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Theoretical background

This section includes the scientific background and a description of conceptions, understandings and algorithmic/conceptual questions, and ends with previous research findings.

Scientific background

Enthalpy H and internal energy U and their changes are related, but the similarities and differences are complex. They are state functions, and the changes include heat and work. The unit is Joule (J) and internal energy is the sum of different forms (Kaper and Goedhart, 2002), but neither enthalpy nor enthalpy change can be transformed into a form of energy. Both ΔU and ΔH can be used to describe what happens during a chemical reaction, for instance bond energy or bond enthalpy, but in upper secondary school and at the undergraduate level enthalpy and its change are often used instead of internal energy and its change. A change in enthalpy is defined as $dH = dU + d(pV)$ or $\Delta H = H_2 - H_1$. Since $d(pV)$ is a change of a product, mathematics states that $d(pV) = p dV + V dp$. The overall change of H does not depend on the path taken from H_1 to H_2 , but dU is path-dependent and $\Delta U = q + w$ is valid for a closed system (Laidler *et al.*, 2003; Atkins and de Paula, 2005; IUPAC, 2007). One reason to introduce enthalpy and its change is the possibility to disregard the expansion work, since $dH = dU + d(pV)$ or $dH = dq + dw + dw' + p dV + V dp$ where d indicates a path-dependent variable and w' , for instance, is electrical work. The above equation probably contains mathematical notions that undergraduate chemistry students are unaware of, and a more simple – although not entirely correct – way is to express the definition as $\Delta H = q + w + p\Delta V + V\Delta p$.

If expansion work is defined as $dw = -p_{\text{ex}} dV$ where p_{ex} is the external pressure (*i.e.* the pressure the system does work against in order to expand), hence $p_{\text{ex}} = p$, the equation becomes $dH = dq + dw + V dp$, which is integrated into $\Delta H = q + w' + V\Delta p$. If the pressure is constant, like in many chemical reactions, $\Delta p = 0$. If no other work is allowed, $w' = 0$, the enthalpy change is heat at constant pressure $\Delta H = q_p$. However, enthalpy changes may also be determined as $dH = dq + dw + dw' + p dV + V dp$, which, at constant volume $dV = 0$ and when no other work is allowed, becomes $dH = dq + V dp$ or integrated $\Delta H = q + V\Delta p$, where $V\Delta p$ is technical work. In many undergraduate textbooks the constant pressure and only expansion work case is emphasized (*e.g.* Chang, 2007; Zumdahl and Zumdahl, 2007), but sometimes this definition is not valid (*e.g.* in a fuel cell where $w' \neq 0$).

Conceptions

Research on conceptions may be “concerned with the qualitative differences among the conceptions that students use to explain scientific phenomena and examine students’ topic-related understanding of scientific concepts” (Duit and Treagust, 1998, p. 6). Conceptions are often viewed as mental models (Petri and Niedderer, 1998; Hartmann and Niedderer, 2005; Treagust and Duit, 2008a, 2008b). Single individuals (Harrison *et al.*, 1999) and groups of students (Thomas and Schwenz, 1998)

have been followed, and students’ conceptions of single concepts (*e.g.* Carson and Watson, 1999), single tasks (*e.g.* Sözbilir, 2001) or a phenomenon (*e.g.* Andersson and Wallin, 2000) have been researched. Different methods and techniques have been used, and the tradition is mostly cognitive or constructivist whereby individuals have parallel conceptions (Petri and Niedderer, 1998; Hartmann and Niedderer, 2005), a conceptual profile (Mortimer, 1995), misconceptions and preconceptions (Driver and Easley, 1978) or intermediate conceptions (Driver, 1989; Niedderer *et al.*, 2007).

The scientific concepts serve as a frame when analysing students’ responses. Then, descriptions of how students perceive the theory differently may be constructed. Alternative conceptions are different from the scientific descriptions (Carson and Watson, 1999) and may arise due to the use of similar words in, for instance, everyday life or formal and informal education, which may lead to robust frameworks such as the physical framework forms of energy, which often describe how students understand chemical thermodynamics (Carson, 2001; Goedhart and Kaper, 2002). However, conceptions are never nonsense (Vosniadou, 2008a), can exist in parallel (Petri and Niedderer, 1998; Hartmann and Niedderer, 2005), and are more likely to occur in some situations (Mortimer, 1995). Therefore, one aim of science teaching is to let students develop a more valid scientific conception, and the conceptual change may be done in many ways (Vosniadou, 2008b). On the path towards the scientific conception, different intermediate conceptions may be identified (Petri and Niedderer, 1998).

Understanding and algorithmic/conceptual questions

Conceptual understanding is a complex phenomenon (Nieswandt, 2007). Often, the question is “Does he/she understand X?” and the answer is yes or no (White and Gunstone, 1992), thus not offering any relevant information. *How* someone understands X is a more valid question. Darmofal *et al.* (2002) summarize conceptual understanding as the ability to apply knowledge to a range of examples and circumstances that are not necessarily known beforehand. Using, adapting and changing the knowledge is also necessary, but teaching is often focused on promoting a fragmented acquisition of discrete facts and algorithms instead of creating a knowledge structure (Claesgens *et al.*, 2002). In research, both tasks/problems or the answer given may be quantitative or qualitative. Also, questions can be solved algorithmically or conceptually (Bowen and Bunce, 1997). For instance:

- Quantitative questions with algorithmic or conceptual answers.

What is the enthalpy change when MgO is formed if 3.4 g Mg is burnt in air? (algorithmic)

If 3.4 g Mg is burnt in air is the enthalpy change more, less or equal to -601.7 kJ? (conceptual)

- Qualitative questions with algorithmic or conceptual answers.

When is the enthalpy change the heat? (algorithmic)

In which set of apparatuses does the measured heat equal the enthalpy change? (conceptual)

In this description, questions with numerical values are quantitative and the answer is either algorithmic (calculation) or conceptual (motivation). Mazur (1997) uses conceptual (theoretical)–conventional (calculation) questions instead. In this study, the terms *qualitative* and *conceptual* are used synonymously in order to describe students' understanding or the characteristics of a question. In Mazur's study about 52% of the students succeed equally well with both kinds of questions, 9% are less fortunate on the conventional questions and 39% are less fortunate on the conceptual questions. But Mazur's results were not unique.

Bodner and Herron (2002) write that "Problem-solving research has provided strong evidence that our students, successful as well as unsuccessful problem solvers, don't grasp the concepts very well. Indeed, one of the most important contributions of research in this area has been the revelation of just how poorly students may understand the ideas underlying problems they have answered correctly. This revelation is despite the fact that teachers frequently justify their emphasis on numerical problem-solving by arguing that it enhances conceptual understanding" (p. 259). Related to Bodner and Herron's statement is how exams are designed (White and Gunstone, 1992), since many teachers believe that numerical problem-solving will enhance conceptual understanding and therefore primarily include calculations in exams. However, algorithmic problem-solving exercises do not promote conceptual understanding and students will, most likely, never get that far (Gabel, 2003). Empirical evidence suggests that a real problem exists since science teaching does not prepare students for conceptual problem-solving (e.g. Kim and Pak, 2002; Gabel, 2003). Students are most likely to succeed in doing chemical thermodynamics calculations, but lack qualitative understanding (e.g. Goldring and Osborne, 1994; Carson and Watson, 1999, 2002; Sözbilir, 2001). The course content must be reduced and qualitative aspects must be addressed prior to algorithmic problem-solving. Carson (2001), Gabel (2003) and Johnstone (2010) argue in a similar manner. In this study, qualitative or conceptual understanding of enthalpy and enthalpy

change is an amalgam of the following statements, which all the written tasks and interviews addressed in some way:

- The student shows that he/she is aware of when and whether enthalpy and enthalpy change are applicable to a certain problem. This corresponds to the purpose of introducing the concepts in the scientific theory.
- The student uses enthalpy and enthalpy change to explain a phenomenon (e.g. reaction or experiment).
- The student uses enthalpy and enthalpy change to predict a phenomenon.
- The student explains the difference between enthalpy, enthalpy change and related concepts.
- The student uses enthalpy and enthalpy change in more than one context.
- The student interprets and analyses a phenomenon with the aid of figures and diagrams.

Previous research findings

In chemistry education researchers have mainly focused on bonds, bond energies and enthalpy change (e.g. Granville, 1985; Boo, 1998; Barker and Millar, 1999, 2000; Boo and Watson, 2001; Galley, 2004). Both Carson (2001) and Sözbilir (2001) argue that there are too few empirical studies investigating undergraduate students' understanding of chemical thermodynamics. The results presented below are obtained from both physics and chemistry education research, and different ages are covered. In the latter part of this section the focus is on results regarding enthalpy, its change, heat and expansion work.

Table 1 shows conceptions of heat and work that are relevant to this study as approximately the same ages are covered. As seen in Table 1, the first law of thermodynamics ($\Delta U = q + w$) is problematic for students: heat and work as states instead of processes and parts of the energy conversion between different forms (e.g. Johnstone *et al.*, 1977; Driver and Warrington, 1985; van Roon *et al.*, 1994; Sözbilir, 2003).

In chemistry, heat and work are energy inputs or outputs and not forms. They stem from the fundamental process known as a chemical reaction, hence bond breaking and bond formation.

Table 1 General results and conceptions of heat and work. Students = undergraduate students. Results about heat are presented first, then energy, and finally work

Results and conceptions	Age	Source	Relevant for conception(s)
Heat is a form of energy	6–13	Sözbilir (2003, p. 28)	F4
Heat is not an extensive quantity but an intensive one	Adolescents and adults	Lewis and Linn (1994)	
Two bodies with the same temperature have the same energy or heat	15–16	Sözbilir (2003, p. 29)	F6
Heat is considered a state quantity instead of a process quantity	15–16	Sözbilir (2003, p. 29)	F6
q , heat, is energy and the unit is Kelvin ($q = T$ or $q = \Delta T$ is used)	Students	van Roon <i>et al.</i> (1994)	F5
The amount of heat liberated does not depend on the work done	Students	Greenbowe and Meltzer (2003)	F4
Energy and work are not separated	~16–18	Johnstone <i>et al.</i> , (1977)	F6, F7
Work is always involved when energy is transferred	13, 16, 18	Driver and Warrington (1985)	F5
Instead of a thermodynamic concept, work is generally considered a mechanical concept	13, 16, 18	Driver and Warrington (1985)	F2
Work is regarded as a convertible form of energy instead of a form of energy conservation	Students	van Roon <i>et al.</i> (1994)	F2
Work is not genuinely seen as a process	Students	van Roon <i>et al.</i> (1994)	F2
The gas leaving the system brings energy with it and this energy is the work	Students	Carson (2001)	F2

Table 2 Results and conceptions of enthalpy, enthalpy change, heat and pV work. Students = undergraduate students

Results and conceptions	Age	Source	Relevant for conception(s)
Endothermic and exothermic are solely based on the sign of ΔH	Students	Granville (1985)	F1, F5
Imprecise terminology regarding enthalpy and enthalpy change	Students	Beall (1994)	F5
Prior to teaching, work is not associated with chemical reactions	Students	Carson (2001)	F2
pV work is unknown prior to teaching	Students	Carson (2001)	F2
Post teaching, work is sensitized but the meaning remained unclear	Students	Carson (2001)	F2
Post teaching, a moving piston or raising of a weight is needed to recognize work	Students	Carson (2001)	F2
Students frequently forget one or several of heat, constant pressure or pV work as they define enthalpy change, making the definition incomplete	Students	Carson (2001)	F1, F6, F7, F8
Enthalpy is a form of energy	Students	Carson (2001)	F4
Enthalpy change is heat at constant volume	Students	Carson (2001) and Sözbilir (2001)	F1, F6, F7, F8
Enthalpy change is heat since no work is done	Students	Carson (2001) and Sözbilir (2001)	F7
Students can calculate the reaction of enthalpy but are not aware that it equals the heat	Students	Sözbilir (2001) and Greenbowe and Meltzer (2003)	F1, F5
The same amount of heat is given out to the surroundings at both constant p and V	Students	Sözbilir (2001)	F6
Bond enthalpies are used in Hess' law instead of formation enthalpies	Students	Teichert and Stacy (2002)	F4
Students separate ΔG from ΔH but they do not know the difference	Students	Ribeiro <i>et al.</i> (1990)	F5
If work is described, the most common way of doing this is without reference to volume and pressure	Students	Nilsson and Niedderer (2012)	F1, F2
When work is described, specific descriptions of volume and its change are more common than specific descriptions of pressure	Students	Nilsson and Niedderer (2012)	F1, F6, F7, F8
Expansion work is not described correctly in actual situations	Students	Nilsson and Niedderer (2012)	F1, F6, F7, F8
Technical work is not often described	Students	Nilsson and Niedderer (2012)	F6, F7, F8

The relationships between bonding and thermodynamics are difficult for upper secondary students to understand and, in fact, students make no links between the two areas (Barker and Millar, 2000).

In Table 2 the main results with respect to enthalpy and its change, (internal) energy and its change, heat and work are summarized. Note that Carson's (2001) results on enthalpy and expansion work can also be read in Carson and Watson (1999). According to Carson (2001), work is sensitized post teaching, even if the meaning is still unclear. Post teaching, four of 22 students explain expansion work acceptably, while eight have a range of alternative conceptions. The most common one, held by three students, is that gas only does work when it pushes a piston. Also, work raises weights and is hence considered a mechanical concept, as previously stated by van Roon *et al.* (1994). According to Carson (2001), one problem is that university teachers assume prior knowledge regarding some concepts (*e.g.* heat and work), and she suggests that thermodynamic entities are defined qualitatively before they are defined quantitatively; for instance, in Carson's study empirical evidence suggests that students have a limited understanding of the expression $\Delta H = \Delta U + p\Delta V$; they read it but do not know the meaning of the symbols.

One issue regarding enthalpy changes is the relationship between enthalpy and reaction heat, since a majority of students do not distinguish between heat and reaction enthalpy (Sözbilir, 2001). A similar result is presented by Greenbowe and Meltzer (2003) regarding calorimetry, system/surroundings and reaction heat. In the calorimeter the measured heat is the enthalpy change due to constant pressure and only expansion work, and the authors state that "It is notable that none of the students in this study acknowledged the fact that since the reactions occurred under conditions of constant pressure, the heat of reaction (q_{rxn}) is equal to the enthalpy

change of the reaction (ΔH_{rxn})" (p. 786). The results expressed by both Sözbilir (2001) and Greenbowe and Meltzer (2003) are comparable since heat and reaction heat, enthalpy change and reaction enthalpy are, in the described situations, identical. Two authors have previously criticized the imprecise terminology of chemists and textbooks (Zemansky, 1974; Beall, 1994). The use of terminology leads to a situation in which enthalpy and enthalpy changes are expressed synonymously, for instance *enthalpy of vaporization* instead of *enthalpy change due to vaporization* (Zemansky, 1974). The result is that students do not realize that Δ indicates a change in enthalpy or free energy. Following Beall's (1994) line of argument, there is a problem in the relationship between the concepts. Enthalpy is related to the process, but Beall does not mention the condition of constant pressure. However, constant pressure is also problematic since students describe enthalpy change as heat at constant volume (Carson, 2001; Sözbilir, 2001). Accordingly, students make connections between enthalpy change and expansion work, arguing that enthalpy change is heat when no work is done ($\Delta V = 0$). Five of 22 students in Carson's (2001) interview study explicitly state constant volume, and Sözbilir's (2001) analysis of questionnaire responses groups this description as one of four that together form one misunderstanding. Recently, Nilsson and Niedderer (2012) have analysed how students use pressure and volume when describing work, expansion work and technical work. Their contextual analysis shows that about 86% and 69% of the descriptions offered by two groups of students, respectively, are either incomplete or incorrect. However, they point out that students more easily relate volume to work than pressure.

Furthermore, Carson (2001) describes that students perceive enthalpy as a form of energy and the framework *forms of energy*, which guides their understanding of enthalpy, entropy and

Gibbs energy (Carson and Watson, 1999, 2002; Carson, 2001). Also, students often describe heat and work as forms of energy (van Roon *et al.*, 1994), which is labelled the forms of energy context and serves as a framework for how students understand thermodynamics (*cf.* Goedhart and Kaper, 2002; Kaper and Goedhart, 2002). In the forms of energy context, energy is transformed between different energy forms and the internal energy is the sum of the different forms. In chemistry education research, it is shown that the different forms are not transferable to a chemistry context (Martins and Cachapuz, 1990).

Research design and methods

Here the design and sampling as well as the different data collections are described.

Design and sampling

The research design was flexible, explorative and small-scale. A flexible design can be characterized as open to input during the research process (Robson, 2002). The design, data collection methods and data analysis affected each other. An explorative design tries to determine what is happening, seeks new insights and searches for possible results that can be further investigated. It generates hypotheses rather than confirmations, and as a consequence the results presented here can be further elaborated. In Fig. 1, a chronological description of the empirical studies is presented. Some general connection to previous research, data collection and the results in the different studies are also shown. The pilot studies are not described in detail here, but both were designed to increase the researchers' awareness of students' preconceptions regarding different contents generally taught in an undergraduate chemistry course. Also, the pilot studies provided details for the development of the main study, for instance a focus on students' understanding of enthalpy, enthalpy change and related concepts as qualitative/conceptual questions were included (*cf.* Bowen and Bunce, 1997; Mazur, 1997; Claesgens *et al.*, 2002; Kim and Pak, 2002; Niaz, 2002; Gabel, 2003).

During ongoing empirical studies, all chemistry programs at the university were cancelled and therefore the design of the main study became small-scale. Instead of $n \approx 60$, a total number of 22 students participated. As a consequence another

small-scale ($n = 10$) follow-up study was conducted at a different university; see more below.

The sampling was always based on voluntary participation and followed the non-randomized principles of "convenience sampling" (Bryman, 2008, p. 183) and "purposive sampling" (Bryman, 2008, p. 458). The difference between these types is that the former is based on available informants and factors the researcher cannot control, while the latter is based on a specific purpose that guides the sampling, and only people relevant to the research questions are included. How participants are chosen affects generalizability and, as volunteering is important, the entire sampling process is to some extent already biased.

With respect to the focused aim from the pilot studies of the main study, categories describing students' answers regarding different contents were created. Here, only categories regarding enthalpy, enthalpy change and related concepts were developed, and in order to saturate them a follow-up study was designed. A comparable group was purposely sought at another university, but the teacher found the tasks too difficult and suggested a group taking a course in chemical thermodynamics at the same university instead. This course was at a more advanced level than the undergraduate course and had fewer students, whom were asked to participate. Table 3 summarizes the data collection instruments and number of participating students in all studies.

Data collection

Here, the data collections in the studies are described, with focus on the main and follow-up studies (see Table 3). In Appendix 1 the most important questions in the study are summarized. During the research process, the ethical guidelines developed by the Swedish Research Council (Vetenskapsrådet, 2002) have been followed.

Table 3 All instruments used and number of participating students. PSs = pilot study with students, HS = main study, FS = follow-up study

Study	Instrument	Number of students
PSs	Questionnaire pre teaching	64
	Interview pre teaching	7
	Video lab open calorimetry and Hess' law	3
	Video lab electrochemistry	2
	Questionnaire post teaching	30
	Video Ellingham diagram	8
	Interview at the end of semester	5
HS	Questionnaire pre teaching (HSE1)	12
	Interview pre teaching (HSI1)	5
	Exam 1a (HST1a)	17
	Exam 1b (HST1b)	16
	Exam 2a (HST2a)	17
	Exam 2b (HST2b)	14
	Questionnaire four weeks post teaching (HSE2)	6
	Interview four weeks post teaching (HSI2)	4
FS	Questionnaire pre teaching (FSE1)	9
	Hand-in 2 (FSInl2)	9
	Hand-in 3 (FSInl3)	7
	Exam (FST)	9
	Questionnaire two weeks post teaching (FSE2)	6

Fig. 1 A general and chronological description of the empirical studies. HT = fall, VT = spring, PSI = pilot study with teachers, PSs = pilot study with students, HS = main study, FS = follow-up study.

Pilot study with teachers and students. The pilot study with teachers included both a questionnaire and a semi-structured follow-up interview (Kvale, 1996). This data collection was open and was aimed at finding interesting features to investigate further and use in order to develop appropriate tasks. Both previous research (e.g. Boo, 1998; Barker and Millar, 1999, 2000; Carson and Watson, 1999; Boo and Watson, 2001) and textbooks (Andersson *et al.*, 2000; Clayden *et al.*, 2001; Atkins and de Paula, 2005) were used, and different subject matter in chemical thermodynamics (e.g. enthalpy, bonds, boiling point, equilibrium, Gibbs energy and entropy) was included. In the pilot study with students, hypotheses were generated for further research.

Main study. The main study was designed to explicitly probe these hypotheses and investigate the effect of introducing qualitative/conceptual questions in exams; hence the aim became narrower. The written questions were formulated to address as many aspects of qualitative/conceptual understanding as possible; see statements above. As a result, different techniques were used (e.g. multiple choice, yes/no, explanatory or descriptive); see more below.

In order to fit the setting, most questions were either new or redesigned from previous research (cf. Thomas and Schwenz, 1998; Carson, 2001; Sözbilir, 2001; Galley, 2004). In some cases, for instance one multiple choice question, the distractors were the results from the pilot study: Question (a) was *Have you previously heard the concept (word) enthalpy?* with the possible answers *Yes*, *No*, and *Don't know*. Follow-up Question (b) was *Which of the following alternatives do you consider to be the best explanation of enthalpy?* with the possible answers (1) *It describes the energy change for a reaction*; (2) *It describes the heat transfer during a reaction*; (3) *It describes a possible state for a system*; (4) *It describes bonds being broken and formed*; and (5) *None of the above, since...* As can be noted, alternatives 1, 2 and 4 are related to enthalpy change instead of enthalpy. Another task was one developed from Sözbilir's (2001) original. It was a key task in the data collections, and the reaction between magnesium metal and hydrochloric acid in a closed apparatus at either constant pressure A or constant volume B was visualized. The questions were (a) *In which set of apparatus, A, B or both, do you think most heat is given out to the surroundings?* and (b) *In which set of apparatus, A, B or both, does energy transferred as heat equal the reaction enthalpy?*

This task, together with a figure, was used during the following data collections: HST1a as Question 5ab and HSE2 as Question 7ab.

Since some questions/tasks were used in exams the course teacher, L3, had the final say on which ones to include and how they were included. In the interviews, the students explained three or more of the following reactions taking place in front of them: the endothermic dissolution of ammonium chloride, the exothermic dissolution of sodium hydroxide, the decomposition of sodium hydrogen carbonate and the reaction between magnesium and hydrochloric acid. These reactions have been used before in chemistry education research (e.g. de Vos and Verdonk, 1986; Boo, 1998; Carson, 2001). In the main study,

categories describing the content-specific understanding were constructed. In total 969 written responses were analysed, resulting in 115 pages of transcripts.

Follow-up study. The follow-up study was designed to explicitly probe the categories constructed in the main study and to saturate them. Hence, the aim was further focused on enthalpy, its change and related concepts. The task based on Sözbilir's (2001) original, used in the main study, was used during FSE1 as Question 3ab and FST10ab. But, the figure in the task was further redesigned and used during FSInl2 as Question 9ab and in FSE2 as Question 4ab due to students' misinterpretation of the figures during the main study (see Conception F9). A total of 222 responses were analysed.

Qualitative analysis

Niedderer's (2001) description of iterative analysis and the analytical methodology of this study are described here.

Qualitative analysis by Niedderer

Fig. 2 shows an applied version of Niedderer's (2001) description of iterative analysis. Iterative means that the analytical process includes both inductive and deductive elements, hence abduction. The aim of the analytical process is to generate theoretical descriptions, conceptions, about students' understanding of some content or phenomenon. The analysis is affected by the researcher's frame of reference and data collected during the research process. Examples of the first are the use of previous research, the scientific content and the wish to offer implications for teaching. These factors influence the researcher to interpret data in a certain way, although Niedderer emphasizes theoretical frames more than is described in Fig. 2. Depending on how the theoretical frames are applied, the researcher can approach the data either deductively or inductively, for instance if hypotheses from previous research form the basis of the analysis or not. If an inductive step is taken, it is not in its most absolute form since there is a frame of reference.

In Niedderer's description, iterative also means that the process is systematic and non-linear. It means that data analysis has a determined purpose but the analytical path cannot be pre-determined. The data and the frame of reference create a process which cannot be predicted but instead has to be described afterwards.

The relationship between this description and the actual analysis is described below, and at the same time the example will clarify the dynamic nature described in Fig. 2. The method of

Fig. 2 The iterative process for generating conceptions about content (cf. Niedderer, 2001).

analysis is complex, and in order to make implicit issues explicit the steps of data analysis are summarized and examples from the authentic analytical process are given. But doing so also means that our description of the analytical process cannot only be traced back to Niedderer's description of iterative analysis; other descriptions of performing qualitative analysis are also of importance (e.g. Glaser and Strauss, 1967; Erickson, 1998; Carson, 2001; Sözbilir, 2001; Bryman, 2008).

The analytical methodology

The general and specific guidelines used during the entire data analysis process are described below. Since the analytical process led to a gradually focused aim, which in turn led to a changed analytical process, this section is characterized by the description of a changed and increasingly focused analytical process. The guidelines are intertwined and should best be viewed as related principles rather than unique ones:

- Compile data

In order to prepare the coding, all data were compiled or transcribed immediately after collection and, if possible, frequencies were calculated (e.g. which answer was chosen).

- Explain wrong answers

Wrong answers to certain tasks were described in a process following Niedderer's (2001) description and the view of an alternative conception; hence, the process explicitly included content in the data-analytical frame of reference. This part of the analysis primarily resulted in conceptions with logical patterns.

- Describe patterns

A greater proportion of data was analysed especially during the main study, and it was not only wrong answers that were analysed. Since the chemical department was shut down, thus lowering the number of informants, both general patterns and specific patterns of certain tasks were sought. During this process, conceptions were constructed to describe both correct and incorrect answers given by students; hence data were analysed without prejudice, which is common in qualitative analysis (e.g. Glaser and Strauss, 1967; Erickson, 1998; Bryman, 2008). Even if an answer is correct it could include incorrect descriptions with respect to scientific theory, but these conceptions are not alternative and logical in the sense that they explain wrong answers. Instead, they describe how students tend to use the concepts (here denoted as underlying).

In the *Results* section, patterns that create the conception are described. Using empirical evidence to support a pattern is like painting a picture for the reader. Sometimes it is almost impossible to give one quote that clearly states *yes, this is the case...*, but through a systematic reading of the data and interpretation of the students' expressions, a picture emerged. Thus, it is important to keep in mind that one student's expression is not evidence of a student conception; instead, it was evidence contributing to the interpretation and the pattern. Interpreting meant twisting and turning the data, a process which was easier with interview transcripts since students had to elaborate on their answers during the interviews. Evidence from questionnaires, hand-ins and exams was

also used in order to deepen and widen the picture. Evidence was included to support the interpretation or sometimes to show that different interpretations were possible.

- Coding and saturation

Data were coded to construct the conceptions. The first step was to become familiar with the data, to start asking questions of the data and then code it in an unprejudiced manner. Words, rows, sentences, passages and the text as a whole were coded, thus labelling different evidence with the same code. The constructed codes changed during the coding process. If similar codes and patterns emerged more general codes and categories were defined, and as the comparison continued the codes and categories became more general and abstract. When necessary additional codes and categories were constructed, some related to old ones and some completely new. Finally, conceptions were constructed, and when no empirical evidence changed the definition or description of a conception as it was applied on the data, each conception was considered to be saturated (*cf.* Glaser and Strauss, 1967).

- Increased generalizability, abstraction, data reduction

The use of more data during the analytical process increased the generalizability, as the constructed conception became more abstract and complex. The conception was used to analyse more data, and during this process generalizability was related to applicability rather than previous research. As codes were merged to form a conception, the analytical process also led to data reduction.

- A gradually changing and increasingly focused aim

The analytical process was driven by the revised aim in the empirical studies. To test the descriptive categories, or conceptions, that had been constructed in the main study, a new empirical study was designed. The aim was therefore gradually revised from chemical thermodynamics in general to enthalpy, enthalpy change and related concepts. To gradually deepen and focus the aim of a study, data collection and data analysis are important in the qualitative research process since data analysis aids in the formulation of interesting questions.

- Content

During the data analysis, reference to the subject content was a principle. Due to the focused research process the researchers' understanding of the content changed, especially during the follow-up study. As students' explanations and descriptions were compared to the definition of enthalpy and enthalpy change, the authors posed questions that forced a revision of their understanding of the content. This process was necessary in order to understand the students' responses. This means that even though the content was in principle the same, the researchers' frame regarding this content changed as the analysis progressed.

- Using literature

Hypotheses, categories and conceptions were formulated as results in the different empirical studies and research literature was included more and more as a comparison and frame. Tasks from the literature were also included throughout the research process.

- Interrater agreement

To increase trustworthiness an interrater reliability test, testing how well two independent researchers categorize the answers,

was performed during the pilot study with satisfactory results. During the main and follow-up studies the second author repeatedly categorized answers to the most relevant tasks. The categorization was done in one of two ways: either questions were categorized using all conceptions, or a conception was chosen and then applied to the data. Whenever answers were categorized differently, the conceptions and definitions were discussed and revised. Due to continuous reviews, almost complete agreement was reached.

A brief example from the analytical process – conception F6.

As the data from the task by Sözbilir (2001) were analysed, the following was the first conception identified:

(1) *When the amount of substance is identical the enthalpy change as heat is identical regardless of the apparatus in which the reaction takes place.* The amount of substance is the key to understanding why students tend to describe the heat as equal in Apparatuses A and B. As the analysis continued the conception changed, and at one stage during the follow-up study it was described with the following sub-conceptions:

Conception 2. If it is the same reaction it is always the same enthalpy change and same heat

F2.1 If same amount of substance then same heat

F2.2 If same reactants/products then same heat

F2.3 Since $C_p = C_v$ q is the same

F2.4 If same state function then same heat

F2.5 Closed valve gives alternative explanations based on F2.1–F2.4

F2.6 Different power but same q

In the *Results* section some features of those described here can still be seen in F6, *The same reaction gives the same enthalpy change and heat*, but for instance F2.5 is now described in Conception F9 instead.

Results

The conceptions constructed are presented in Table 4 and the presentation is elaborated below, where the salient aspects of the conceptions are given. Conception F3 is excluded in this presentation since it was based on another analytical method (authors, in press).

Conception F1. The mantra of enthalpy change as heat at constant pressure

Students have learned to express parts of the definition by heart and the conception includes two subcategories: first F1.1, *that the required demand for constant pressure is explicitly expressed but disregarded as the answer is given*, whereby students explicitly state that enthalpy change is heat at constant pressure but argue for a case in which the pressure is not constant. For instance, S11 (HST1a, Question 5a), *Both give off the same amount of heat because the Enthalpy does not change if the same*

Table 4 The conceptions constructed in the study. In F6, R stands for state function/reaction/amount of substance/reactant and products. The frequencies are based on the number of answers categorized as the conception/total number categorized answers to all tasks where the conception is present. For F1 the frequencies are presented for each sub-conception, but for all other conceptions the frequencies are for the entire conception

Conceptions	Sub-conception (F) or pattern (M)	Frequencies HS	Frequencies FS
F1. The mantra of enthalpy change as heat at constant pressure	F1.1. The required demand for constant pressure is explicitly expressed but disregarded as the answer is given. F1.2. The required constant pressure is not mentioned as the enthalpy change as heat is explained.	F1.1 24% (12/51) F1.2 27% (21/79)	F1.2 11% (1/9) F1.2 29% (12/42)
F2. If a visual change in the position of an artefact cannot be observed, work during a chemical reaction is difficult for students to identify.	M1. When a chemical reaction occurs, the work is difficult to identify since it is abstract. M2. When an artefact moves, for instance a piston, work is easier for the student to identify.	17% (14/82)	36% (25/69)
F4. Enthalpy is a form of energy.	M1. Enthalpy and enthalpy change are implicitly and explicitly described synonymously with energy-energy change. M2. Enthalpy and enthalpy change follow the first law of thermodynamics, $\Delta H = q + w$. M3. Enthalpy and enthalpy change are described as forms of energy, for instance as taking place in energy transformations.	26% (23/90)	27% (13/49)
F5. Enthalpy and enthalpy change describe similar aspects of a chemical reaction.	—	12% (6/50)	16% (7/43)
F6. The same reaction gives the same enthalpy change and heat.	M1. Same $R \Rightarrow$ same q M2. Same $R \Rightarrow$ same $\Delta H \Rightarrow$ same q M3. Same $R \Rightarrow$ same $q \Rightarrow$ same ΔH	Question A 29% (5/17) Question B 12% (2/17)	—
F7. Enthalpy change is heat when no work is done.	M1. Enthalpy change is heat in Apparatus B since $\Delta H = \Delta U + p\Delta V$ and $\Delta V = 0$, hence $\Delta H = q$ as the work is 0 (incorrect choice/incorrect argument). M2. Enthalpy change is heat in Apparatus A since $\Delta H = q + V\Delta p$ and $\Delta p = 0$, hence $\Delta H = q$ as the work is 0 (correct choice/incorrect argument).	26% (6/23)	39% (13/33)
F8. Enthalpy change is heat since the energy transferred as heat is ΔU	—	Question B 35% (6/17)	13% (4/30)
F9. An alternative interpretation of the apparatuses provides an alternative logic	M1. Efficiency/flow M2. Static figures M3. An open or closed system	21% (7/34)	47% (7/15)

products and reactants are involved $\Delta H = \Delta H_{\text{prod}} - \Delta H_{\text{reac}}$ (which is only valid at constant pressure). S11 explicitly states that the equation is only valid at constant pressure, but argues that the heat is the same in both Apparatuses A (constant p) and B (constant V).

The second subcategory is F1.2, where the requirement constant pressure is not mentioned as the enthalpy change as heat is explained, whereby students do not use the definition of enthalpy change as heat at constant pressure (when only expansion work is allowed) when answering questions explicitly addressing the definition. For instance, S7 (HST1a, Question 5b), *It must be B too, since the volume is constant, thus no work is done and all energy is heat*. Here, enthalpy change is related to constant volume instead of constant pressure. The definition of enthalpy change is not explicitly mentioned, which indicates sub-Conception F1.2.

Conception F2. If a visual change in the position of an artefact cannot be observed, work during a chemical reaction is difficult for students to identify

The conception indicates that a common case in chemistry, expansion work against the surroundings (atmosphere), is not regarded as work by students. Also, the abstract boundary between a system and its surroundings, where the actual expansion work is taking place, is easier to understand when the movement of a randomly chosen artefact, for instance a piston, can be identified by the naked eye. The two patterns that have emerged are M1, *When a chemical reaction occurs, the work is difficult to identify since it is abstract*, and M2, *When an artefact moves, for instance a piston, work is easier for the student to identify*. One example of M2 is the answer given by SK3 (FSIn12, Question 9a): *It ought to be System B that is giving away the most heat. In System A, energy will be used to push the piston, hence energy will be spent on that and not as much can be transferred as heat*. Here, the student tells in which set of apparatuses, A, B or both, the most energy is given as heat. The correct alternative is chosen, and in the explanation of work an artefact (piston) is affected (M2). In the following transcript it can be noted that S7 identifies that no work is being done. However, work is described as the energy transformation between different forms in terms of transformation of potential energy. At the same time, something should do the transformation. This something may push something if the pressure is increased; hence something may be interpreted as an artefact, especially if it makes a turbine run (M2). S7 (HSI2, parts of excerpt from $t \sim 5.20\text{--}7.20$, ammonium chloride dissolving in water, I = interviewer, S = student):

I: [...] is any work done[?]

S: no, I don't think so

I: no, how come[?]

S: because [silence 2 sec] no work is done [silence 2 sec] in some way there's no [silence 2 sec] transformation of potential energy or something like that, so no, I don't think any is done

[...]

I: but if you were to explain the concept of work, what do you mean by saying work [?]

S: work, then [silence 2 sec] something should do a transformation of energy [silence 7 sec] you do so something gets a higher energy [silence 4 sec], for instance if the pressure increases and you push something so it moves, then...

I: ok

S: ...I think work is done [...] You make a turbine run

I: but here we have a chemical reaction

S: hmm

I: but isn't it...

S: but no work

It is noted that Conception F2 is primarily found for tasks investigating the artefact's importance for work. In the interview, S7 identifies that no work is done because nothing interacts. In fact, in both pre and post interviews, even though gas is produced the students describe an absence of work since no artefacts are included.

Conception F4. Enthalpy is a form of energy

The conception indicates that enthalpy, energy, heat and work are related to each other and that students describe, apply and explain the concepts as if they are forms of energy. This means that students tend to understand enthalpy as related to physics and the forms of energy framework in which different forms are transformed into each other. Three patterns have emerged: M1, M2 and M3. In M1, *enthalpy and enthalpy change are implicitly and explicitly described synonymously with energy/energy change*. The following transcript shows one of a series of statements made by S1. Returning to a previous statement regarding enthalpy and its change, S1 stated that *it is measured in joules per mol*, which is true, but as *joule is energy* it is possible to use both energy and enthalpy and since Joule is the unit, enthalpy must be energy. S1 (HSI2, short excerpt from $t \sim 11.50\text{--}12.50$, ammonium chloride dissolving in water, explain using energy and enthalpy, I = interviewer, S = student):

I: [...] because now in your explanation you began with enthalpy and endothermic and then you went on using energy

S: [laughs]

I: what [silence 2 sec] how is it possible that we can talk of both energy and enthalpy for one and the same reaction [?]

S: [silence 2 sec] yeah, I just think they're almost the same but I don't know [...] it's measured in joules per mol or something like that and [...] joule is energy [laughs]

The other two patterns are M2, enthalpy and enthalpy change follow the first law of thermodynamics, $\Delta H = q + w$, and M3, enthalpy and enthalpy change are described as forms of energy, for instance as taking place in energy transformations. The answer from SK8 serves as an example of both patterns: SK8 (FSIn12, Question 9b): *In B since the reaction is taking place in a closed vessel, then no mass transfer will take place and the enthalpy change will be transformed into heat*. SK8 explains that enthalpy change is transformed into heat (M3). But, Apparatus B is actually the wrong answer and the heat does not correspond to the enthalpy change as heat. In B no work is done; hence pattern (M2) is exemplified.

Conception F5. Enthalpy and enthalpy change describe similar aspects of a chemical reaction

This conception is based on all collected data and describes both correct and incorrect answers as well as how students use the concepts in discussions. The picture emerging in the analysis is as follows. Enthalpy has the same meaning as enthalpy change and is sometimes used as an abbreviation for, for instance, reaction enthalpy. This means that students use enthalpy to describe the process or actual reaction instead of the state before and after a reaction. In the following example the student argues that the most heat is given off in Apparatus B, which is correct, but uses the state function enthalpy $H = E + PV$ to describe an enthalpy change: S8 (HST1a, Question 5a): *B gives the most heat to the surroundings since in Case (A) energy is used for work. $H = E + PV$. The same tendencies hold for other concepts as well, for instance in the following example where enthalpy (H) and Gibbs free energy (G) are expressed as ΔH and ΔG . Negative enthalpy means $\Delta H < 0$, not $H < 0$. S1 (HST2b, Question 3): *Enthalpy ΔH , Gibbs free energy ΔG and entropy S [...] Gibbs free energy ΔG can be: [...] the reaction with negative enthalpy (ΔH) [...] The reaction with positive enthalpy must have had $\Delta H < T\Delta S$...**

Conception F6. The same reaction gives the same enthalpy change and heat

This conception is related to the tasks based on Sözbilir's (2001) original. The common denominator is the conclusion that the same reaction (amount of substance and/or reactants and products) will always give the same heat regardless of whether the process is carried out at a constant pressure or volume. Hence, students draw the wrong conclusions about heat, change in internal energy, enthalpy change and the meaning of a state. Three patterns have emerged: M1, *Same $R \uparrow \Rightarrow$ same q* ; M2, *Same $R \Rightarrow$ same $\Delta H \Rightarrow$ same q* ; and M3, *Same $R \Rightarrow$ same $q \Rightarrow$ same ΔH* .

In the following example, molar enthalpy seems to be a valid description of how the students describe the same heat in Apparatuses A and B (M2). The argument is that the path taken is unimportant, which is the opposite of the scientific view.

S12 (HST1a, Question 5a): *At constant pressure the amount of heat, change in enthalpy, will be equal to the energy of the system. Same reaction, same amount of substance, same reactants. When all reactants have reacted, the sum of the same – that is the path the reaction takes – is unimportant. All reactants have been used in both cases. The heat to the surroundings should be the same.*

Conception F7. Enthalpy change is heat when no work is done

This conception offers insight into some answers to the task designed from Sözbilir's (2001) original. Here, students describe that enthalpy change is heat when no work is done. Two related patterns have emerged. The first is M1, *enthalpy change is heat in Apparatus B since $\Delta H = \Delta U + p\Delta V$ and $\Delta V = 0$, hence $\Delta H = q$ as the work is 0 (incorrect choice/incorrect argument)* – for instance in the answer by S7 (HST1a, Question 5b), *it must be B too, because the volume is constant and therefore no work is*

done all energy is transformed into heat. Here, constant volume is explicitly addressed and the student chooses the wrong Apparatus, B. However, it is true that all energy is transferred as heat in Apparatus B due to constant volume. Here we argue that the student bases the argument on $\Delta H = \Delta U + p\Delta V$, which is only valid at constant pressure, and since $\Delta V = 0$ and $p\Delta V = 0$ the logical answer seems to be enthalpy change as heat when no work is done. The other pattern is M2, *enthalpy change is heat in Apparatus A since $\Delta H = q + V\Delta p$ and $\Delta p = 0$, hence $\Delta H = q$ as the work is 0 (correct choice/incorrect argument)* – for instance given by SK6 (FSInl2, Question 9b), *Apparatus A, since $dH = dq + Vdp$ where $dp = 0$.* Here the student chooses the correct apparatus but uses a formula for constant volume when volume increases.

Conception F8. Enthalpy change is heat since the energy transferred as heat is ΔU

This conception, a deepening of Conception F7 in which enthalpy change is heat when no work is done is the foundation, describes that $\Delta H = \Delta U = q$ instead of $\Delta H = q$ and the fact that energy transferred as heat is denoted ΔU (or ΔE). S1 (HST1a, Question 5b): *in Case (B) the volume is constant $\rightarrow \Delta H = \Delta E$. In Case (A) the volume varies and the expansion requires energy otherwise given to enthalpy $\Delta H \neq \Delta E$.*

The student shows $\Delta H = \Delta U$ (ΔE) instead of $\Delta H = q$, implicitly indicating that the energy transferred as heat is ΔU (ΔE). The student also identifies constant volume in B and varying volume in A. Since the student expresses that *volume is constant $\rightarrow \Delta H = \Delta E$* it is reasonable to assume that the student bases the explanation on the definition of enthalpy change at constant pressure $\Delta H = \Delta U + p\Delta V$.

Conception F9. An alternative interpretation of the apparatuses provides an alternative logic

Students have interpreted Apparatuses A and B in a different way than anticipated. The analysis of the interpretations gave the three following patterns: M1, *Efficiency/Flow*, in which answers regarding the greatest efficiency or flow instead of heat are grouped; M2, *Static figures*, is best described as a picture. Here, both apparatuses have a specific constant pressure and volume, hence students describe them as states instead of as ongoing processes; in M3, *An open or closed system*, answers in which students describe an open valve as an open system are included, as described in the following example: S19 (HST1a, Question 5b), *B energy transfer as heat should be the same as enthalpy change in Case (B) with a closed valve but not with the configuration. The explanation is based on $\Delta H^\circ = -464 \text{ kJ/mol}^{-1}$, which multiplied by mol/amount of substance for the products gives the heat transfer in kilo-joule/kJ. Since the connection between the two is based on molar amounts, they can only be the same if no substances are leaking out, something which will surely happen if the valve is open, since hydrogen gas/ $\text{H}_2(\text{g})$ would leak out and change the molar amounts compared to a closed valve keeping the hydrogen there.*

In this response there is a passage to an open valve, or tap, indicating that the amount of substance changes (M3). Again, molar enthalpy seems to be a valid description and an open

valve is an open system and not a closed system at constant pressure. At the same time, a closed valve means a closed system instead of a closed system and constant volume.

Discussion and concluding remarks

In this section the contribution to the knowledge base, different methodological considerations and implications are addressed.

The constructed conceptions – contribution to the knowledge base

The conceptions constructed during the analytical process describe qualitative differences (*cf.* Duit and Treagust, 1998) and follow Carson's and Watson's (1999) description that no matter how small the differences are from the scientific conceptions, the label is an alternative conception. The scientific frame is described in order to make the analysis possible; thus, how students perceive the theory relates to the comparison between the answer and the theory. The frequencies are based on the number of answers categorized as the conception/total number categorized answers to all tasks in which the conception is present. Thus the frequencies may seem higher or lower than they actually are, but according to research they are probably more common than expressed here (Mortimer, 1995).

There are different ways to contribute to the knowledge base. New conceptions can be constructed; other conceptions have been constructed before but new data provide new insights; and finally, previous conceptions can be generalized as they are.

Conception F1, *The mantra of enthalpy change as heat at constant pressure*, has not been stated before. It firstly describes how students express constant pressure but argue for a case in which constant pressure is not valid, and secondly it includes the absence of constant pressure when it is explicitly asked for. Both expressed patterns give a clearer picture of how students apply the definition of enthalpy change and constant pressure. The entire conception is of the underlying type, according to the description of a mantra (Nationalencyklopedin, 2012), which means that F1 does not govern how students argue; instead, it is a description of how they include/exclude different statements in their answers as they argue another case. As noted, the mantra differs from the scientific definition since *only expansion work* is left out. Although it has not been described previously, some similarities with previous research exist; for instance, Greenbowe and Meltzer (2003) note that none of the students in their study equate reaction heat with enthalpy change as processes are carried out at constant pressure. Carson (2001) expresses a similar finding based on the fact that only two of 22 students describe enthalpy change completely. Carson states "The special importance of constant pressure and the limitation to pV work appeared not to have impinged on students" (p. 114). Nilsson and Niedderer (2012) show results similar to those found by Carson (2001), since expansion work is not explained correctly in actual situations and since students relate volume to work more easily than pressure. Also, Carson (2001) and Sözbilir (2001) report that

students frequently state that enthalpy change is heat at constant volume, indicating that there is a general problem with constant pressure and only expansion work. Earlier, Granville (1985) reported that students tend to focus only on the sign ΔH when determining whether a reaction is endothermic or exothermic, and miss the fact that the definition is only valid if the only work allowed is expansion work.

Learning to express things by heart is an example of algorithmic learning, and the mantra is no different. Researchers have suggested that the problem is how the theory is applied rather than how the calculations are done (*e.g.* Bowen and Bunce, 1997; Mazur, 1997; Claesgens *et al.*, 2002; Niaz, 2002; Gabel, 2003).

Conception F8, *Enthalpy change is heat since the energy transferred as heat is ΔU* , also provides new insight into how students argue when enthalpy change is the heat given off in an apparatus. As described above, Conception F8 is an elaboration of F7. As it seems, students actually argue for when ΔU is the energy transferred as heat. This means that students end up choosing an incorrect answer. Thus far, no evidence of this conception has been found, and Sözbilir (2001) only describes results similar to Conception F7, as does Carson (2001). However, when analysed with Nilsson and Niedderer's (2012) matrix, the examples given would yield both incomplete and incorrect descriptions of the expansion work. Therefore, it is possible that this conception deepens previous results regarding why students argue that enthalpy change is heat at constant volume. Logic shows that the student argues when $\Delta H = \Delta U$ instead of $\Delta H = q$, implicitly stating that $\Delta U = q$.

Another way to contribute to research is to describe conceptions that are similar or identical to previous research results. Conception F6, *The same reaction gives the same enthalpy change and heat*, has been stated before but this study has provided new insights. Students argue that the heat and enthalpy change is equal in both Apparatuses A and B (constant p vs. constant V). It has previously been identified that students frequently forget one or more of the factors heat, constant pressure and expansion work as they define enthalpy change (Carson, 2001). This study supports this finding, since students tend not to focus on constant pressure and expansion work as they argue why the heat must be the same. Nilsson and Niedderer's (2012) matrix shows how students use pressure and volume when explaining work, expansion work and technical work, and stress the importance of using the general definition of enthalpy change since it is difficult for students to argue for a constant volume/varying pressure case if they have only been introduced to $\Delta H = \Delta U + p\Delta V$. This finding is in accordance with Carson's (2001) and Sözbilir's (2001) results that enthalpy change is heat at constant volume. Johnstone *et al.* (1977) also showed a result among younger students that the amount of heat does not depend on the work done.

In Sözbilir's (2003) review heat is an intensive quantity, but this study contradicts this since molar enthalpy can be used to explain students' answers; hence, heat is an extensive quantity. Also, Sözbilir (2001) reports that students confuse total energy with heat and for Question A in the post test a frequency of 5%

is reported. Even though a limited number of students participated in this study, empirical evidence suggests that answers to Question b can be included in the categorization, at least in the main study.

Like F6, Conception F9 – *An alternative interpretation of the apparatuses provides an alternative logic* – provides similar but not identical insight to previous research. The conception indicates that students interpret the questions and figures in alternative ways, and as a result the conception is fruitful from both a methodological and conceptual point of view. The fact that the figures have been interpreted as static in the main study led to a change in the follow-up study: Conception F9 was still present, but the pattern indicating static figures did not appear. However, patterns showing students' descriptions of efficiency and/or flow were identified in both studies as well as in one of Sözbilir's (2001) misunderstandings. A key issue regarding the patterns seems to be how systems are described in textbooks. In some common textbooks open, closed and isolated systems are presented according to the test-tube principle (Atkins and de Paula, 2005; Chang, 2007) and visual differences between system/surroundings/universe (Laidler *et al.*, 2003; Atkins and de Paula, 2005; Chang, 2007; Zumdahl and Zumdahl, 2007), but tasks to prepare students for differentiating between these fundamental aspects of a chemical system are seldom included. Differentiating between properties of the system and the surroundings is important, but Carson (2001) shows that students have difficulty separating a system from its surroundings, although results suggest that post teaching the situation has improved. However, Greenbowe and Meltzer (2003) show the opposite result. In their study, 22% (of $n = 207$) correctly identify the chemical reaction as the system while only 6% correctly identify the surroundings. Although research shows some opposing tendencies, the common ground is to differentiate a system from its surroundings in order to identify the properties of the reacting systems.

The last four conceptions generalize previous research findings. Since scientific knowledge is based on different authors showing similar results, this result is important since the different studies concern different countries, educational levels and methodologies. Below, the last four conceptions are related to previous research findings.

Conception F2 – *If a visual change in the position of an artefact cannot be observed, work during a chemical reaction is difficult for students to identify* – shows the importance of an artefact when identifying expansion work since work against the surroundings (atmosphere) is disregarded. We do not argue against the obvious fact that work is done, but merely describe that without the artefact no work is done. Work, as described in chemistry, has been found to be difficult for students to identify. Carson (2001) describes that "students had difficulty in associating work with chemical reactions" (p. 118), and presents findings such as work equals bond breaking, the presence of a piston or raising weights. Nilsson and Niedderer (2012) show that in their two groups 59% and 37% of the answers regarding work are left blank. This could be interpreted as students having difficulty seeing the work actually being done. Empirical evidence suggests

that work is done when gas and an arbitrarily chosen artefact interact. The formation of gas that expands is not regarded as work. The results here, together with Carson's results, indicate that the description of work by van Roon *et al.* (1994) as a mechanical concept still seems to be the best and, sometimes, the only valid description of how students perceive work in chemistry.

Conception F4, *Enthalpy is a form of energy*, describes when enthalpy and its change are described and applied in a similar way to (internal) energy and its change and hence no differentiation is made between the concepts. Neither enthalpy nor enthalpy change is a form of energy by definition (Kaper and Goedhart, 2002). Also, neither enthalpy nor enthalpy change follows the first law of thermodynamics. However, it is true that the first law of thermodynamics is a fundamental part of enthalpy change. In this study students commonly express enthalpy, Gibbs energy and entropy as forms of energy and, in the explanation of the framework forms of energy, transformation is a key concept (Carson, 2001). In a review it is shown that students base their perceptions of different concepts on transformations, and the framework is robust (Goedhart and Kaper, 2002). Therefore, university students accept new thermodynamic concepts as part of the framework (Carson, 2001). The following interpretation of students' answers sheds some light on why it might be easy to include enthalpy as part of the framework: if heat is a form of energy and enthalpy change is heat then, surely, enthalpy change must be a form of energy.

In Conception F5, *Enthalpy and enthalpy change describe similar aspects of a chemical reaction*, both $H = U + pV$ and $\Delta H = \Delta U + \Delta(pV)$ are used, for instance, to describe changes, and when students use enthalpy it is related to changes. Beall (1994) reports similar findings for enthalpy and Gibbs energy, and students forget to indicate the change for internal energy (van Huis and van den Berg, 1993). More recently, Sözbilir (2001) reports that students use reaction heat, enthalpy change and enthalpy similar to Beall's (1994) findings, and like Sözbilir (2001), Greenbowe and Meltzer (2003) show that students have difficulty relating reaction heat to the enthalpy change. Long ago, Driver and Warrington (1985) showed similar patterns for work and energy since students do not tend to separate them. However, the present study differs from most previous ones since both correct and incorrect answers are analysed. A feature of the conception is how students use the concepts in actual settings, and even though the students choose/give a correct answer the concepts may be used incorrectly. Improper use does not necessarily result in an incorrect answer.

In Conception F7, *Enthalpy change is heat when no work is done*, both patterns indicate that students pick an alternative that does not correspond to the definition of enthalpy change they themselves are using. This in turn leads to contextually correct descriptions of volume but incorrect descriptions of pressure (e.g. if $\Delta V = 0$ then $p\Delta V = 0$ even if the context is $\Delta p \neq 0$ and $\Delta V = 0$). Nilsson and Niedderer (2012) show that students often correctly relate volume to work, but pressure is not mentioned often. Also, Carson (2001) and Sözbilir (2001) describe results similar to those presented here. In the latter study a

misunderstanding is present in 47% and 36% of the answers on the pre and post questionnaires, respectively, where one sub-conception of four is similar to F7. In Carson's (2001) interview study, five of 22 students explicitly state that enthalpy change is heat when the volume is constant since no work is done. Although related to the previous results, the different educational levels in this study provide further insight into students' understanding of the relationship between work and enthalpy change.

Based on the results presented and the contribution to the knowledge base, it is possible to conclude that enthalpy and its change do not necessarily offer students new ways of solving, anticipating and explaining problems in chemistry.

Relationships between the conceptions

During the data analysis, the labels *underlying* and *logical* were used to group the conceptions; see Table 5. More general tendencies were denoted as underlying, whereas alternative logics to the scientific conception were denoted as logical. Grouping the conceptions also means that they are each placed on one side of a continuum, but in reality they should be regarded as more/less underlying/logical. When arguing for the different conceptions, it became obvious that the division is rather rough. However, the main idea was to show how students used the concepts (*i.e.* underlying) or argued for a certain incorrect answer when there was a predefined correct answer (*i.e.* logical). Also, the underlying conception is more general and unprejudiced than a logical conception, more fluid on the continuum and goes beyond the correct/incorrect answer to a certain task. However, it is still an alternative conception since it deviates from the scientific frame. Since underlying and logical conceptions are constructed in similar ways, as described in the data analysis, they may seem more alike than they actually are since the idea of a conception is to describe a characteristic, which means that statements based on the definition of the conception are either included or excluded. The grouping may also be traced back to the methods, tasks and questions used (*e.g.* Carson, 2001; Sözbilir, 2001). Carson (2001) formulates conceptions based on interview data and a validated list of statements. Sözbilir (2001) formulates conceptions of different tasks based on a coding scheme. One reason for the need to divide the conceptions into underlying and logical is the use of different tasks and data collection methods. The data reduction led to some general patterns, the underlying

conceptions and some task specific conceptions, the logical ones. In retrospect, the data analysis carried out can perhaps best be described as a synthesis of Carson's (2001) and Sözbilir's (2001) analyses.

The conceptions are related to each other in different ways, but each describes unique properties of the students' answers. Three relationships between the conceptions are described below.

- Relationship R1: evidence of two conceptions in one answer

One answer may act as evidence of two different conceptions, since an answer can contain different theoretical aspects. An example of this is Conceptions F4 and F5, which can be used in parallel. Theoretically they are mutually exclusive, but they can be used to describe the same answer, as described here:

S1 (HST1a, Question 5b): *In Case (B) the volume is constant $\rightarrow \Delta H = \Delta E$. In Case (A) the volume varies and the expansion requires energy otherwise given to enthalpy $\Delta H \neq \Delta E$.*

Conception F4 is applied, since the *expansion requires energy otherwise given to enthalpy*. Conception F5 is applied since *enthalpy* is expressed but related to $\Delta H \neq \Delta E$.

- Relationship R2: conceptions that are logically alike

If conceptions are logically alike it means that one conception leads to another, since they share some logic. An example of this is Conceptions F7 and F8:

S1 (HST1a, Question 5b): *In Case (B) the volume is constant $\rightarrow \Delta H = \Delta E$. In Case (A) the volume varies and the expansion requires energy otherwise given to enthalpy $\Delta H \neq \Delta E$.* Here F7 is activated, since volume is constant $\rightarrow \Delta H = \Delta E$ which implicitly indicates that $p\Delta V = 0$. Conception F8 gives a deeper understanding of the answer, since the student argues for the case when $\Delta H = \Delta U$ (ΔE) instead of $\Delta H = q$. As a consequence, volume is constant and no work is done (F7). However, not all answers categorized as F7 can be categorized as F8.

- Relationship R3: conceptions facilitate each other

These conceptions are mutually exclusive but facilitate each other. An example of this is Conceptions F6 and F1 (F1.1), since F6 facilitates F1:

S11 (HST1a, Question 5a): *both give off the same amount of heat because the Enthalpy does not change if the same products and reactants are involved $\Delta H = \Delta H_{\text{prod}} - \Delta H_{\text{reac}}$ (which is only valid at constant pressure).* The student explicitly states that the equation or statement is only valid at constant pressure, indicating that constant pressure is known. At the same time, the actual argument is that both apparatuses give off

Table 5 Different types of conceptions

Type of conception	Conception
Underlying	F1. The mantra of enthalpy change as heat at constant pressure F2. If a visual change in the position of an artefact cannot be observed, work during a chemical reaction is difficult for students to identify F4. Enthalpy is a form of energy F5. Enthalpy and enthalpy change describe similar aspects of a chemical reaction
Logical	F6. The same reaction gives the same enthalpy change and heat F7. Enthalpy change is heat when no work is done F8. Enthalpy change is heat since the energy transferred as heat is ΔU F9. An alternative interpretation of the apparatuses provides an alternative logic

the same heat. The relationship between the conceptions exists, since F6 facilitates F1.

Decisions during the data analysis – a gradually focused aim

This study used local opportunities to develop teaching and construct new conceptions. Since the pilot study with teachers and students was designed to develop a frame for the study (*e.g.* identify preconceptions and develop relevant tasks), the original idea to follow one course and its teacher was kept even though the chemistry department was shut down just prior to the main study. Also, since only a limited number of studies about undergraduate students' conceptions of enthalpy and its change and related concepts can be found (*e.g.* Carson and Watson, 1999; Carson, 2001; Sözbilir, 2001; Greenbowe and Meltzer, 2003; Nilsson and Niedderer, 2012), the research design was kept but was adjusted to the decrease in participants. The explorative, flexible design allowed for this, and the aim was gradually narrowed, which is also common in qualitative research (Glaser and Strauss, 1967; Robson, 2002). However, in retrospect some things could have been done differently, for instance the data collection.

Since we wanted to keep the study within the developed frame (*i.e.* L3's aims), we chose not to include data from other universities during the main study. Instead a larger group was sought for the follow-up study, but the new teacher found the tasks too difficult for the students and recommended another, more advanced, course with fewer students instead. Although we find the categories to be saturated, additional data may shed new light on the categories developed.

A different approach would be to use Carson's (2001) or Sözbilir's (2001) research designs, which would offer an opportunity to quantitatively analyse the data, or at least use the authors' developed categories. However, with this study design and the focus of the pilot study with students (*i.e.* chemical thermodynamics in general), the authors' categories would not have corresponded with most data. The use of pre-designed categories could also have hindered one outcome in the research process, namely the first author's ability, through a systematic re-reading of the data, to assign definitions and categories to the patterns emerging from the data. This ability must be developed during a research process, and this was considered important. However, the tasks developed from Sözbilir's (2001) original should have been used in interviews as well in order to allow for students to fully describe their answers and justifications.

Different techniques were used (*e.g.* multiple choice, yes/no, explanatory or descriptive) to address the description of qualitative or conceptual understanding. However, it became obvious that some techniques were more fruitful than others; for instance, the multiple choice question in the main study with the distractors taken from the pilot study with students, in which an almost identical open question was answered by the students. Hence, it is possible that all answers appealed to some students but since only one answer could be chosen there is a possibility that the frequencies of other distractors are higher than we can show. The yes/no questions served as a complement to other questions, but in retrospect it was easy for the students to guess correctly.

The explanatory or descriptive questions were developed during the research process. As the analysis shows, different conceptions were activated, sometimes more than one in one answer. New possibilities therefore exist; see below.

Generalizability and trustworthiness

As noted above, one indication of the quality of this research is the generalizability of the results. Not surprisingly, similar results have been found

- by different authors in different countries,
- at different educational levels, and
- with different data collection methods (triangulation).

The use of previously developed tasks and methods increases generalizability since the results are comparable. As some tasks were used both in the main study and follow-up study, generalization across educational levels is possible. Although important from a methodological perspective, the re-designing of the task based on Sözbilir's (2001) original decreased the generalizability. However, the conceptions have been shown to be applicable to different data and situations (*i.e.* questionnaires, exams, hand-ins and interviews), which increases generalizability.

Generalizability is the possibility that the results are valid in a larger population, and since this study shows similarities to previous studies in the field we believe the results presented here are valid outside the range of this study, in some cases even in upper secondary education.

In this research project, different methodological and analytical choices have been argued and discussed. The empirical evidence included has always been based on a scientific frame of reference and personal interpretations. The personal frame of reference and the interpretations are clarified in the qualitative analysis, but personal values have not guided the analysis. In constructing a conception, the researcher is always the constructor; therefore, it is obvious that a researcher cannot be completely objective, but the researcher's personal views should not have affected the research process or results. It is thus important to stress that the iterative research process was based on empirical evidence interacting with a frame of reference.

The credibility of research is increased when recommendations are followed and other researchers partake in the research process. The design, methodological concerns, data analysis, theoretical frames and conceptions have been discussed at conferences with supervisors, experienced teachers and other PhD students. Using different methods and data triangulation also increases credibility (Robson, 2002). However, using different methods may lead to difficulties in comparing data due to different units of analysis. In order to increase credibility, evidence from interviews was part of the definition of a conception, but the interviews were not analysed in the same way as the written data. Also, Sözbilir's (2001) way of including data from interviews was followed.

Implications for research and teaching

Research on the teaching and learning of thermodynamics at different educational levels has long been discussed (*e.g.* Duit and Haeussler, 1994; Lewis and Linn, 1994; Kaper and Goedhart,

2002; Millar, 2005; Engström, 2008; Johnstone, 2010). For chemical thermodynamics and higher education Carson (2001), Sözbilir (2001) and Goedhart and Kaper (2002) give more specific suggestions, and we support the idea that qualitative discussions should precede quantitative manipulations of variables (White and Gunstone, 1992; Carson and Watson, 1999; Carson, 2001; Bodner and Herron, 2002; Gabel, 2003; Johnstone, 2010).

According to Carson (2001) (and we agree), one problem is that university teachers assume prior understanding of heat and work. They should do this, of course, since fundamental concepts like (internal) energy, heat and work are included in upper secondary education, but it is possible that students' prior understanding is not in accordance with teachers' beliefs. Discussing these concepts first will most likely illuminate the differences, and calculations should be excluded in the first step (*cf.* Carson, 2001; Gabel, 2003). Also, as enthalpy and its change are introduced using a frictionless piston in a cylinder together with an algorithmic derivation, empirical evidence suggests that the purpose of introducing enthalpy in chemistry will most likely evade students (*cf.* Carson, 2001; Sözbilir, 2001). Work, especially expansion work, must be further emphasized and exemplified in teaching since one purpose of introducing enthalpy and its change is related to expansion work.

In theory, it is also possible to exclude the abstract concept of enthalpy from teaching altogether, but in practice it seems more difficult. Some students need enthalpy further along their educational path as well as in future employment. Hence, it is difficult to give clear suggestions concerning whether or not to exclude enthalpy. However, one hypothesis is that most students will understand the more fundamental parts of chemical thermodynamics better if enthalpy is excluded.

In Sweden, enthalpy is introduced at the upper secondary level and in most examples used it is not needed as a theoretical foundation. In fact, most students are already in the forms of energy framework (Goedhart and Kaper, 2002), and chemistry teachers can therefore use energy, heat, work and the first law of thermodynamics to prepare them for the chemical perspective. In order to bridge the gap to physics and find similarities, it is also possible to consider energy quality (and entropy) as parts of the chemistry curriculum (*cf.* Engström, 2008). However, bridging the gap requires teachers' awareness of how different science subjects use the concepts (*e.g.* the forms of energy framework and biology) and how they are used in everyday life.

Following Beall's (1994) line of argument about scientific terminology, we believe in a revision of how enthalpy changes are expressed. Long ago, Zemansky (1974) proposed that *enthalpy of vaporization* should instead be expressed as *enthalpy change due to vaporization*. One step in this direction has been made, with IUPAC (2007) changing the index of the process from ΔH_{vap} to $\Delta_{\text{vap}}H$, thus indicating that the enthalpy of a system changes due to vaporization. However, many standard textbooks still use the old expression.

Although the previous suggestions were intended for policy-makers, closing the gap between secondary- and tertiary-level chemistry education is of importance since the same content is covered (de Jong, 2000). Enthalpy is a commonly used concept

in both upper secondary- and tertiary-level chemistry, and it is surprising how limited the research is on the actual teaching-learning process. Since this research has been carried out at the tertiary level, the research suggestions offered here are relevant to higher education.

We propose three research suggestions: firstly, use the same tasks in order to collect more data, whereby discussions in classrooms may provide new insight; secondly, develop new tasks in order to refine old results and construct new ones. Both these suggestions can be carried out within the frame of a university chemistry course; thirdly, use theoretical triangulation in order to gain different theoretical insights (Robson, 2002).

We chose to continue the discussion of continuous content-related research as posed by Carson (2001), Sözbilir (2001) and other researchers in chemistry education research. In light of the development during the past decade, one suggestion is to address socio-scientific issues in relation to enthalpy and its change. Our empirical evidence indicates that energy, heat and work can be used by undergraduate students to explain different socio-scientific issues, whereas enthalpy and its change cannot.

Appendix 1. Selected tasks translated into English

The first task was developed during the research process. It also includes a question, C, that was a calculation using Hess' law. The task was used in HST1a as Question 4ab; FST as Question 3ab and FSTE2 as Question 3ab. During HS, ΔE was used to describe the change in internal energy (*cf.* Zumdahl and Zumdahl, 2007) whereas ΔU was used in FS. Below, only ΔU is used.

As a chemical reaction occurs, the enthalpy change ΔH for the reaction sometimes differs from the internal energy change (ΔU) for the reaction.

- Give an example of a reaction that fulfils $\Delta H \neq \Delta U$. (2p)
- Motivate why the chosen reaction fulfils $\Delta H \neq \Delta U$. (3p)

The second task was based on Sözbilir's (2001) original. It was used in HST1a as Question 5ab; in HSE2 as Question 7ab; in FSE1 as Question 3ab; and in FST as Question 10ab.

The third task was developed during the research process. The situation presented here is analogous to the interview tasks in which exothermic/endothermic reactions took place in front of the students. The task was used in HST2b as Question 3.

Assume two identical beakers filled with the same volume of water. Add 1 mol of solid sodium hydroxide to one beaker and 1 mol of solid potassium iodide to the other beaker. A while later an increase in temperature is observed in the beaker with sodium hydroxide while the temperature decreases in the beaker with potassium iodide. The temperature in the surroundings is constant during the experiment. The beakers cannot affect each other's temperature.

Please explain how both reactions can occur despite the increase in temperature in one beaker and decrease in the other. Base your explanation on the concepts enthalpy, Gibbs free energy, entropy and bonds.

Consider the reaction

taking place in each set of apparatus shown below. In A the tap is open, and in B the tap is closed. Equal amounts of reactants are used in each case.

Consider that the reactions are completed and the systems are cooled down to their initial temperature, and you are able to measure the heat given out to the surroundings by the reaction. Based on the information given, please explain:

- In which set of apparatus, A, B or both, do you think most heat is given out to the surroundings? Explain your answer as carefully as you can.
- In which set of apparatus, A, B or both does energy transferred as heat equal the reaction enthalpy? Explain your answer as carefully as you can.

(A) Open tap (the pressure inside the syringe equals the pressure outside the syringe)

(B) Closed tap

The fourth task was presented as HSE2 Question 9. A similar one with magnesium and hydrochloric acid was presented in HSE1, but in this case the questions concerned temperature, energy and enthalpy. Below, the term *spontaneously* is used in the question since it is used by both Teacher L3 and Zumdahl and Zumdahl (2007).

Consider the following reaction $2\text{Na(s)} + \text{Cl}_2\text{(g)} \rightarrow 2\text{NaCl(s)}$ which occurs spontaneously at 25 °C.

Consider the reaction

taking place in each set of apparatus shown below. In A the tap is open, and in B the tap is closed. Equal amounts of reactants are used in each case.

Consider that the reactions are completed and the systems are cooled down to their initial temperature, and you are able to measure the heat given out to the surroundings by the reaction. Based on the information given, please explain:

- In which set of apparatus, A, B or both, do you think most heat is given out to the surroundings? Explain your answer as carefully as you can.
- In which set of apparatus, A, B or both does energy transferred as heat equal the reaction enthalpy? Explain your answer as carefully as you can.

(A) Open tap (the pressure inside the syringe equals the pressure outside the syringe)

Before reaction

After reaction

(B) Closed tap

Before reaction

After reaction

(a) Is it exothermic or endothermic? Describe how you arrive at your answers and the assumptions you make.

(b) What happens to the bond energy during the described reaction (from reactants to products)? Please explain as thoroughly as possible.

(c) Please explain why the bond energy and bond enthalpy do not have the same numerical value.

The fifth task is based on Sözbilir's (2001) original and the results in the main study of students interpreting the figures differently (see Conception F9). The task was used in FSInl2 as Question 9ab and in FSE2 as Question 4ab.

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† Here R is short for state function/reaction/amount of substance/reactants and products.

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