Adjustment of the Event Bush Method to Chemical and Related Technological Tasks

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Abstract. Chemistry, despite its high level of formalization, benefits from implementation of knowledge engineering tools. “Static” (or object-based) methods have been successfully used in this science, but the character of chemical knowledge urges one to look also for “dynamic” (event-based) methods, especially in experimental and industrial domains. Still, quite a work is needed to make the application of event-based methods in chemistry as perfect and correct as that of object-based ones, and adjustment of the said methods to this science may considerably contribute to the theory that underlies them. In particular, new solutions have been found at testing the method of event bush by chemical tasks. These solutions may optimize the method for use in a wide range of fields.

Keywords. Chemistry, knowledge engineering, dynamic knowledge, event bush method, experiment.

1 Introduction

Since the genius discovery of Dmitry Mendeleev expressed in his periodic table of elements, chemistry became one of the best-organized fields of knowledge the humankind ever had. Nevertheless, abundance and diversity of combinations of “allowed” bonds between the elements, especially in organic, bio- and geochemistry, make this field, despite its internal regularity, rather loose and hard-to-span. This claims for application of special methods of organization of knowledge, and such methods have been successfully applied in chemistry.

The most extended and powerful tools of knowledge organization developed for chemistry and related fields (biochemistry, medicine) are Chemical Entities of Biological Interest (CHEBI) ontology [5], nomenclatures of compounds produced by International Union of Pure and Applied Chemistry [3], chemical divisions of ChemID Plus, Medical Subject Headings [10] and some other search systems. In some of them not only lingual but also visual means of representation (structural formulae of compounds) are implemented (e.g., in CHEBI [4]) that is an unusual solution for the ontology design.

Nevertheless, these developments generally fail to encompass one important feature of chemical knowledge – its dynamic character. Indeed, nomenclature of elements or compounds is, in fact, only an introduction to understanding of possible chemical reactions, this well-ordered miracle of transformation of one substance into another. Verbal and graphic explication of this order is useful for understanding of various branches of chemistry, for planning the experiments and, of course, for industrial applications. This is why there were a number of attempts of using the event-based methods in chemical or related issues. Event trees and Bayesian networks are involved to model hazards and disorders at chemical factories [1], flowcharts (sensu stricto or sensu lato, sometimes quite informally), to describe experiments [2; 6] and even to perform classification of compounds [7] – i.e., to approach a "static" task from "dynamic" side.

Still, these methods, as was argued by Pshenichny and Mouromtsev [9], contrary to the object-based ("static") ones, need better rethink and formalization of grammar of event description in the nodes. In such a formalized domain as chemistry, this "under-formalization" of knowledge engineering approaches becomes especially evident. One method of dynamic knowledge engineering, the event bush, has got the most evolved verbal grammar and related structural rules of event combination [8]. In our paper an opportunity of formalization of record of events, processes and scenarios in chemistry by means of the event bush method will be examined. For this, first there will be considered a trivial task from inorganic chemistry, and then, it will be transformed into a hypothetic experimental/technological application, which also will be modeled by event bush.

2 An Example of Formalization of Simple Chemical Reaction

For the beginning, one of the simplest and best-known chemical reactions was considered, that of acid and alkali with formation of salt and water – e.g., $HCl+NaOH=NaCL+H_2O$; $H_2SO_4+CaO=CaSO_4+H_2O$.

On the one hand, the case looks obvious for application of the event bush method. For this, we shall conceptualize this equation as a possible scenario in some environment of directed alternative changes, in which we define the "key players" (primary internal, or ia events) as primary, non-unique inputs, and external "actors" (primary external, or ib events) that may put some constraints on the behavior of "key players" [8]. This "distribution of roles" looks straightforward in the considered case – one of the participating compounds is "key player", while the other, "external actor".

However, on the other hand, there is a semantic complication in this seemingly trivial case. Both the alkali ad acid enter reaction symmetrically, and there is no ground to prefer one as "key player". Be acid affected by alkali or alkali affected by acid, the result (salt+water) would be the same. Still, this complication gives us a methodologically beautiful opportunity to compose two event bushes, in which the ia and ib events change places. The result is shown in Fig. 1 a,b.

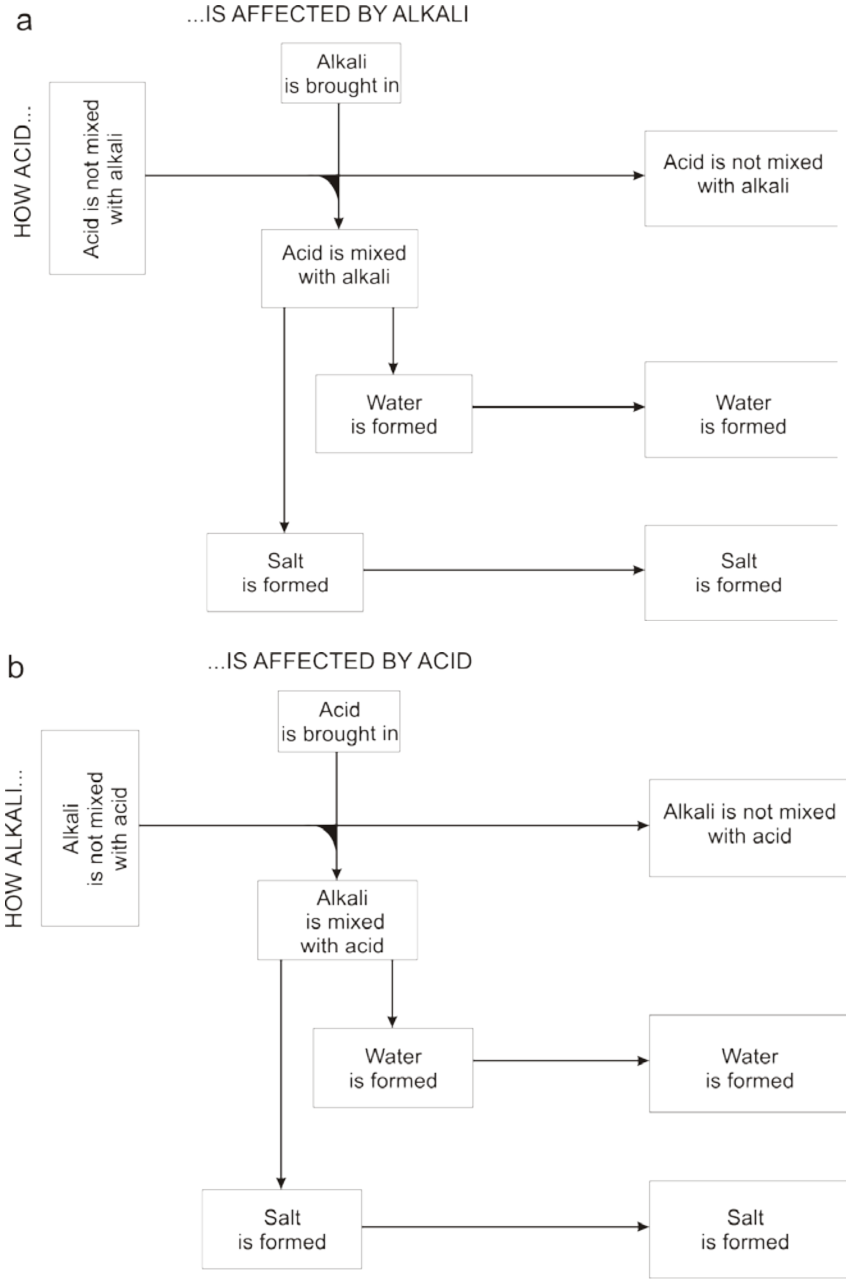

Fig. 1. Two alternative event bushes describing similar reaction of acid and alkali. See comments in the text.

In accordance with the character of the reaction, the two bushes look quite symmetrical. In both of them two incompatible scenarios are seen: one, the mandatory "nothing happens" scenario (if compounds are not brought together – in the event bush semantics, either alkali is not added to acid, or vice versa), and the other scenario that depicts the reaction resulting in simultaneous formation of salt and water. As a methodological experience, one may conclude that dealing with a case that two events happen simultaneously, equally influencing each other and symmetrically determining the future course of events, a couple of event bushes with symmetrical structure has to be expected as shown in Fig. 1 a,b. Because of similarity of consequences, it can be postulated that "Acid is mixed with alkali" is equivalent to "Alkali is mixed with acid". (Though, the meaning of equivalence so far is understood here rather informally; there is not enough ground to appeal to definition of equivalence used in any existing formal system, e.g., in classical logic, because the event bush has not been entirely interpreted in terms of any of such system.)

One may suppose that considering a reaction involving three or more compounds may represent a problem because the event bush semantics implies only two types of primary events, primary internal (ia) and primary external (ib), and this division is related to the binary subject-predicate structure of statements representing events in the event bush [8]. Still, it looks unlikely that three or more agents interact with each other exactly in one time, and if not, there should be one-to-one collisions, and the whole reaction can be represented by successive or parallel *couple interactions*, i.e., be well modeled by event bush (or a pair of bushes).

The above example shows an ability of event bush to cope at least with some basic issues of pure chemistry. Below an applied issue will be considered.

3 Experimental and Technological Application

To address an applied chemical issue, suppose a very simple example of experiment or production – a tank filled with two liquids (fluids) divided by an impermeable screen. The screen is removed; fluids contact each other and mix (Fig. 2).

This simple case represents a purely mechanical process and may be remarkable only by the use of one more, optional connective of the event bush, the conflux (see the bottom of Fig. 2). However, along with the "pure-chemical" case depicted in Fig. 1, this is just an "introduction" to an "applied chemical" case. Suppose that one fluid in a tank is acid and the other, alkali. What happens then is modeled by the event bush in Fig. 3.

To build this bush, "Fluid A" in the bush from Fig. 2 was changed to "Acid", and "Fluid b", to "Alkali". In all the rest, the upper part of the resulting bush repeats the bush in Fig. 2. Hence, the new bush was derived from the previous one by substitution of two subjects. In other words, given this substitution, the bush in Fig. 2 *is the rule* for construction of the upper part of the new bush. However, when replacement reaches the event "A mixture of fluid A and fluid B is formed in the tank", this results in event "A mixture of acid and alkali is formed in the tank" of the new bush. From this point, based on the meaning of the considered events, one may postulate that the

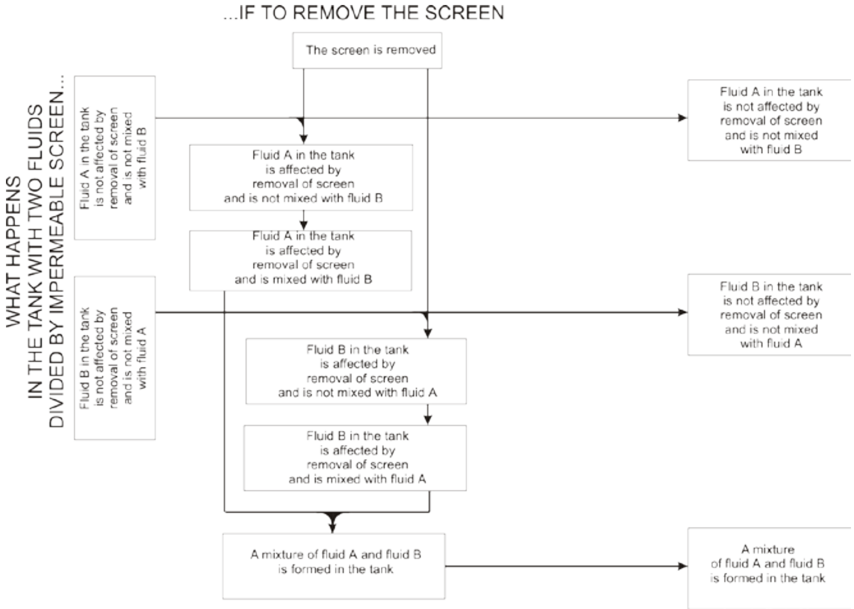

Fig. 2. An event bush describing the behavior of two fluids in a tank (see comments in the text)

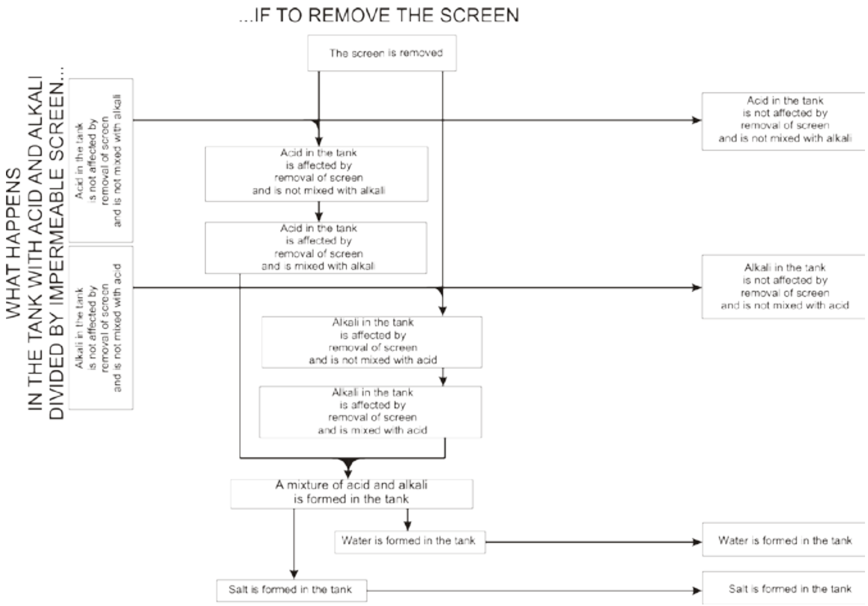

Fig. 3. An event bush describing the behavior of acid and alkali in a tank (see comments in the text)

Fig. 2 bush does not apply as a rule anymore for the newly constructed bush. Instead, it looks reasonable to postulate that the event “A mixture of acid and alkali is formed in the tank” is a kind of (or a particular case of) event “Acid is mixed with alkali” or its equivalent “Alkali is mixed with acid”. Then, the rest of the bush will be composed based on the corresponding part of the Fig. 1/Fig. 2 bushes. Thus, there is no tertiary event that would correspond to “A mixture of fluid A and fluid B is formed in the tank” of Fig. 3 bush, but instead there are secondary statements that are particular cases of “Water is formed” and “Salt is formed” Fig. 1/Fig. 2 bushes – “Water is formed in the tank” and “Salt is formed in the tank”, correspondingly, and the same-formulated tertiary results.

Despite the triviality of the case, it demonstrates an important methodological novelty. Some event bushes serve as the *rules of composition* for another bush.

4 Discussion

The rules of composition of one event bush based on others need to be formalized to become independent of meaning of particular events. This seems to become feasible with complete formalization of event description grammar and algorithmization of building the event bush. Nevertheless, what can be definitely said now is that having a number of event bushes constructed, one can *obtain new knowledge* combining them, binding them with additional axioms and thus constructing new bushes. (Another issue is how well this knowledge would be supported by data.)

One way of building a bush based on another bush is specification of events and substitution of genus by differentia in subjects or predicates of some events, e.g., “Fluid A” to “Acid” or, possibly, “Acid” to “Formic acid” in Figs. 1 a,b. If to continue this approach and descend down to instances, e.g., to “Formic acid sample no. 49276” instead of “Formic acid”, the event bush may be transformed into a data-storing facility. Also, attributing quantitative values to the events of the bush and attributing computational sense to its connectives, one may create a tool for computation of chemical reactions or physical-chemical or technological computation [8].

Theoretical findings made at adjustment of the event bush method to pure-chemical and applied chemical tasks (a couple of equivalent bushes and understanding of event bush as a rule for composition of another bush) emerged at the very beginning of application of this method in chemistry. It looks highly probable that further research in this direction will bring the results that will enrich the theory of event bushes and serve in many other fields to organize existing knowledge and, perhaps yet more importantly, obtain new one.

5 Conclusions

1. A methodological novelty brought by testing of the method of event bush by modeling simple chemical reactions is an opportunity to construct a couple of equivalent event bushes that model similar environment equally well but should be

considered in pair to reflect the observed symmetry of primary internal and primary external events.

2. Putting a primitive experimental/technological task in terms of event bush has revealed an important opportunity to use one bush as a rule of composition of another and therefore obtain new knowledge combining existing event bushes.

3. At present, building new event bushes based on existing ones is performed largely by intuition and for trivial tasks; formalization of this procedure will open wide opportunities for dynamic knowledge engineering in various fields.

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