



An interactive approach to the notion of chemical substance and the case of water

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Abstract

From organic synthesis to quantum chemical calculation, chemists interact with chemical substances in a wide variety of ways. But what even is a chemical substance? My aim is to propose a notion of chemical substance that is consistent with the way in which chemical substances are individuated in chemistry, addressing gaps in previous conceptions of chemical substance. Water is employed as a case study to develop the account, not only because it is a familiar example of a chemical substance, but also because its structural peculiarities make it an ideal test case for drawing out potential issues and limitations. Examining four distinct views of chemical substance—the microstructural, thermodynamic, purification, and a functional/relational account—I conclude that each has considerable drawbacks when used as a standalone concept. However, these accounts are not rendered obsolete, but are combined into a semi-pluralist conceptual patchwork. My interactive account of chemical substance is consistent with existing substance descriptions and chemical practice.

Keywords Chemical substance · Concepts · Water · Ontology of chemistry · Pluralism · Pragmatism

Introduction

No one really understands water. It's embarrassing to admit it, but the stuff that covers two-thirds of our planet is still a mystery.
(Ball 2008)

Chemists interact with chemical substances in a multitude of ways: we produce and manipulate them in the laboratory, measure their properties with elaborate instruments, simulate them on computers and use a wide range of diagrams to represent, describe and reason about them. But what lies at the centre of all these activities? What is a chemical substance?

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In the broadest possible sense, a chemical substance is a category of matter within a broader system of categorisation that is central to the discipline of chemistry. My project of articulating a notion of chemical substance is predominantly concerned with explicating the workings of this broader system. Of course, not all matter can be meaningfully described in chemical terms. Chemistry is not concerned with categorising and describing the inner workings of fundamental particles like neutrinos and certain astronomical objects like black holes, but it applies to almost everything in between. Every material we encounter in our daily lives can be described in terms of the chemical substances it consists in. For example, coffee comprises a variety of chemical substances, such as water, caffeine, pyrazine, and quinic acid. Chemistry is a science, so there is some method to the madness of categorising substance—it is entirely uncontroversial that individual substance categories are systematically related in some way. However, it is hotly debated in the philosophy of chemistry what this system actually looks like. In developing a novel, interactive account of chemical substance based on Wilson's (2006) account of concepts, I aim to answer this question.

Water is an especially supportive case study for developing a semi-pluralist, interactive account of chemical substance. Of course, water is ubiquitous and easily recognized. We reference or interact with it in a very broad range of circumstances. Nevertheless, water is rather exceptional with regards to its complex microstructure and thermodynamic anomalies, still posing some unanswered questions that are the object of active scientific investigation (Stanley et al. 2007). In the discussion of different notions of substance, these complexities can be used to draw out nuances and limitations. Furthermore, water can serve as an extreme test case for a novel account. The ability to aptly capture a chemical substance as eclectic and multi-faceted as water can be considered an indication of a promising breadth of applicability of a proposed account.

Water works particularly well as a challenging test case because it is very firmly understood as a chemical substance despite its complexities. One strategy of dealing with difficult test cases is denying that something is a substance by definition to keep the internal consistency of an account intact. Such a move is certainly justifiable in some cases, but it seems untenable in the case of water. Scientists and laypeople alike share a strong conviction that water is to be classified as a chemical substance. A notion of chemical substance that aims to track the actual use of the term to any extent should not be in opposition to such a widely shared classification of a substance as ubiquitous as water.

Beyond just the case of water, any reasonable system of chemical substance should be broadly consistent with naming conventions in chemistry. One can refer to chemical substances using multiple, more or less systematic, representational tokens. These include common names, systematic names, sum formulas, structural formulas, and even physical models. Out of these, only structural formulas and systematic names are derived from a standardised system and considered generally unambiguous. Structural formulas are especially popular, as they are much easier to decipher even at a glance. Throughout the paper, I use H_2O as a shorthand for the structural formula of water.

In this paper, I outline an interactive approach to the notion of chemical substance. Using the example of water, I develop a semi-pluralist notion of chemical substance that is both coherent and applicable to a broad range of contexts. In Sect. "[Existing accounts](#)", I begin by entertaining multiple views of chemical substance: the microstructural account (Sect. "[The Microstructural account](#)"), the thermodynamic account (Sect. "[The thermodynamic account](#)"), the purification account (Sect. "[Further macroscopic criteria and the purification account](#)"), and a functional/relational account (Sect. "[A Functional/relational account](#)"). I argue that each has considerable drawbacks when used as a

standalone concept. In Sect. “[To choose or not to choose](#)”, I show that these accounts are neither mutually reducible, nor co-extensive. However, there are considerable overlaps that enable smooth shifts and productive combinations of different conceptions in practice, demonstrated in Sect. “[An Interactive Patchwork](#)”. Ultimately, I argue that we need not forego any conception of chemical substance in favour of another but may instead embrace a semi-pluralist conceptual patchwork, held together by interactions. A chunk and permeate approach ensures that such a patchwork is feasible despite global inconsistencies.

Existing accounts

The microstructural account

In the microstructural view, chemical substances are ultimately characterized by their microstructure, meaning the spatial and topological arrangement of atoms on the molecular scale, as described using molecular and structural formulas. In this view, one might hold that water is essentially H_2O . In philosophy of science, this claim was famously made by Kripke (1972) and Putnam (1975), who relied on water as a foundational example for their account of natural kinds.

There are several ways in which the rather simplistic conception of water as H_2O fails. First, how we think of the makeup of water is historically contingent. Chang (2012) convincingly argues that we might have come to think of the elemental composition of water much differently than we do today, showing that H_2O might plausibly have come to be designated as HO instead. Secondly, self-ionisation complicates the picture. At 24 °C and zero ionic strength, the concentration of OH^- and H_3O^+ ions is 10^{-7} M each in any body of pure water. Furthermore, H_2O , OH^- and H_3O^+ are not present as isolated single units, but form hydrogen bonds, resulting in a very broad range of rapidly shifting superstructures (Ignatov and Mosin 2013; Keutsch and Saykally 2001). On a structural basis, it is decidedly inaccurate to state that water is simply H_2O . If the notion of any given chemical substance were directly and solely tied to the molecular structure associated with its structural formula, an honest look at the evidence would lead us to abandon water as a chemical substance rather than reduce it to H_2O .

A more sophisticated microstructural account has been proposed by (Hendry 2006), trying to save the microstructural view of water. Hendry acknowledges that interatomic geometry is not rigid but only forms vague-bounded, overlapping clusters of chemical structures. To circumvent the self-ionisation and superstructures, he posits an isolated molecule: “water is the substance formed by bringing together H_2O molecules and allowing them to interact spontaneously” (Hendry 2006). In other words, water is whatever happens when you put isolated H_2O molecules together.

The proposed definition is unidirectional, going from the microscopic to the macroscopic assemblage, the latter being inconsequential. Of course, bringing single H_2O molecules together to form a body of water is not a task we typically engage in when handling water. In order for the conception to be of any use, it must be applied to actual bodies of water counterfactually. How does one tell if a substance could have been produced by putting together single H_2O molecules? The criterion is only viable if there is a possibility to go in the other direction, to isolate single molecules. If one, hypothetically, were to isolate just one molecule from a liquid body of water, there is an (admittedly small) chance that it is not H_2O . However, there are states in which a body of water resembles an aggregate

of isolated H₂O molecules more closely. IR spectroscopy attests that hydrogen bonds still exist in the gas phase, but do so more rarely and form smaller structures (Maréchal 2007), depending on temperature and pressure. Water may still form superstructures even in a molecular beam (Dyke and Muentner 1972), a method commonly employed to conduct single molecule experiments. Single H₂O can also be isolated by enclosing it in fullerene structures (Varadwaj and Varadwaj 2012), but in this case still interacts, albeit weakly, with the fullerene. In practice, it is surprisingly difficult to separate any macroscopic amount of water into nothing but single H₂O molecules, even when using procedures designed to do just that.

The procedures that may result in obtaining single, isolated H₂O molecules are far removed from the ways in which scientists analyse and recognize water in practice. The presence of hydrogen bonds by no means obfuscates the identification of water. Not only are the resulting structures causally connected to many unique and recognisable features of water, but they are also observed in its analysis. For example, the rotational bands in the IR spectrum of water depend on the extent to which hydrogen bonds are present (Maréchal 2007). They also influence the OH stretching band (Schmidt and Miki 2007). Of course, such methods do contain ample evidence for structures in which an oxygen is linked to two hydrogen atoms. However, the H₂O is only isolated from hydrogen-bonded structures conceptually in the interpretative process, not by any material process of isolation. I am not arguing that this simplification is unjustified or that such a link is impossible to establish. However, the reduction of water to H₂O is post hoc in most actual contexts: relying on the presupposition of H₂O as a meaningful entity and foregoing other conceptions or structures that may also be supported by the data, purely because the neat simplification of water to the theoretical entity H₂O already exists. When H₂O remains a theoretical entity, defining water as what happens when these theoretical molecules are put together becomes nonreferring, as the reference to actual material substance is lost. It is at least troubling for Hendry's conception that the conceptual connection is rarely established with reference to the analysed substance in practice but relies on roundabout counterfactuals instead.

It seems reasonable to demand that a concept of water is in some way tied to how water is identified in practice, although one must be careful not to conflate concept and criteria for recognition. Here, Hendry's definition encounters another problem: water was recognized as a chemical substance long before chemical structure, the idea of molecules as actual microscopic building blocks, or even hydrogen and oxygen as elements ever caught on. One might argue that previous concepts of water were based on stereotypes as opposed to an underlying principle we recognise today, but such a belief seems difficult to reconcile with the remarkable constancy of the concept of water across time, especially relative to the much more dynamic history of chemical theories. Conceptualizing water as H₂O is in line with a sophisticated theoretical backdrop that comes with simplifying assumptions. This theoretical backdrop has shifted over time and is by no means a unified construct, but it has remained stable enough to assume that H₂O refers to a meaningful theoretical entity. However, this entity does not neatly fit the complicated and heterogenous microstructure of actual water in light of current evidence. The convention to re-assert that water is one unified chemical substance is in tension with its complex microstructure. In Hendry's proposal, reference is established via a more direct and less contentious relation between the formula H₂O and a single water molecule that conforms to it. However, the cited single water molecule remains counterfactual for the most part, and thus within the theoretical framework. The microstructural conception does less to support the reference between actual macroscopic substances and the referential tokens used in chemistry than one might expect.

The thermodynamic account

The thermodynamic view is a competing approach to chemical substance, which foregoes reliance on microstructural properties altogether. It is most strongly defended by Needham (2000; 2002; 2017). Thermodynamically, chemical substances are individuated by their characteristic phase changes, which can be plotted against temperature and pressure in phase diagrams. Melting and boiling points at atmospheric pressure can be induced and observed even with very simple equipment, hence these two points of a phase diagram usually suffice for individuation in practice. The choice of phase change as a criterion rests on the premise that chemical substances retain their identity during phase change. On a theoretical level, the macroscopic individuation is often justified with reference to Gibbs' paradox, which holds that quantities of different chemical substances exhibit an entropy of mixing when mixed isothermally, whereas quantities of the same chemical substance do not (Needham 2002, 2000). Proponents of the account need neither deny the existence of microfeatures in general, nor do they oppose the use of microstructural abstractions in chemistry (Needham 2000), but do not take them to be a reliable basis for individuating chemical substances.

The case of water illustrates some gaps in the thermodynamic view. An isolated molecule cannot have a melting or a boiling point, as phases only emerge due to the relative movement of multiple molecules to each other. In a strictly thermodynamic view, a volume of water that only comprises a single H₂O molecule could consequently not actually be considered water. This conclusion seems counterintuitive to chemists.

The view has some unclear implications for chemical substances that vary in isotopic composition. There are several stable isotopes of both hydrogen and oxygen, all of which are usually present in water. However, the isotopic composition may vary, either for natural reasons (see e.g. Dotsika et al. 2010) or because it has been artificially enriched. Heavy water contains only the heavier deuterium (²H) in place of the lighter and more common hydrogen isotope protium (¹H). Isotopic composition influences chemical reactivity and physical properties such as melting and boiling points in very subtle ways. These effects are most pronounced in the case of hydrogen, as additional neutrons have the strongest relative effect on the atomic weight. Given its composition, isotope effects are particularly noticeable in water, although by no means unique to it. The phase diagram of heavy water is markedly different from the standard phase diagram of water (Bridgman 1935). Given these discrepancies, must heavy water not be considered a different chemical substance in the thermodynamic view? If so, where would we draw the line in the distribution of possible isotope ratios?

Mirroring the somewhat flimsy counterfactual connections in the microstructural account, there are circumstances in which the thermodynamic one makes substance assignments seem overly speculative. Although these cases do not challenge the internal consistency, they demonstrate the limited applicability of the accounts. Melting and boiling points are dramatically influenced by impurities. Such shifts do not pose a theoretical challenge to the thermodynamic view—the aberrant thermodynamic behaviour of mixtures indeed lies at the very core of its theoretical foundation. However, a direct reference is technically only established when melting and boiling points of pure¹ substances are measured. When such a measurement is not possible,

¹ Of course, ideal purity is not attainable but must be approximated.

they cannot simply be inferred using other analytical techniques. Even attempts to calculate them using molecular structure are fairly limited, especially in the case of melting points (Yalkowsky and Alantary 2018). Measuring samples with a high degree of purity does not pose a problem in the case of water, but there are many substances that are only stable in solution. Some substances disintegrate in a chemical reaction at temperatures and pressures far below potential melting or boiling points. In these cases, melting and boiling points cannot be measured. Nevertheless, there are many analytical techniques, such as IR spectroscopy, that are routinely used to identify such substances and that can be used even when a substance is present in solution. In fact, modern chemistry tends to rely on these techniques even when melting and boiling points are available. Interpreting the results of these types of analysis is essential to substance chemistry. These techniques are clearly seen as a solid basis for substance classification, so it seems arbitrary to introduce the availability of melting and boiling point as an additional criterion.

One could argue that the microstructural conceptions are only extensions of patterns established in and ultimately reliant on previous thermodynamic investigation. Yet, modern analytical techniques such as NMR spectroscopy can hardly be meaningfully interpreted without at least some realist commitment to microstructures. The refusal to directly incorporate microstructural evidence makes many compounds seem more speculative than they actually are.

Further macroscopic criteria and the purification account

Chemical substances have many macroscopic features beyond thermodynamic ones, upon which we may draw to recognize and define them. For example, liquid water is colourless and clear. It (arguably) does not have a smell or taste. Its viscosity can be estimated or measured, as well as its refraction index. One can assess solid water, or ice, along a range of measures of hardness and flexibility. In our day to day lives, these properties are used much more frequently to recognize water than either microstructure or thermodynamics. These largely sensory criteria cannot be used to establish a scientifically justified basis for a taxonomy of chemical substance, as there is no theoretical foundation that would warrant any specific choice of criteria.

A broad macroscopic set of features is recognized in Schummer's (1998) purification view of chemical substance, a macroscopic conception in which chemical substances are individuated via purification. Distinct chemical substances are those which cannot be further purified by any means available at the time. Purification commonly involves thermodynamic separation techniques. Thus, the purification view is not dissimilar from the thermodynamic view. However, additional macroscopic interventions and criteria are admitted, which may for example include enantioselective chromatography, colour, or crystal shape.

The purification view inherits many limitations from the thermodynamic account. Macroscopic purification criteria are not applicable to isolated molecules and may thus not be used to individuate them. Furthermore, there are in fact means to isolate heavy water, which may again render it a distinct chemical substance according to this view. Lastly, a direct referential link can technically only be established when a substance is actually purified.

A functional/relational account

Beyond microstructure and macroscopic criteria such as thermodynamical properties or purification, a functional/relational view of chemical substance is at least conceivable. A functional/relational view does not consider individual substances in isolation, but according to their roles in broader systems. Such classifications are already employed in some chemical subdisciplines, for example in protein biochemistry. A functional/relational account may plausibly bridge microscopic and macroscopic features. Such a view has, to my knowledge, not been proposed in the literature thus far and it is not my intent to sketch out what exactly it might entail here.

In the case of water, a functional/relational view would likely feature its life sustaining properties and role in biochemical processes. These are closely tied to the physical and chemical features discussed in the above section. Hydrogen bonds as well as the density anomaly of water evident in its phase diagram are crucial to sustaining life on earth. There are some open questions regarding the generalizability across time and space if these features are expressed in functional or relational terms. Nevertheless, the account seems promising for some circumstances not covered by the accounts outlined thus far, particularly in the case of biomolecules that only assemble in water and assume different structures depending on their molecular environment (Tobin 2010).

A functional/relational account might be of interest for some intents and purposes, especially in biochemistry, where biomolecules are often classified by function rather than composition already. However, there are many open questions, especially regarding concentration. Purified water is toxic to most organisms in large amounts. Yet it would go against all of established chemistry (with the possible exception of biochemistry) to argue that impure and pure water are distinct chemical substances. A functional/relational account may work in specific local circumstances but can hardly be applied to all contexts. Any such account needs to be established relative to a specific chemical purpose of inquiry and can function well for this purpose. However, there is no single purpose of inquiry that holds across all of chemistry. Therefore, any particular functional/relational account is unlikely to generalise across the field.

Moving forward

To choose or not to choose

To summarise the above, we are left with at least four distinct conceptions of water, all of which are usefully applied to some but not all contexts in which one may analyse or otherwise encounter water. The microstructural view allows us to include single molecules and, using somewhat roundabout and often counterfactual links, any aggregate in which these may feature, no matter whether it may be considered pure or impure. Both the thermodynamic and the purification account are far less reliant on counterfactual reasoning, and thus left less vulnerable to inaccurate theorising. However, they imply an evidential gap between substances that can be isolated and those that cannot be. This gap seems difficult to uphold in face of the prowess of modern analytical techniques, which heavily rely on microstructural interpretations. The possibility of a functional/relational approach was only briefly brought up. It may potentially perform well in areas not adequately covered

by any of the other accounts discussed. Any functional/relational account is embedded in local circumstances, for which it can be advantageous. For example, a functional/relational account could feasibly be constructed for polymer chemistry or nanochemistry. Particular functions and relationships are integral to any such account, so these cannot just be stripped for the purpose of generalising the account across subdisciplines. Thus, the use of functional/relational accounts remains limited.

The accounts of chemical substance are not mutually reducible. Each account has a distinct foundation for the individuation of substance. I have argued that these foundations are connected but one cannot be used to infer the basis of another. Most obviously, any functional/relational account requires contextual information that is neither provided nor can it be processed in any of the other accounts. One may assume that the information provided by the thermodynamic and the purification account can be reduced to a microstructural concept, but this is not the case. There are trends that correlate certain microstructural features with melting or boiling points. For example, larger and more polar microstructures correlate with higher melting and boiling points. For some substances, numerical predictions may even be made with some accuracy based on known series of similar substances or quantum mechanical calculations. However, there is no single method that is both accurate and universally applicable to all substances (Yalkowsky and Alantary 2018). Similarly, predictions are commonly made for specific purification procedures based on microstructural considerations, but these are heuristic in nature and tend to be qualitative rather than quantitative. Conversely, the molecular structure of a chemical substance can only be inferred from melting or boiling points given ample additional information on its reactivity and/or further measurements. Purification procedures and assumptions about molecular structure mutually inform one another, thus one cannot replace one with the other. Out of all combinations, the thermodynamic and the purification accounts are perhaps the most similar. Still, the purification account incorporates a broader range of input. Unlike the thermodynamic account, the purification account is able to incorporate new criteria for the individuation of substances, as is the microstructural account.

Conceding mutual reducibility, one may still hold that it is permissible to arbitrarily choose one account or use them in parallel if the resulting taxonomies were co-extensional. Again, the functional/relational account most obviously diverges from the others, as it covers grounds in biochemistry that only partly overlaps with the other conceptions. Though the classifications resulting from each of the other accounts are largely in agreement, there are special cases in which they are not, for example in the case of allotropes and nanoparticles. There are conflicting opinions as to whether allotropes should be considered unique chemical substances (van Brakel 2012). Allotropes are different forms of an element in the same physical state, such as diamond and graphite, metallic and non-metallic Zinc or the numerous forms of elemental sulphur. While these do have different three-dimensional microstructures, they are converted into one another in a way that is generally considered a phase transition. Most nanoparticles are assemblages that are microstructurally no different than much larger lumps of the same material. Yet, they often show vastly different behaviours in macroscopically observable physical properties, such as colour, melting point (Buffat and Borel 1976) and chemical reactivity. Both allotropes and nanoparticles would thus be categorised in different ways depending on whether one uses a micro- or macrostructural account of chemical substance.

Acknowledging that the accounts are neither mutually reducible nor co-extensional, the two remaining options are either to pick the most advantageous account or to embrace some kind of pluralism about chemical substance. The former currently remains a viable if disadvantageous option. The most pressing drawbacks of each account have been discussed

in Sect. “Existing accounts”. The flaws can be considered serious, but they are not fatal. At this stage, one could further weigh the advantages and disadvantages of each individual account and deem one of them preferable over the others, but it is clear that the result would not be very satisfactory either way. Besides, cutting out an account just because it does not look promising may even impede scientific progress (Chang 2012). Instead, I use the last section to sketch a semi-pluralist picture that is able to connect the different accounts and that can be used to resolve local inconsistencies.

An interactive patchwork

In order to connect and at least partly reconcile the different accounts, I adopt a contextualist view based on Wilson’s (2006) account of concepts. I propose that accounts of chemical substance are invoked locally to facilitate interactions, meaning both the interactions of scientists with substance and resulting interactions of substances with each other.

Wilson (2006, chap. 6) argues that concepts are in many cases not simple means to reach a classificatory goal. Instead, groups of predicates often subdivide into localised patches that are formally inconsistent with one another (Wilson 2006), and are interconnected by bridges. Collectively, the patches and bridges form uneven facades of interconnected meaning. A concept is especially prone to splitting into patches in order to allow the description of complex systems using a manageable number of descriptive terms (Wilson 2006). In scientific reasoning, bridges and patches can be constructed using a chunk and permeate approach (Brown and Priest 2004, 2015; Friend et al. 2018). This paraconsistent reasoning strategy deals with global inconsistency by separating locally consistent chunks and operating within these. A limited amount of information is allowed to permeate between chunks. The approach keeps the patchwork intact and prevents arbitrary conclusions despite global inconsistencies.

In the case of chemical substance, the outlined accounts may be understood as such localised patches, as they are mutually inconsistent yet connected via extensional overlaps and bridges of mutual interdependence. By extensional overlaps, I mean chemical substances in contexts for which the above accounts are in agreement. For example, the thermodynamic and the microstructural account are in agreement when classifying a litre of purified water. When a volume comprising only a single H₂O molecule is isolated from this litre of water, only the microstructural account is able to meaningfully bridge the two contexts, whereas the thermodynamic account loses traction. Conversely, a distillation after an unknown reaction derives its justification as a goal-directed intervention purely from the thermodynamic or purification account, whereas a microstructural reference cannot be established at this moment, pending further investigation.

The interaction-based dynamic aggregate actually is much closer to chemical practice than any singular account. In the laboratory, chemist’s smoothly move between experimental procedures such as purifying chemical substances with thermodynamic procedures, and reasoning about the occurring processes by abstracting them to structural formulas. Experimental procedures are adjusted in response to the microstructural reasoning, which would make little sense without a realist commitment to the microstructural reference of structural formulas. On the other hand, structural formulas remain open to adjustments if observed properties are not coherent with expectations. To the practicing chemist, both microstructural theory and experimental procedures remain malleable and are continuously adjusted to each other. These activities can be understood

using a chunk and permeate approach. Consistency is demanded locally within a chunk, but not globally. Thus, each interaction remains coherent.

Even seemingly irreconcilable differences in extension can be overcome with a narrow focus on the interaction at hand to construct a separate chunk. For example, one need not commit oneself to a stance on the universal substance status of allotropes, when planning a catalytic reaction involving allotropes. If the relevant feature involves reactivity exhibited by one allotrope but not another, it may be more pertinent to adopt the microstructural view. If, however, the reaction involves a phase transition, it may be more useful to conceptualise them as a single substance.

Letting go of global consistency in favour of a broader, adaptative scope and local fit may seem like a rather daring step. However, global consistency is a value that need not be adopted unquestioningly (Longino 1995). Inconsistencies are common across science. They can be rationally navigated using a chunk and permeate approach (Friend et al. 2018). In fact, global consistency is not a value that chemists seem to particularly care about. For example, many chemists still routinely employ a shell model of the atom for simple approximations of reactivity, fully aware that it is inconsistent with current theory and evidence. An even more brazen example is the use of different, conflicting scales of electronegativity depending on subfield and research goal. It is far from unusual in chemistry to forego broader theoretical consistency in favour of practical aims. Pluralism of theories and methods that is contextually adapted to coherently fit the subdiscipline and research question is already widespread in chemistry. A matching notion of chemical substance therefore seems like a fitting next step.

Conclusion

In summary, my discussion of the microstructural, thermodynamic, purification, and functional/relational accounts of chemical substance has uncovered a range of drawbacks to each, using water as a challenging test case. Yet, none of these drawbacks amount to fatal flaws. Each account is useful in certain circumstances notwithstanding gaps in other areas. I have shown that the accounts are not mutually reducible. Furthermore, they cannot be considered to be co-extensional, although they largely result in intersecting classifications. Instead of dismissing some accounts in favour of others, I have demonstrated that they can be combined into one semi-pluralist patchwork based on interactions, taking context and purpose into account. My interactive account of chemical substance shows that it is not necessary or even useful to unite all of chemistry under one rigid notion of chemical substance.

We need not forego any particular conception of chemical substance already in use in favour of another. Instead, contextual notions of chemical substances can be aggregated to form a dynamic set of interconnected notions. There need not be one single shared relation that consistently holds all chemical substance classifications together. The problematic implications of global inconsistencies are avoided with the use of a chunk and permeate approach. Local coherence can be maintained via a radically contextual focus on interaction.

My semi-pluralist account has far-reaching implications for understanding not only present uses but also the history of the notion of chemical substance. Any rigid account of chemical substance runs the risk of becoming further and further removed from chemical practice as novel techniques are introduced that rely on properties of chemical substance not

considered in the central tenets of the account. This effect can currently be observed in the thermodynamic account of chemical substance, which arguably captures dominant ideas of chemical substance in the early to mid-twentieth century very well, but increasingly has trouble keeping up with modern analytical techniques, that are increasingly removed from melting and boiling points. In contrast, a patchwork account can accommodate new input and gradual shifts in focus. Obsolete patches can be slowly disbanded, while new ones can still be informed by them and gain import gradually, allowing smooth transitions with a chunk and permeate approach. My proposed notion of chemical substance can thus account for the remarkable persistence of most substances even over several dramatic theoretical and experimental shifts in chemistry over the last 200 years and the continuing relevance of a notion of chemical substance to this day.

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Declarations

Conflict of interest The author has no relevant financial or non-financial interests to disclose.

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