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A Model of Early Chemical Reasoning[1]

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1. Introduction

During the 18th Century, one of the primary goals of chemistry was to determine the *components* of substances. This was a long and painstaking process, during which many different models were proposed and rejected. Throughout most of the 18th century combustion was believed to involve the decomposition of the combustible body, and this was one of the central tenets of the theory of *phlogiston*. Only in the last two decades of the 18th century was the phlogiston theory challenged and eventually replaced by the *oxygen* theory. In this paper we describe STAHL, a cognitive simulation that models the inferences made by early chemists. The system is named after G. E. Stahl (1660 1734), one of the principal formulators of the phlogiston theory. In the following pages we describe STAHL in terms of its component heuristics, and trace its reasoning on a number of episodes from the history of the phlogiston theory.

2. An Overview of STAHL

STAHL's input consists of a set of reactions, each represented by a simple schema. For instance, the reaction of sulphur and iron to form sulphuretted-iron would be represented as (react (input sulphur iron) (output sulphuretted-iron)). STAHL's goal is to determine the components of all non-elemental substances involved in the given list of reactions. In the table below we present six heuristics used by STAHL in inferring the componential models of substances.

STAHL's heuristics for inferring the components of substances.

INFER-COMPOSITION
If A and B react to form C,
or if C decomposes into A and B,
then infer that C is composed of A and B.

REDUCE
If A occurs on both sides of a reaction,
then remove A from the reaction.

SUBSTITUTE
If A occurs in a reaction,
and A is composed of B and C,
then replace A with B and C.

EQUATE-DECOMPOSITIONS
If A is composed of B and C,
and A is composed of D and E,
then infer that B and C react to form D and E.

IDENTIFY-COMPONENTS
If A is composed of B and C,
and A is composed of B and D,
then identify C with D.

IDENTIFY-COMPOUND
If A is composed of C and D,
and B is composed of C and D,
then identify A with B.

The most basic of the rules, INFER-COMPOSITION, deals with simple synthesis and decomposition reactions, and lets the system unambiguously infer the components of a compound. For example, given the sulphuretted-iron formation reaction, this rule would infer that sulphuretted-iron consists of sulphur and iron. Of course, the INFER-COMPOSITION rule can also deal with cases in which three or more substances unite to form a simple compound, and with similar decompositions.

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For more complex reactions, STAHL employs other rules to transform these reactions into simpler forms, so they can eventually be matched by INFER-COMPOSITION. Thus, the REDUCE heuristic is responsible for "cancelling out" substances occurring on both sides of a reaction, leading to a simplified version. For instance, given the input (react (input calx-of-iron vitriolic-acid water) (output vitriol-of-iron water))[2], the REDUCE rule would produce the simplified description (react (input calx-of-iron vitriolic-acid) (output vitriol-of-iron)). In turn the INFER-COMPOSITION rule would conclude that vitriol-of-iron consists of calx-of-iron and vitriolic-acid.

The third heuristic (SUBSTITUTE) initially leads to more complex statements of reactions, but may enable the REDUCE rule to apply. This rule draws on information about the components of a substance that have been inferred earlier. Eg. suppose that, in addition to the last example, STAHL knows that (react (input iron vitriolic-acid water) (output vitriol-of-iron inflammable-air water)). Now, by REDUCE (applied to water) and then by SUBSTITUTE (applied to vitriol-of-iron) the system infers that iron consists of calx-of-iron and inflammable-air. This is in fact the conclusion drawn originally by Cavendish [1766], after he discovered hydrogen while dissolving metals in acids.

Let us now, based on the three rules described above, consider the origins of the theory of phlogiston early in the 18th century. G. E. Stahl adopted the ancient view that fire is a manifestation of a common principle which leaves a body during combustion. Therefore, any reaction involving combustion was viewed as a decomposition; for instance, burning charcoal was interpreted as decomposing it into phlogiston (another term for the matter of fire) and some residual ash. G. E. Stahl succeeded in proving the usefulness of the notion of phlogiston in explaining many reactions that were by no means reactions of combustion, and in justifying the presence of phlogiston in substances that were not combustibles.

Let us examine the path taken by STAHL in ariving at the initial conclusions of the human Stahl's theory of phlogiston. We present the system with two facts: (react (input charcoal air) (output phlogiston ash air)) and (react (input calx-of-iron charcoal air) (output iron ash air))[3]. Given both reactions, STAHL immediately applies its REDUCE heuristic to the first fact, giving the revised reaction (reacts (input charcoal) (outputs phlogiston ash)). The system then applies the same rule to the second fact, giving the reduced reaction (reacts (input calx-of-iron charcoal) (output iron ash)). After this, the first of these revisions, combined with the INFER-COMPOSITION rule, leads to the inference that charcoal is composed of phlogiston and ash, which was one tenet of the early phlogiston theory. Having arrived at this conclusion, STAHL applies SUBSTITUTE, generating the expanded relation (reacts (input calx-of-iron ash phlogiston) (output iron ash)). At this point, REDUCE is used to remove ash from both sides of the equation, giving (reacts (input calx-of-iron phlogiston) (output iron)). Finally, INFER-COMPOSITION leads STAHL to infer that iron is a compound composed of calx-of-iron and phlogiston. If, at this point, STAHL is given the reaction (react (input calx-of-mercury iron) (output mercury calx-of-iron)), in which neither phlogiston nor charcoal is explicitly present, the system infers that mercury consists of calx-of-mercury and phlogiston.

Now we are able to reproduce a historically valid application of EQUATE-DECOMPOSITIONS. Sulphur, as a combustible, was believed to contain phlogiston. To demonstrate that its remaining component is vitriolic-acid, G. E. Stahl refers to the following reactions [Partington, 1961, p. 671]:

(react (input vitriolic-acid potash) (output vitriolated-tartar)),
(react (input sulphur potash) (output liver-of-sulphur)),
(react (input vitriolated-tartar charcoal) (output liver-of-sulphur)).

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[2] The following "dictionary" may be helpful in understanding our historic examples: metallic calxes are 18th century terms for metallic oxides, inflammable air is hydrogen, dephlogisticated air is oxygen, vitriol of iron is iron sulphate, vitriolated tartar is potassium sulphate, and liver of sulphur is a mixture of potassium polysulfides with potassium thiosulfate.

[3] Chemists of the early 18th century acknowledged the necessity of air in combustion as the acceptor of phlogiston and believed that combustion in a closed vessel stops at some point when air gets saturated with phlogiston and cannot accept more of this principle.

All three reactions match the INFER-COMPOSITION rule, and as the result, STAHL produces two different decompositions of liver-of-sulphur. This activates the EQUATE-DECOMPOSITIONS rule and now STAHL considers the additional reaction: (react (input sulphur potash) (output vitriolated-tartar charcoal)). In this reaction, SUBSTITUTION applies to both vitriolated-tartar and charcoal, creating (react (input sulphur potash) (output vitriolic-acid potash ash phlogiston)). Reduction of potash on both sides enables INFER-COMPOSITION to apply, and to conclude that sulphur consists of vitriolic-acid, and phlogiston (and ash, unless we ignore residual substances or use soot instead of charcoal, as the (almost) pure source of phlogiston. STAHL in its present form cannot deal effectively with residual substances or impurities).

The final two heuristics are responsible for postulating that two substances that were originally thought to be different are in fact identical. For instance, the IDENTIFY-COMPONENTS rule matches when STAHL learns that a compound can be decomposed in two different ways, where these decompositions differ by a only single substance. Our examples enable it to apply this rule to iron, for which STAHL has already inferred two different compositions: into calx-of-iron plus inflammable-air and into calx-of-iron plus phlogiston. Identification of inflammable-air with phlogiston, made at this point by STAHL, was indeed a historic fact, and was claimed from 1766 until the final rejection of the phlogiston theory in the 1790's.

Given a set of reactions as input, STAHL applies its heuristics to these reactions until it has made as many inferences as possible. Then the system halts, but it can accept additional input reactions and can make additional inferences. At any given point during the computation, the system's knowledge consists of some mixture of observed reactions, transformed reactions, and componential models. One of the system's interesting features is the manner in which its heuristics interact. Note that the SUBSTITUTION rule (and some other rules, too) requires knowledge of a substance's composition, so that some inferences about composition must be made before it can be used. We have also seen that complex reactions must be rewritten by the REDUCTION and SUBSTITUTION rules before some composition inferences can be made. This interdependence leads to a "bootstrapping" effect, in which inferences made by one of the rules enable further inferences to be made, these allow additional inferences, and so forth. This process begins with one or more simple reactions, but after this the particular path taken depends on the data available to the system.

3. Automated Self-Correction

Although STAHL's heuristics provide useful direction through the space of possible chemical models, they are not guaranteed to produce correct inferences. For instance, the system may apply the REDUCE rule when different quantities of a substance occur on both sides of a reaction, leading to errorful conclusions. However, similar confusions also occurred in the history of chemistry. As late as 1810, Gay-Lussac and Thenard [1810] argued that potassium was a compound of potash and hydrogen, contrary to Davy's claim that potash was a compound of potassium and oxygen. They based their argument on the following reactions:

(react (input potassium water) (output caustic-potash hydrogen water)),
(react (input caustic-potash water) (output potassium oxygen)),
(react (input potassium ammonia) (output hydrogen green-solid)),
(react (input green-solid water) (output caustic-potash ammonia water)).

Only the second reaction is not acceptable from today's point of view. The motivation for this description was Gay-Lussac's and Thenard's disbelief that potash, known to have an extremely strong affinity to water, can be totally destitute of water. Given these four reactions, STAHL is capable of inferring their conclusion about the composition of potassium in three independent ways: from the first reaction alone, from the second reaction (if it is known in advance that water consists of hydrogen and oxygen), and from the last pair of reactions.

Of course, chemists eventually realize their errors and recover from them, and STAHL incorporates strategies to do the same. If, during the computation, a reaction is transformed to the form of empty input: (react (input) (output A)), STAHL enters its error-recovery procedure. There are several other states of the system's knowledge that activate the same procedure: obviously (react (input A) (output)), but also, for