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Use of computational thermodynamics in process engineering education

Case: HSC Chemistry and its possibilities

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***Abstract* —** Thermodynamics can be widely used in various areas of science and practice. For instance, it is widely considered as one of the key elements in the higher education of process (or chemical) engineering. However, there is no general agreement on how thermodynamics should be taught. Some curricula focus on theory and scientific principles, whereas others emphasize the role of utilisation of thermodynamics in various applications. The programme of process engineering at the University of Oulu in Finland is based on a so-called DAS-formalism, in which studies proceed from descriptive studies to holistic synthesis via analysis-studies, that form the main core of the B.Sc. level curriculum. Methodological skills and knowledge (needed in R&D of process engineering) are emphasized in an attempt to bind theory with practical elements of engineering. It has been noticed that this helps to motivate also practice-oriented engineering students to study theoretical topics such as thermodynamics. Engineering courses emphasizing the methodological skills may be based on e.g. experiments, analyses or modelling. In comparison to experiments and analyses, modelling and simulation often offer an easier, safer and cheaper way to introduce methodological aspects to engineering curricula. This paper focuses on the possibilites to use computational thermodynamics (CTD) at different stages of higher engineering education using HSC Chemistry –software as an example.

***Keywords* —** *engineering education; process and environmental engineering; thermodynamics; curriculum*

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Keywords—engineering education, process and environmental engineering, thermodynamics, curriculum

I. INTRODUCTION

Thermodynamics, and physical chemistry in general, are an essential part of process and chemical engineering [e.g. 1,2,3]. However, despite its universal nature there is no consensus on how thermodynamics should be taught in different fields of science [e.g. 3,4,5,6]. One example to classify the different perspectives to teach thermodynamics, as well as other natural sciences, is to divide thermodynamics education in three categories in which either classical theory, fundamental sciences, and scientific research (CFS), numerical methods, virtuality and computerization (NVC) or experience, practice, empirics and heuristics (EPE) are emphasized [6]. Furthermore, teachers and researchers of engineering education tend to emphasize the importance of practical relevance as well as the context in which thermodynamics is taught, learned and utilized [3,4,5]. One of the challenges of thermodynamics education is to find a balance between different approaches [6] and it has also been claimed that the overemphasis of analytical scientific skills in the engineering education has led into so-called excessive *scientification* due to which some other significant areas of engineering expertise have been neglected in the engineering education. Excessive *scientification*, together with inability to see the differences between science and technology, has been considered to be a serious problem in several academic engineering curricula [3,4,7,8,9,10,11]. Hence, it is important to ensure that in addition to theoretical and scientific approach (CFS), computational (NVC) as well as practical (EPE) approaches are also included in the engineering curricula.

The B.Sc. level process engineering curriculum at the University of Oulu in Finland has been planned according to a so-called DAS-formalism, which consists of descriptive, analytical and synthesis phases, through which the education is carried out. In comparison to more conventional engineering curricula, in which the analytical skills are emphasized and considered as a fundamental basis for further studies, one of the key issues in the DAS formalism is to begin the engineering studies with a descriptive phase, during which the focus is not on the analytical skills, but rather on the description of the phenomena and the processes that are to be mastered in the further studies. In other words the first phase of the DAS formalism focuses on outlining the relevant engineering field through description and the educational field is covered conceptually. This helps students to understand the meaning and relevance of the skills and concepts that are included in their curricula. Computational and analytical skills (“the mathematical arsenal”), even though central in engineering, are not introduced until the second phase. During this analytical phase, the educational goal is to learn to use tools and different functional approaches to solve technical and scientific problems. Finally, the aim of the last phase is to create a synthesis by binding the learned analytical skills into an entity. Progression of engineering studies according to DAS formalism is illustrated in Figure 1. [12] The B.Sc. level studies are followed by M.Sc. level studies during which students are specialized on more specific fields of process engineering such as process metallurgy.

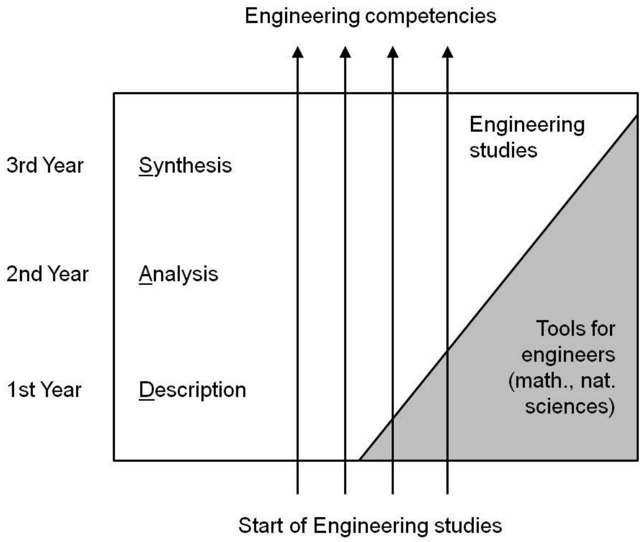

Fig. 1. DAS formalism in engineering education [modified from 12].

At the University of Oulu, Finland, it has been noticed that the curriculum based on the DAS formalism helps students to understand the engineering context in which analytical - or scientific - skills are used. This has led to better motivation in comparison to previous, traditional curriculum that began with analytical courses of mathematics, physics and chemistry. [12] The purpose of this paper is to illustrate how computational thermodynamics can be utilized in the different phases of the DAS formalism in the engineering education. The case studies presented in this paper are based on the use of commercial HSC Chemistry -software in the process engineering education at the University of Oulu.

II. Computational Thermodynamics at Various Stages of Higher Engineering Education

A. Descriptive studies

The purpose of descriptive studies is to describe the context and the key concepts of the process engineering. In thermodynamics, this means answering to the following questions:

1. What is thermodynamics and what does its key concepts mean?

2. In which applications is thermodynamics used in process engineering? What do you get as results?

3. What is the role of thermodynamics in process engineering? Why is it important to process engineers?

Obviously these topics could be dealed with different kind of educational approaches, but this chapter focuses on how computational thermodynamics (CTD) software could be used. It is worth noting, that although using CTD to answer these questions, it is not necessary for students to use software themselves at this stage of curriculum. Selected examples and cases from the research and development can be included in the education in order to presenting the use of thermodynamics in actual R&D problems within process engineering. According to the basic idea of the descriptive phase, it is not relevant to focus too much on how the results are obtained, but to emphasize the problem and the context in which thermodynamics is used, to present the actual problem for which CTD can offer solutions and to show students what kind of results may be obtained with CTD. By explicitly showing the context of the problems in which CTD is being used, it is also possible to include “engineering elements” to the curriculum and thus avoid the excessive *scientification* which may cause motivational problems with the engineering students as mentioned in introduction. Using this approach, the key concepts of thermodynamics (such as enthalpy or free energy) are not learned (only) via mathematical definitions, but by realizing what is their role in solving actual engineering problems.

HSC Chemistry contains several modules suitable at this stage of studies. For example modules used to compute equilibrium compositions of given systems (Gem) and create mass and heat balances (Bal) are often used R&D and hence the results obtained from these modules could be easily used as examples on how thermodynamics is used to solve engineering problems. As an analogy from another field, teacher could for example tell students, that whereas artificial intelligence expert system tells the medical doctor the name of the disease, when doctor has specified the symptoms, a process designer can solve what comes out from the chemical reactor after specifying the raw materials and conditions to the software. With a meaningful choice of examples, the very same results that illustrate the use of CTD in engineering R&D can also be used to illustrate certain fundamental principles such as the influence of temperature and pressure on the equilibria of chemical reactions according to the Le Chatelier's principle or effect of oxygen enrichment on the adiabatic flame temperature. A few examples on the use of Gem and Bal modules are shown in Figures 2 and 3.

In addition to the above mentioned Gem and Bal modules, other HSC modules could also be used at this stage for illustrative purposes. For example Dia module can be used to quickly draw diagrams in which various thermodynamic properties for different compounds are presented as a function of temperature. This feature can be used to illustrate the connection between Gibbs free energies and stabilities of different states (as presented in Figure 4) or to show how heat capacities of different kind of compounds change when temperature is increased (as shown in Figure 5).

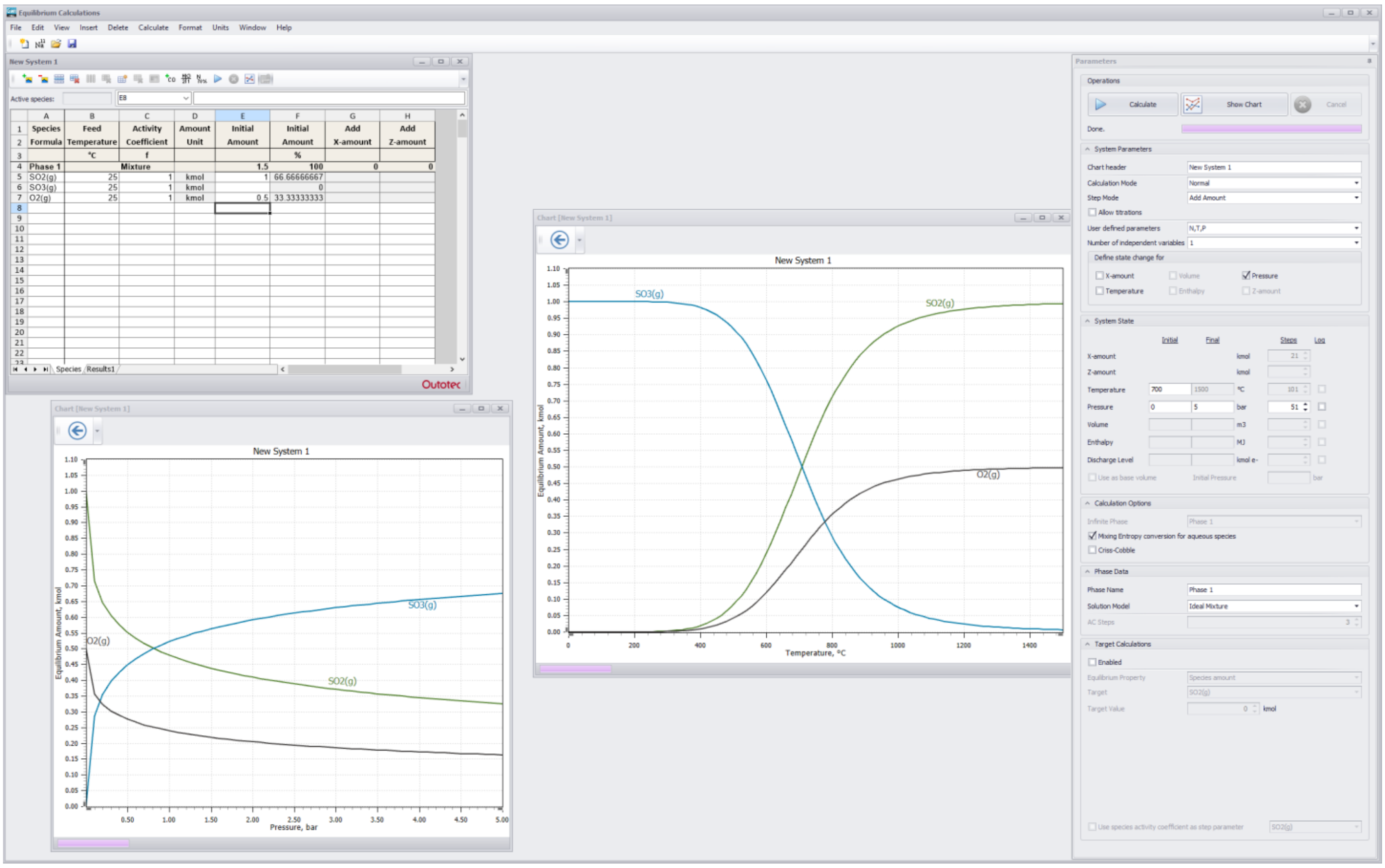

Fig. 2. Example on the use of the Gem module in HSC Chemistry. This example illustrates the Le Chatelier's principle by showing the effects of temperature and pressure on the chemical equilibrium between sulphur dioxide (SO_2) and sulphur trioxide (SO_3).

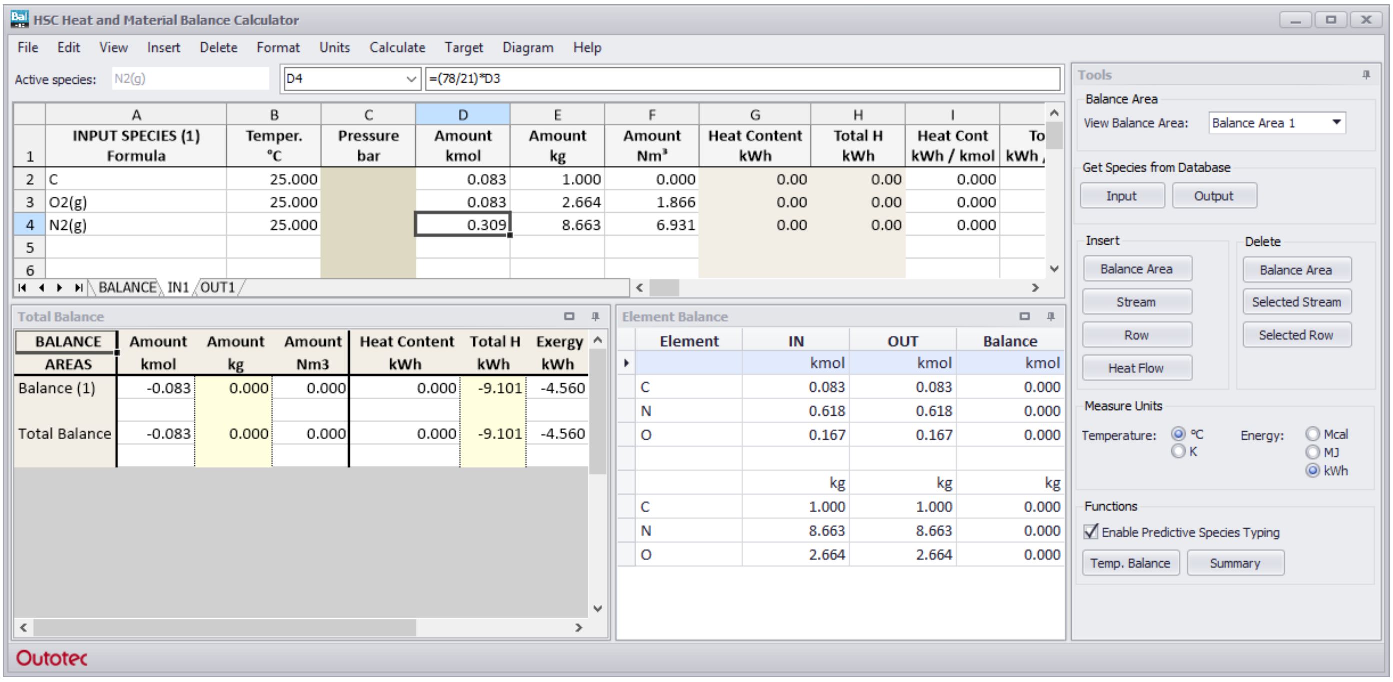

Fig. 3. Example on the use of the Bal module in HSC Chemistry. This example illustrates how much heat is released when burning carbon with air.

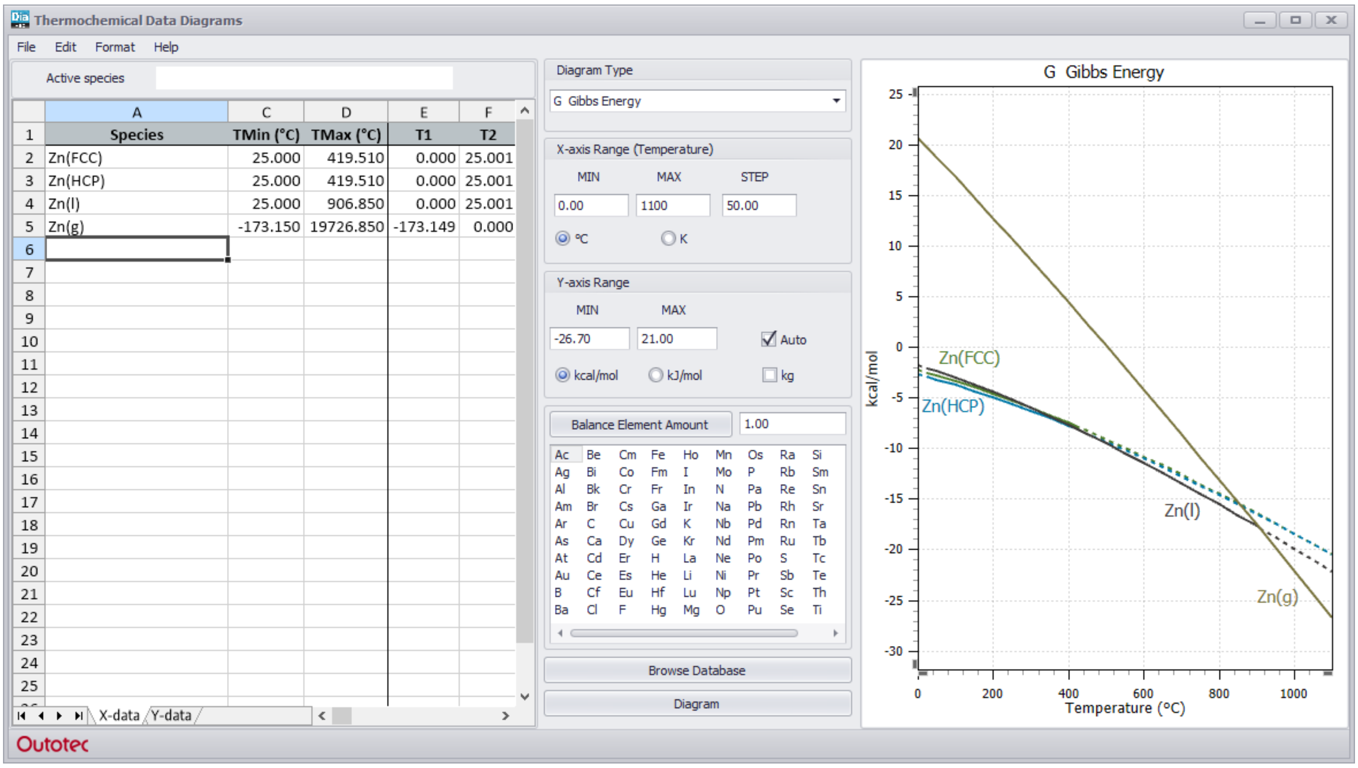

Fig. 4. Use of the Dia module of the HSC Chemistry to illustrate the Gibbs free energies of different states of zinc as a function of temperature. The phase with the lowest value of Gibbs free energy is the most stable in each temperature.

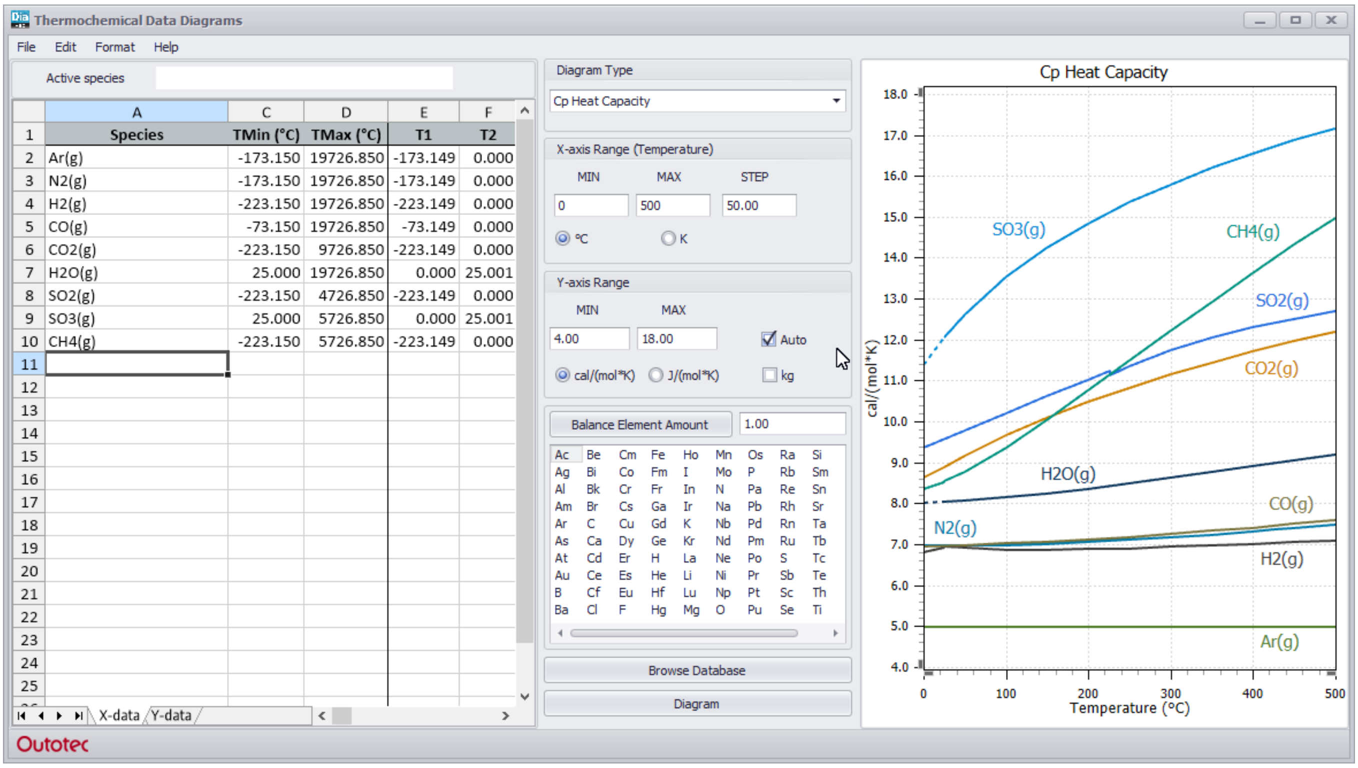

Fig. 5. Use of the Dia module of the HSC Chemistry to illustrate the change of heat capacities as a function of temperature for selected gas components. The figure illustrates how the values of heat capacity are increased with the increasing complexity of the gas molecules.

B. *Analytic studies*

The purpose of analytic studies is to learn to use tools and different functional approaches to solve technical and scientific problems. In thermodynamics, this means that students are required to learn for example:

1. How to create and solve mass and energy balances for systems with practical relevance?

2. How to solve chemical equilibrium for a given system?

3. How to consider the stabilities of different phases in given conditions (T, p) and how to define conditions in which given phases are stable?

Same modules of the HSC Chemistry that could be used during the descriptive studies (mainly Gem and Bal), can also be used during the analytic studies. However, at this stage students are given exercises and they are required to use the modules themselves in order to solve the given problems. In engineering problems it is common that mere calculations are not enough: it is equally important to be able to "quantify" real-life-problems into a form in which they can be solved computationally and also to interpret the results of the calculations in order to find solutions for the original problems. Although the students are not expected to be equipped with this kind of skills in their full scale at this stage of studies, the exercises are nevertheless chosen in a way that requires more than mere calculation. An example of system definition in the Gem module is shown in Figure 6.

Although the use of CTD software is a common practice in R&D, exercises solved without a software are also needed in order to properly learn the basics of thermodynamic computations. This kind of exercises help students to understand what kind of initial values are needed in the calculations, what kind of assumptions are required in order to use certain computational methods or models, how these initial values and assumptions have an effect on the results and so on. The open database of the HSC software (cf. Figure 7) is a valuable source of thermodynamic data needed in the creation of new exercises. In addition to this, the software can also be used to check the results of the "hand-made calculations". Additionally, Periodic chart (Ele; cf. Figure 8) and Measure units (Mea; cf. Figure 9) can be used to obtain properties of the elements and to make unit conversions.

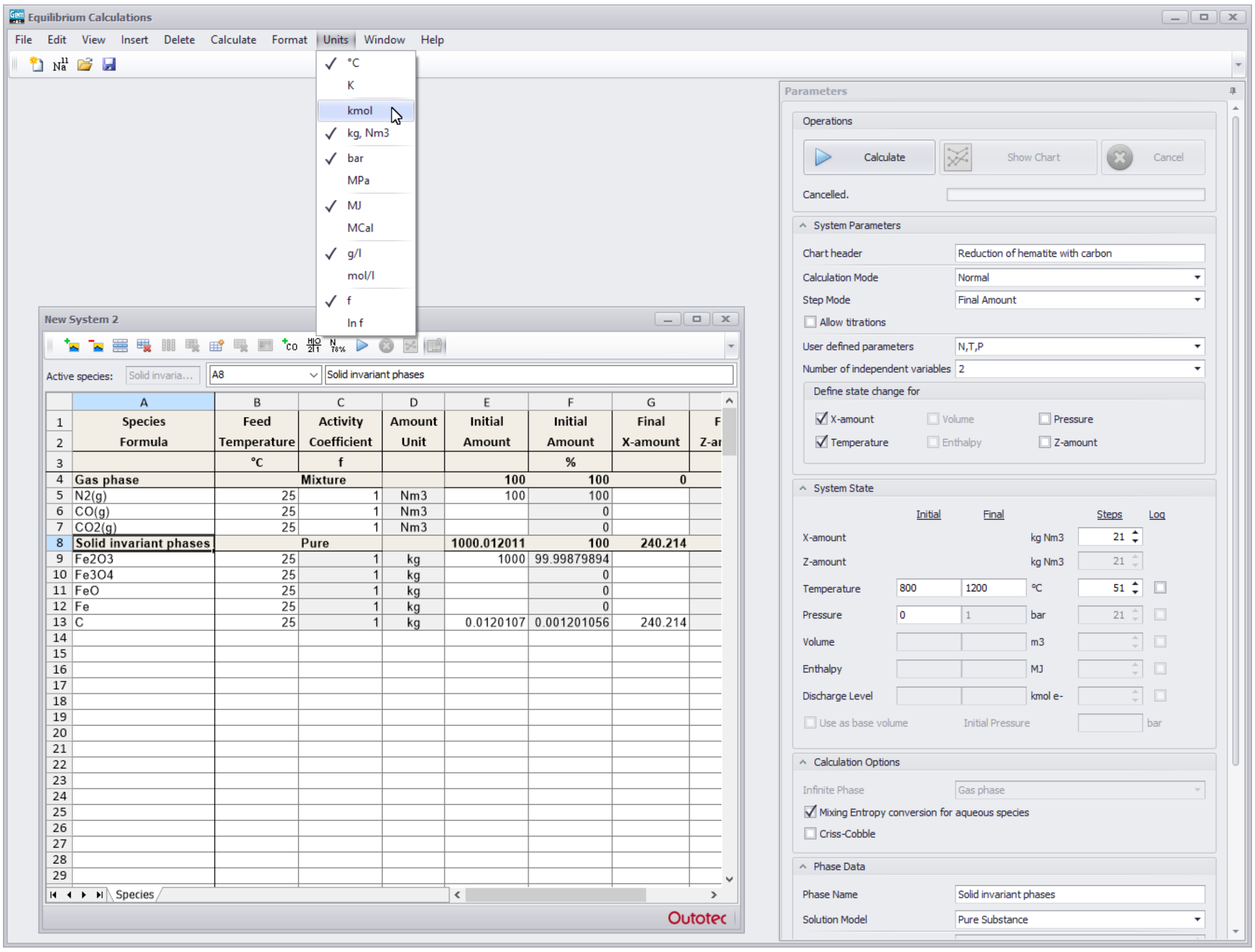

Fig. 6. Example of system definition in the Gem module of the HSC Chemistry. The purpose of this example is to study the reduction of hematite (Fe_2O_3) with carbon in different temperatures.

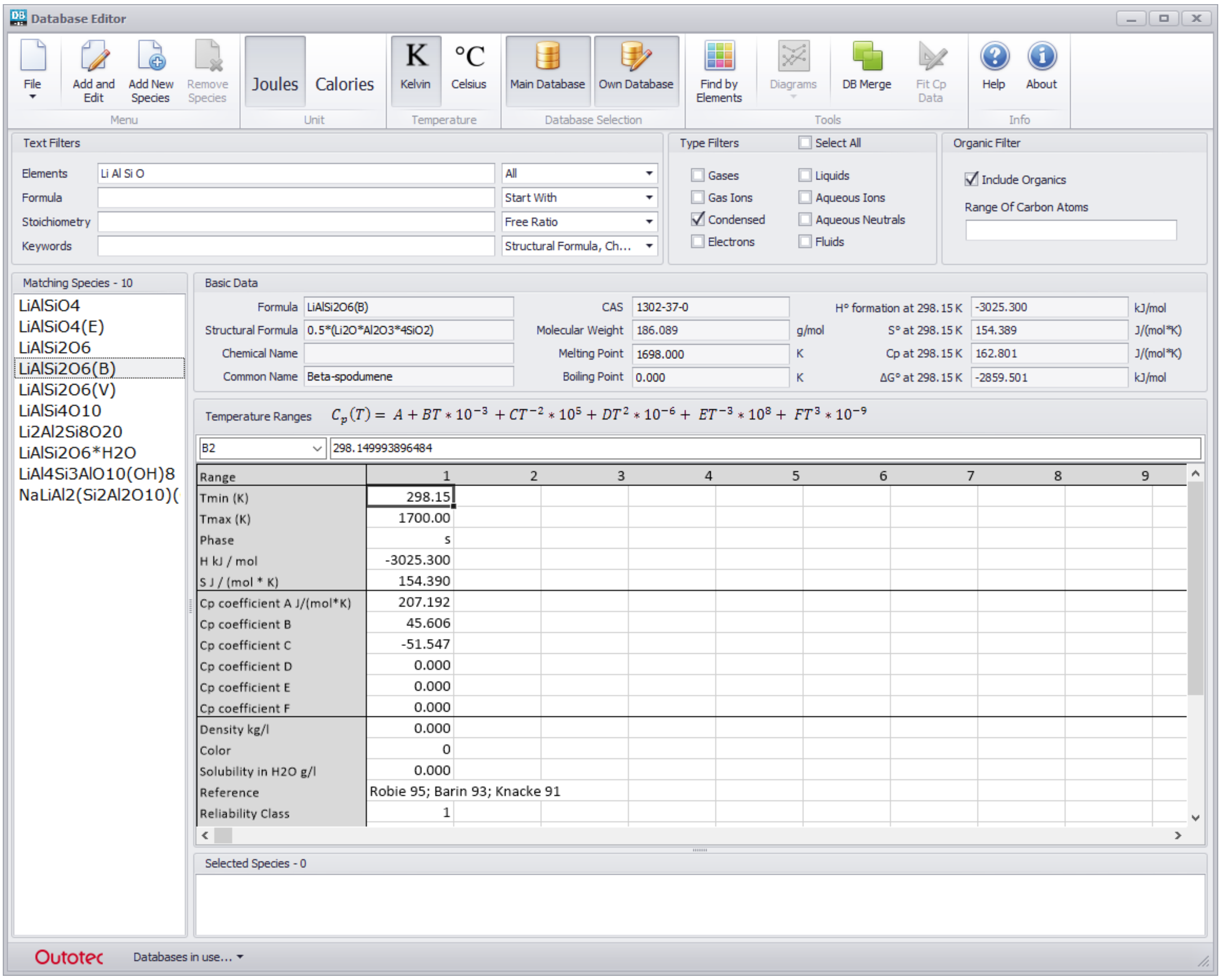

Fig. 7. Example of thermodynamic data (thermodynamic properties of β-spodumene) in the HSC Chemistry database.

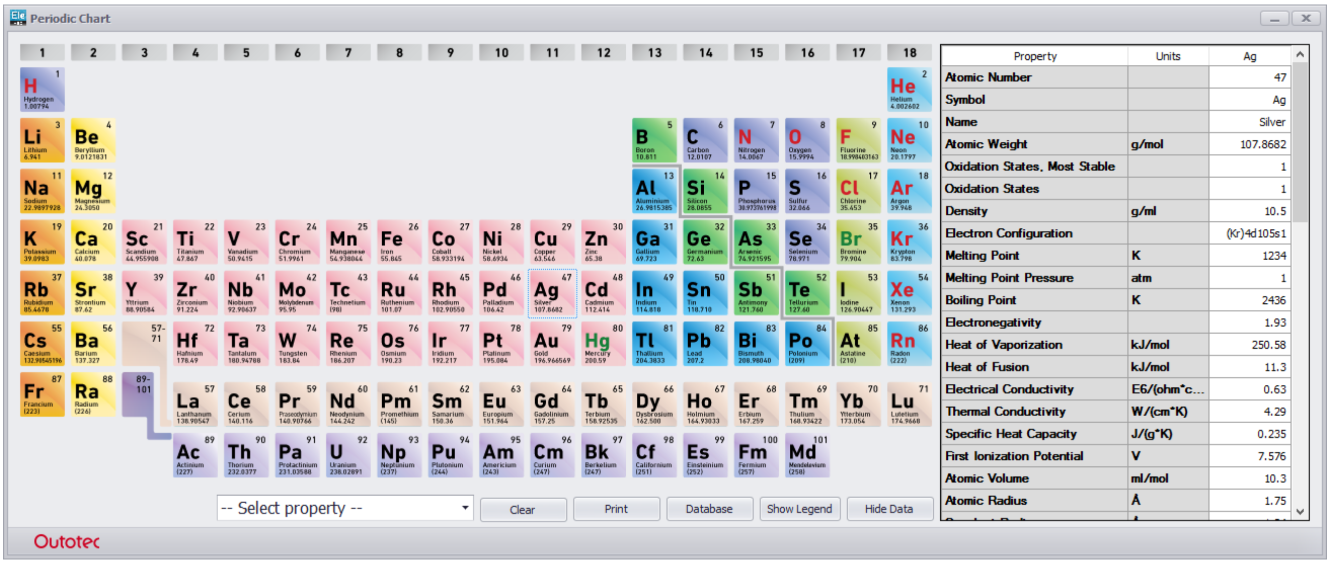

Fig. 8. Properties of silver as an example on the use of the Ele module in the HSC Chemistry.

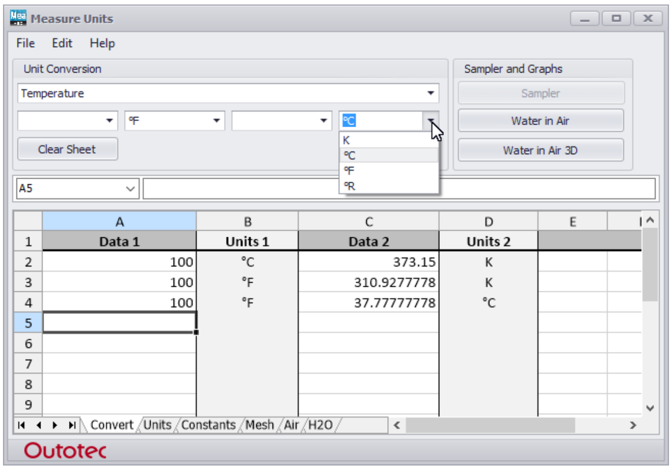

Fig. 9. Example of unit conversions using the Mea module in the HSC Chemistry.

HSC software contains several modules that can be used to create diagrams illustrating the stabilities of phases of given systems as a function of conditions. For example so called Ellingham, Kellogg and Pourbaix diagrams can be made using Dia, Lpp or Tpp and EpH modules, respectively. Examples of these diagrams are shown in Figures 10, 11 and 12.

With these kind of stability diagrams, it is easy to estimate as well as illustrate the influence of conditions (such as temperature, pressure or gas composition) on the stabilities of different compounds and phases. Due to fast and easy user interface, students can quickly make various estimations themselves and see the effect of changing variables and initial values on the results.

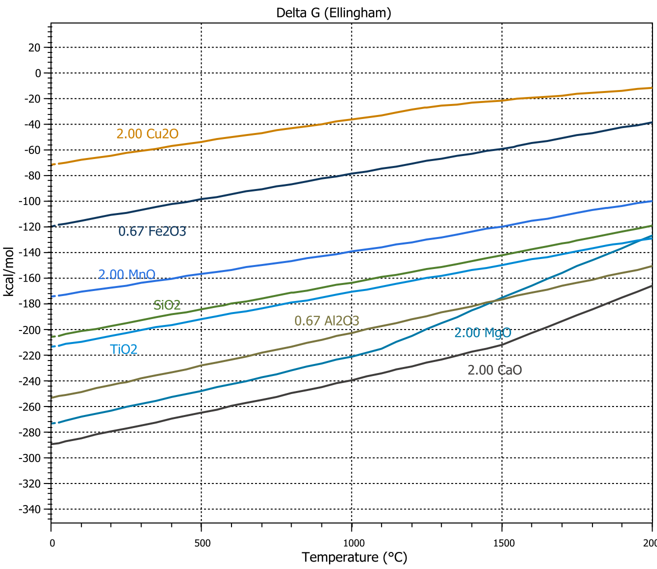

Fig. 10. Ellingham diagram drawn with the Dia module of the HSC Chemistry.

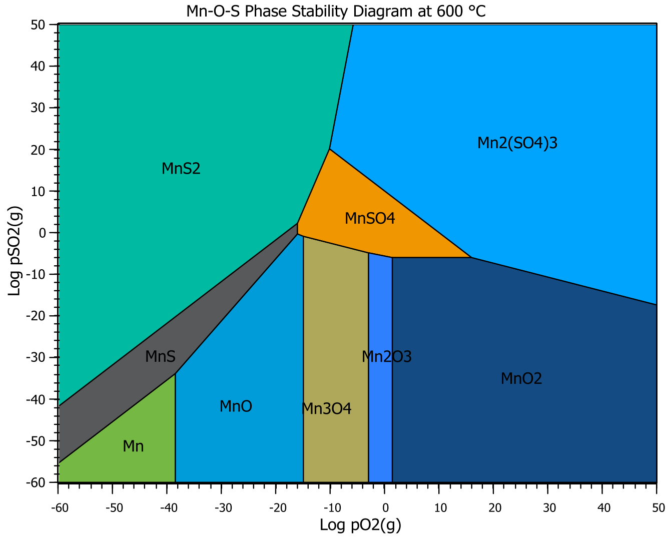

Fig. 11. Kellogg diagram drawn with the Lpp module of the HSC Chemistry.

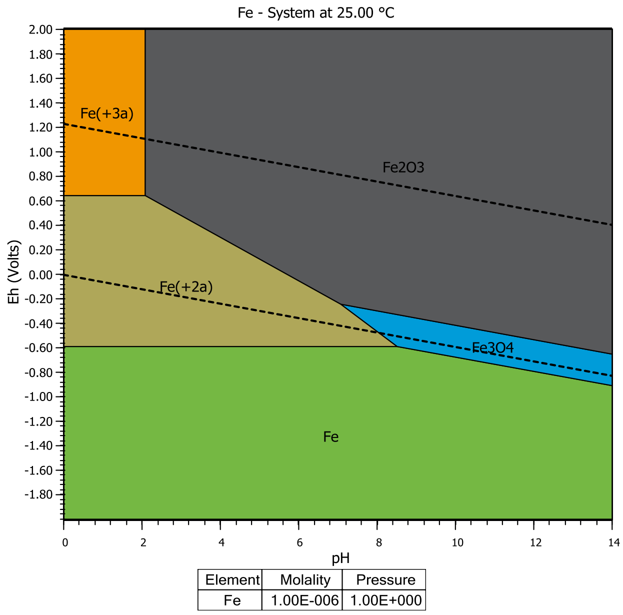

Fig. 12. Pourbaix diagram drawn with the Eph module of the HSC Chemistry.

C. Synthesis studies

The purpose of synthesis studies is to create a synthesis by binding the learned analytical skills into an entity. In thermodynamics, this means answering to following questions:

1. How CTD is used as a part of R&D in process engineering?

2. What are the possibilities and limitations of CTD?

3. How to interpret and utilize the results of CTD to find solutions to problems with practical relevance?

At this stage of studies Gem and Bal modules are still used to study chemical equilibria as well as heat and material balances, respectively. Since the learning outcomes of this stage emphasize larger entities, it is required to connect the results of various calculations together in order to solve the exercises at this stage. This means that to solve a certain problem or exercise a student is required to use several modules of the HSC software, as well as other modelling and/or experimental tools, and then find a result based on all the results. At this stage of studies, students could also be required to find some of the needed initial values themselves, i.e. all the initial values are not given with the exercise (as very rarely are in "real life"). One characteristic feature of the problems and exercises at this stage is the lack of unambiguity: there might be more than one equally correct ways to solve the given problems. Typical problems are related to e.g. process design in which thermodynamic considerations are used in addition to other methods (such as reaction kinetics and fluid dynamics).

Another HSC module that is very useful at this stage of studies, is the Sim module, that allows user to simulate the behavior of larger process systems. It is typical to HSC Sim exercises that students are required to find more information about the studied processes in order to be able to complete the tasks.

Generally speaking the exercises in the synthesis studies emphasize meaningful definition of studied systems as well as their correspondence with the real systems that are being considered, whereas the correct technical use of different modules was more emphasized during the analytic studies.

D. Advanced studies and theses

The B.Sc. level studies are followed by M.Sc. level studies during which students are specialized on more specific fields of process engineering such as process metallurgy, chemical engineering or automation engineering. The studies at the M.Sc. level depend very heavily on the area of specialization that the students have chosen. Hence, different things are emphasized in the education of thermodynamics, too. In general, larger exercises and more open-ended problems are used in comparison to more limited exercises during the B.Sc. level studies. At its best, M.Sc. level exercises can be part of research, while students work as research assistants in projects in which use of CTD is required.

III. DISCUSSION

The so-called DAS formalism consisting of descriptive, analytical and synthesis studies has been a basis for the B.Sc. level curriculum of the process engineering programme at the University of Oulu since 2005. Although computational thermodynamics was a part of some courses already before 2005, the methodological skills – including the use of CTD and other simulation tools – have been emphasized more heavily after the introduction of the DAS formalism. Generally speaking, there has been positive changes in both passing percentages and student feedback in the courses of thermodynamics since the change from more theoretical approach to more practical orientated courses and increased use of simulation tools. However, it would be difficult to distinguish – not to mention quantify – the effect of the use of CTD on the improved passing percentage and feedback, since more comprehensive studies concerning the connection between the use of simulation tools and learning outcomes has not yet been made.

The purpose of this chapter is to give a short overview on the roles and skills required from both teachers and students when dealing with the increased use of simulation tools in the education of thermodynamics. Overview is based on teachers' experience as well as student feedback.

A. Teacher's perspective on the use of CTD

Concerning the teacher's role in simulation oriented education of thermodynamics, it is essential to reserve enough time and to be prepared for guidance and tutoring (at the expense of mere lecturing) – especially in more open-ended problems of the synthesis studies and the advanced M.Sc. level studies. The CTD software, such as HSC Chemistry presented in this paper, have usually user interfaces that are relatively easy to use and fast to learn. Hence, the guidance is usually not focused so much on the use of software itself, but on how the given real-life problems are "quantified" into forms that can be solved computationally and how the results of the computations are interpreted. Additionally, students are usually not qualified to make validation of the simulation results themselves and need help on how to verify that the modelling has given them results that are realistic and relevant for the original problem. Since everything cannot be instructed individually for every student, it is important to consider in advance which topics and issues can be taught for larger groups, what students can study individually before the simulation exercises (for example with the help of short videos made available for the students) and what is taught and learned during the exercises themselves.

Since one of the goals of using simulation oriented education is to motivate engineering students with real-life problems, one of teacher's challenges is to be able to create problems and exercises that have enough practical relevance. Whereas actual industrial problems might be too large or too complicated for students to solve (at least during the earlier stages of studies), oversimplification of these problems might make them lose their practical relevance. Finding a balance between realisticity and simplification requires both pedagogical skills as well as knowledge on how (and in which applications) CTD is used in actual research and development. According to our own experience, a close co-operation between teachers and researchers as well as industrial and other partners has helped to find actual problems to be used as exercises.

Obviously one of the practical challenges in the use of CTD software is the updating of the software so that it truly is in line with methods and tools used in actual research and development. This requires not only economic resources to acquire new versions of the software, but also teachers to maintain and develop their skills in the use of the software. Use of an outdated software might have a negative effect on the students' motivation.

Finally, it should be noted that although (according to our expericence) the use of CTD is a suitable approach to teach thermodynamics in various stages of engineering education, one should be careful not to neglect other aspects of thermodynamics. Instead of excessive *scientification* it is quite possible to be guilty for excessive emphasis on numerical methods and simulations as well. Within individual courses, sufficient theoretical background and depth of core issues must be ensured in addition to practically relevant simulation exercises. Furthermore, co-operation between teachers of different courses is needed in order to ensure the functionality of the curriculum as a whole.

B. Student's perspective on the use of CTD

Similar to teachers, more active role is required also from the students in simulation oriented education in comparison to more theoretical approaches. Courses with simulation exercises are often based on continuous assessment, which requires students to take part actively throughout the whole course. According to student feedback, some students feel simulation oriented courses more demanding in the beginning, but most of them realise that the continuous assessment is actually not so heavy as the course advances.

Concerning the required skills, most CTD software have an easy user interface (as mentioned above) and, after a short introduction, the use of the software itself does not cause any difficulties for most of the students. However, most students need help while turning practical problems into problems that can be computed with the software. Therefore it is essential to reserve enough time for the exercises. According to the student feedback, sufficient time reserved for the exercises is one of the most essential prerequisites for the succesful use of CTD software.

Although simulation oriented approach with practically relevant exercises seems to be motivating for most of the engineering students, there are always some students that would have prefered an approach that would give less focus on the practical applications and more emphasis on theoretical background and thermodynamics as a whole. According to our experience, it has been helpful for these students, when they have been instructed to familiarise themselves with a textbook that gives a more comprehensive outlook on thermodynamics. In many cases it has been enough for them to get acquainted with just the contents of the textbook in order to get an overview on the different aspects of thermodynamics. This overall picture has helped them to see the role of simulation exercises as a part of thermodynamics and thus increased their motivation for the simulation exercises as well.

IV. SUMMARY

Use of simulation exercises is an essential part of the engineering education curricula. Methodological skills related to modelling and simulation create connections between theory and practice [cf. 13, 14], which helps students to understand the role and relevance of theoretical studies (such as mathematics, physics and chemistry) when they have a chance to apply their theoretical knowledge in real-life-related problems using tools that are actually used in R&D projects. Obviously, the connection between theory and practice could also be achieved using other methods such as experiments, analyses and process campaigns, but in the end it is easier, cheaper and more flexible to use simulation exercises. Concerning the education of thermodynamics, CTD software such as HSC Chemistry offer a versatile tool that could be used in various stages of education as described in the previous chapters.

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