, or sulfato-complexes with elements like uranium, americium, neptunium, technetium, or plutonium in different oxidation states.

The potential of ChemApp to cope with the Pitzer formalism is also used in two other applications. One deals with a salt-based material under development referred to as SVV ("Selbst Verheilender Verschluss"), which upon contact with free water reacts to a tight seal for boreholes [95, 96]. To model the penetration of NaCl-saturated brine into SVV, an interface between RockFlow [97] and ChemApp was developed. The SVV-filling was modeled using a mesh of finite elements. As a result of flooding, the dissolution and precipitation of secondary minerals was predicted by the model. The second application is concerned with mass transport in hydrothermal systems [98]. Here, again, saturated salt solutions are encountered, this time at elevated temperatures.

3.9. Nuclear materials

The investigation of chemical interactions between corium and concrete is of vital importance in calculations on the safety of nuclear power plants. Kothe et al. have used ChemApp within the framework of a data assessment project aimed at formulating standardized property data for compounds and solutions relevant in thermochemical modeling of corium–concrete interactions [99].

In his research on the temporary melt retention in the reactor pit of the European Pressurized Water Reactor (EPR), Nie [100] made use of ChemApp within the framework of the COSACO code, since thermochemical phenomena which influence the behavior of the MCCI (molten core concrete interaction) constituted a principal element of the new modeling approach. In analyzing the interactions between the core melt and sacrificial concrete, this approach provided a coherent description of the mutual dependencies between thermal hydraulics and thermochemical phenomena.

3.10. Thermophysical properties

While thermochemical data and the method of Gibbs energy minimization are normally used for the calculation of phase equilibria, it is also possible to employ this technique in the evaluation of other physical properties, for instance in the calculation of surface tensions of liquid solutions. Tanaka et al. [101] have used ChemApp in their procedure to calculate the surface tension of binary liquid alloys using the system Bi–Sn as an example. In further work Pajarre et al. [102] developed a model by which the calculation of the surface tension can be completely embedded into the Gibbs energy minimization process. This is achieved by adjusting the chemical system to contain separate thermochemical descriptions of the bulk and the surface phase, while the constraint of constant surface area is included by adding an additional pseudo system component. For details, see the contribution of Koukkari et al. [12] elsewhere in this volume.

At PYROSEARCH, ChemApp is also used in a custom-designed computer software package estimating the viscosity of slags in the system Al_2O_3–CaO–'FeO'–SiO_2 [103, 104]. The newly developed slag viscosity model enables the viscosities of homogeneous (completely molten) liquid slag systems, as well as heterogeneous (partially crystallized) slag systems, to be predicted as a function of the bulk slag composition and operating temperature over the complete range of conditions at iron saturation. ChemApp was used to develop the customized software program PyroSoft which calculates the viscosities and presents the result to the user in a graphical form. ChemApp was also used in their development of a structurally based viscosity model for fully liquid silicate slags [105]. The model links the slag viscosity to the internal structure of melts through the concentrations of various anion/cation structural units.

3.11. Lamp chemistry

High-intensity discharge (HID) lamps are chemical reactors which exhibit extreme thermal conditions. ChemApp is used as a module of a HID lamp model developed at Philips Research [106]. Local chemical equilibrium calculations using ChemApp in combination with the solution of transport equations (using the CFD package FIDAP) are carried out in an iterative procedure to obtain the stationary distributions of radiating species in the lamp. These in turn allow for the calculation of light-technical properties of the lamp.

3.12. Materials development and constitutional thermochemistry

Soon after ChemApp became available it was used for the simulation of casting and solidification processes. Greven et al. used it in their simulations for the macroscopic modeling of the microstructural evolution in castings [107]. This approach combined macroscopic calculations using an in-house 3D-FEM-program with a micro model that predicts the dendritic solidification of ternary alloys.

Schneider et al. [108, 109] have used ChemApp in the simulation of the precipitation kinetics during homogenization of commercial Al-alloys. During heating of as-cast ingots up to homogenization temperature a variety of phases are formed, thus a model was developed which is capable of describing the simultaneous nucleation, growth, coarsening, and compositional changes of several types of precipitates.

Hack et al. [110] have used ChemApp in a project that demonstrates the potential of three-dimensional phase diagrams, using up-to-date computer graphics techniques. Different from the past, perspective diagrams can now be generated from quantitative calculations of phase equilibria for systems with any number of components. New visualization techniques from the field of virtual reality (VR) are used to make the complex data easier to understand by displaying them in three dimensions. If time is incorporated in the visualization it is even possible to display four-dimensional diagrams, for example the change of the constitution of a ternary system with temperature.

4. Conclusion

Since its initial development, ChemApp has been successfully applied in a multitude of projects, in particular to model the thermochemical aspects of processes involving inorganic, complex solution phase chemistry. The general modeling approach in most cases is the division of the entire process into equilibrium reactors localized with respect to space and/or time, and the subsequent modeling of matter and energy exchange between them. Once a process can be conceptually described in this fashion, the successful application of

ChemApp depends solely on the availability of quality thermochemical data for the chemical system in question. However, there are also applications of ChemApp in modeling thermophysical properties of liquids as well as in taking phase diagram calculations into the third dimension.

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