# Action Based ABox Update: an Example from the Chemical Compound Formulation

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**Abstract.** The Chemical Formulation Problem (Compounding Problem) consists in modifying the chemical formulation of a compound in order to obtain a new compound showing a set of desired performances. This paper presents a computational model for the Compounding Problem based on the interpretation of transformation actions on the compound structures as ABox updates. Possible transformations of the compounds are defined as transitions of a Labelled Transition System (LTS), and the Compounding Problem has been defined as a Heuristic Search Problem. In order to reduce the complexity of the search space the paper presents an approach based on: (i) the representation of the ontological constraints on the compounds' structure in a TBox, and the representation of compound formulations as ABoxes. (ii) The representation of the transitions of a LTS as a set of actions producing updates on ABoxes; (iii) the definition of an algorithm to check ABox consistency with respect to a specific axiom schema in order to prune inconsistent branches of the search space.

## 1 Introduction

The Chemical Compound Formulation Problem (Compounding Problem) consists in modifying the chemical formulation of a *chemical compound* in order to obtain a new compound showing a set of desired performances. Reasoning on the structural and behavioral change dynamics of chemical compounds is a very hard combinatorial problem, even when a small number of chemical elements are taken into account. In fact, although there are a number of mathematical methods for computational chemistry based on quantitative and micro-level physical representations exist, their computational cost grows largely with the complexity of the investigated substances [1]. For this reasons it is challenging to overcome the computational intractability of the quantitative, mathematical, compound representations, exploring a higher-level qualitative approach to the Compounding Problem. This approach is based on the elicitation of the knowledge involved in the practice of experts working in the field. According to a mereological point of view, a compound is a blend of atomic chemical ingredients in various proportions (its "formulation"), where each ingredient is chosen according to its different chemical and physical properties. This perspective on chemical compounds has been supported by repeated observations of expert practices, and can be naturally supported by an ontological representation based on DL; DL formulas provide a tool to specify both the

ontological boundaries of the domain (TBox) and the representations of specific compounds (ABox). Within this perspective, the structural representation of compounds and their components need to be connected with their representation in terms of performances and behavior, on the basis of which a compound is chosen.

The computational model is defined as a product of $n$ possible labelled transition systems (LTSs), each representing the domain entities at a given level of representation, and a set of morphisms between the LTSs. The *states* of each LTS are ABoxes representing compound formulations, while *transitions* are compound transformation actions. *Morphisms* establish relations between the different levels of representation in order to associate, e.g. a set of performance parameters to a structural representation of the chemical compound. Three representational dimensions are particularly relevant for a number of different industrial compounds (e.g. drugs, rubber compounds, and so on): (i) the *structural dimension* - a list of ingredients together with their quantity; (ii) the *behavioral dimension* - a description of the outcomes of artificial lab tests, and (iii) the *teleological dimension* - a description of the outcomes of tests conducted in the final application environment.

An instance of a Compounding Problem consists in acting on a specific LTS in order to obtain a compound fulfilling the requirements specified at other levels of the representation. Given the morphisms between the three levels introduced above, our goal is to produce changes on the structural level in order to meet the requirements specified at the behavioral level and at the teleological level. This problem can be easily interpreted as a Planning Problem within the Heuristic Search paradigm [2]: the structural representation of the given compound is the initial state, transitions represent possible actions and the goal test is defined on the behavioral and teleological representation associated to compounds; however, the great number of actions that is possible to take on every compound drastically boosts the branching factor compromising the feasibility of the algorithmic approach.

The computational effort that is needed to explore this structure can be significantly reduced by pruning the branches producing non admissible states, according to ontological criteria. A compound formulation can be considered *ontologically consistent* if it does not violate domain specific constraints imposed on its mereological composition. Our approach consists therefore in: (i) representing the ontological constraints on the compounds' structure in a TBox and the compounds structure in a ABox; (ii) representing the structural-level LTS as a set of actions producing updates on ABoxes; (iii) formally define the notion of admissible action according to notion of ABox satisfiability; (v) define an algorithm to check ABox satisfiability with respect to a specific axiom schema in order to prune inconsistent branches of the search space.

The present computational model, developed in the context of a project made in collaboration with the Business Unit Truck of Pirelli Tires [3], led to the design of a system for the automatically resolution of chemical formulation problems in the industrial domain of rubber compounds for tires [4]. In this paper we focus on the DL-related aspects of our approach, and in particular on the interpretation of compound transformations as ABox updates, and on the algorithm for checking consistency of the updates; while for further details about the implementation of the search algorithm we refer to [4]. The next section presents the axioms defining the ontological integrity conditions

for a chemical rubber compound formulation at the structural level. Section 3 further describes the heuristic search space based on DL descriptions. Section 2 describes the interpretation of the LTS transitions as ABox updates, and introduces the algorithm for the ABox updates consistency checking. Concluding remarks end the paper.

## 2 TBox and ABox in the compounding knowledge scenario

For a comprehensive description of the TBox we refer to [5, 6]. In the following, we present some core aspects of our ontological representation in the domain of tread rubber compounding. The following formulas are expressed in the $\mathcal{SIQ}$ DL under Unique Name Assumption. Let $\prec$ be a primitive role standing for "is a functional part of"; $\prec$ is a "composed" part-of relation in the sense of [7] (i.e. a part-of relation that is both *integral* and *functional*). In particular, $\prec$ is *not reflexive*, *not symmetric*, and *not transitive*. It is useful to introduce the inverse role "has functional part" ($\succ$) as $\succ \doteq \prec^{-}$. The axioms in the structural-level TBox guarantee that if a model exists, then the model describes the structure of a compound devoted to the production of tire in the industrial field of interest.

$$\begin{aligned}\texttt{TreadCompound} \equiv \texttt{Compound} &\sqcap (= 1 \succ .\texttt{PolymericMatrix}) \\ &\sqcap (= 1 \succ .\texttt{Vulcanization}) \\ &\sqcap (= 1 \succ .\texttt{ProcessAid}) \sqcap (= 1 \succ .\texttt{Antidegradant}) \\ &\sqcap (= 1 \succ .\texttt{ReinforcingFiller}) \\ &\sqcap ((\geq 0 \succ .\texttt{Softener}) \sqcap (\leq 1 \succ .\texttt{Softener}))\end{aligned}$$

It is standard that a rubber compound devoted to tread tire production is made of at least five essential systems [8]: (1) the `PolymericMatrix`; (2) the `Vulcanization` system; (3) the `ProcessAid`; (4) the `Antidegradant`; (5) the `ReinforcingFiller`[1].

$$\texttt{PolymericMatrix} \equiv \texttt{System} \sqcap (= 100 \succ .(\texttt{NaturalRubber} \sqcup \texttt{ButadieneRubber}))$$

$$\begin{aligned}\texttt{Vulcanization} \equiv \texttt{System} &\sqcap ((\geq 1 \succ .\texttt{Sulphur}) \sqcap (\leq n \succ .\texttt{Sulphur})) \\ &\sqcap ((\geq 1 \succ .(\texttt{GroundElement} \sqcap \textit{hasFamilyName}.\texttt{Accellerant})) \\ &\sqcap (\leq m \succ .(\texttt{GroundElement} \sqcap \textit{hasFamilyName}.\texttt{Accellerant}))) \\ &\sqcap ((\geq 2 \succ .\texttt{ZincOxide}) \sqcap (\leq p \succ .\texttt{ZincOxide})) \\ &\sqcap ((\geq 2 \succ .\texttt{StearicAcid}) \sqcap (\leq p \succ .\texttt{StearicAcid}))\end{aligned}$$

The `PolymericMatrix` is a system having 100 parts as a blend of natural and synthetic rubber or, alternatively, 100 parts of natural or synthetic rubber alone. Parts of the `Vulcanization` system are the Sulphur, the Oxide Zinc and the Stearic Acid in a predefined *quantity*. A vulcanization system contains a given quantity of a element in the family of the `Accellerant`.

$$\begin{aligned}\texttt{ButadieneRubber} \equiv &\texttt{GroundElement} \sqcap (= 1 \prec .\texttt{PolymericMatrix}) \\ &\sqcap \textit{hasStructure}.(\texttt{Cis} \sqcup \texttt{Trans}) \sqcap \textit{hasFamilyName}.\texttt{Polymer} \\ &\sqcap \textit{hasMolecularWeight}.\texttt{NumericalValue}\end{aligned}$$

[1] Since the syntax of $\mathcal{SIQ}$ does not admit individuals in the TBox; the $m, n, p$ symbols of the following formulas are interpreted as placeholders for appropriate integers according to specific compounding domains.

`ButadieneRubber` is a ground element and an exclusive part of the polymeric matrix system. Butadiene rubber, that is member of the family of Polymers, is characterized by having a specific configuration (*Cis* or a *Trans*), and a *molecular weight*.

Descriptions of specific compounds are represented by means of ABox assertions. Concept atoms in the ABoxes are all *defined names* of the TBox. Structural-level representation of compounds is completely represented by the mereological role assertions in the ABox, i.e. the assertions in the ABox concerning the $\succ$ and $\prec$ roles between the domain individuals. Moreover, the ABox specifies the quantity of all the ingredients available for a given compounding process[2].

## 3 The heuristic search space

Within a Heuristic Search paradigm, the compound formulations (ABoxes) represent the *states*, while the *transitions* are interpreted as admissible transformation actions of these formulations. The state space is defined as a product of LTSs.

**Definition 1 (Labelled Transition System).** *A labelled transition system $\Gamma$ is a structure $\langle S, i, \Lambda, \rightarrow \rangle$, where (i) $S$ is a set of states, with initial state $i$, (ii) $\Lambda$ is a set of labels, and (iii) $\rightarrow \subseteq S \times \Lambda \times S$ is a ternary relation of labeled transitions. If $p, q \in S$ and $\alpha \in \Lambda$, then $(p, \alpha, q) \in \rightarrow$.*

If the states of the LTSs are represented by sets of ABox assertions, the transitions between these states (*quantity increase* and *reduction*, and *substitution* actions) that define compound transformation actions can be viewed as ABox update operations. Let $\theta$ be a transformation action whose effect is to *increase* the quantity of a given ingredient[3].

**Definition 2 (Increase Transformation Action).** *Given a LTS $S = \langle S, i, \Lambda, \rightarrow \rangle$, and a state $s \in S$, let $\mathcal{A}_s$ be the ABox associated to $s$. Let $\mathcal{A}_s$ contain a set of assertions of the form $\succ (\mathtt{sys}^i, \mathtt{ing}^j)$, where $\mathtt{sys}^i$ and $\mathtt{ing}^j$ are individuals respectively of the classes $i$ and $j$, with $i \sqsubseteq \mathtt{System}$ and $j \sqsubseteq \mathtt{GroundElement}$, and $j$ is a* base symbol *in the definition of the concept $i$. A transition $\theta_{i,j} \in \{\rightarrow\}$ is an* increase transformation action *for a given ingredient iff its application $\theta_{i,j}\mathcal{A}_s$ returns an updated ABox $\mathcal{A}_{s'} = \mathcal{A}_s \cup \succ (\mathtt{sys}^i, \mathtt{ing'}^j)$, where $\mathtt{ing}^j \neq \mathtt{ing'}^j$.*

Once the levels of representation have been chosen and the respective LTSs have been defined, the problem solving knowledge can be formally represented by means of two *morphisms*, mapping states to states and transitions to transitions of the different systems. Morphisms codify expert causal knowledge linking structural transformations on the compound to behavioral and teleological ones; they forecast the behavioral and teleological effects of a structural transformation (e.g. a quantity increase of Silica worsens the abrasive and resistance behaviors).

[2] Ingredients can be intuitively considered as chemical "bricks" with a proper name, where a brick is a fixed quantity of a given chemical substance.

[3] The transformation actions of quantity reduction and substitution of chemicals have been defined as ABox updates in a similar way.

A morphism $\Gamma \rightarrow \Gamma'$ between transition systems can be introduced as a pair $(\sigma, \lambda)$, where $\sigma$ is a function on states, preserving initial states, and $\lambda$ is a partial function $\lambda$ on the transition labels. The morphism maps a transition of $\Gamma$ to a transition of $\Gamma'$: if $(p, \alpha, q)$ is a transition in $\Gamma$ then $(\sigma(p), \lambda(\alpha), \sigma(q))$ is a transition in $\Gamma'$ provided that $\lambda(\alpha)$ is defined. Provided the suitable constraints on the transitions by means the introduced morphisms, the definition of the product of *n* labelled transition systems is as usual [9]. Suppose that the states $s = \langle c, l, h\rangle$ and $s' = \langle c', l', h'\rangle$ are elements of a product of three LTSs (where, $c$ stands for *c*ompound structure, $l$ for *l*ow-level behaviors and $h$ for *h*igh-level performances). Let $\tau = (\sigma, \lambda), \tau' = (\sigma', \lambda')$ are compounding morphisms such that $\sigma(c) = l$ and $\sigma'(l) = h$; these morphisms represent that a compound structure $c$ is associated to specific compound behaviors $l$ and performances $h$. Morphisms are necessarily given as inputs of the compounding problem. Then, the application of the transition $\lambda_i$ to $s$ (creating a new state $s'$) is generated by the application of a structural transformation action $\lambda_C \colon C \rightarrow C$ (mapping compound structures to compound structures) such that $\lambda_C(c) = c'$. But the application of $\lambda_C$ leads to a partial state $\langle c', l, h\rangle$ that is not well defined. In order to obtain a well defined state $s'$, representing a feasible solution of the compounding problem, morphisms are exploited applying the transformations associated to $\lambda_C$ to obtain the other involved dimensions ($l'$ and $h'$). Formally, the notion of "well defined transition" is introduced as follows:

**Definition 3 (Well Defined Transition).** *Given the compounding morphisms $\tau, \tau'$, two states $s = \langle c, l, h\rangle$ and $s' = \langle c', l', h'\rangle$ in the product, and a structural transformation action $\lambda_C$. The triple $(s, \lambda_i, s')$ is a well defined transition, written $(s, \lambda_i, s') \in \rightarrow$,* iff *$\lambda_C(c) = c'$, $\tau(c') = l'$ and $\tau'(l') = h'$. The state components $l'$ and $h'$ are obtained by mapping the transition $\lambda_C$ to appropriate transitions $\lambda_L$ and $\lambda_H$. In particular, if $\tau(c) = l$, and $\lambda_C(c) = c'$, then there exists a state $l'$ such that $\lambda_L(l) = l'$, for some $\lambda_L = \tau(\lambda_C)$, with $\tau(c') = l'$.*

## 4 The compounding actions as ABox updates

Let us start with an example of update concerning the reinforcing filler system. Let $\mathcal{T}$ be a TBox containing only the following terminological axiom (stating that a reinforcing filler system must contain *at least* one and *at most* two parts of carbon black):

$$\texttt{ReinforcingFiller} \sqsubseteq \texttt{System} \sqcap ((\geq 1 \succ .\texttt{CarbonBlack}) \sqcap (\leq 2 \succ .\texttt{CarbonBlack}))$$

Let $s$ be a state of the LTS associated to $\mathcal{T}$. The following set of assertions $\mathcal{A}$ is a fragment (that takes into account the composition of the reinforcing filler system) of the complete description of a compound formulation: $\{\texttt{ReinforcingFiller(rf0a01)}$, $\texttt{CarbonBlack(cb0a01)}, \texttt{CarbonBlack(cb0a02)}, \texttt{CarbonBlack(cb0a03)}$, $\succ (\texttt{rf0a01}, \texttt{cb0a01}), \succ (\texttt{rf0a01}, \texttt{cb0a02})\}$.

Let $\theta$ be a transformation action whose effect is to *increase* the quantity of the carbon black contained in the reinforcing filler system. Considered as an ABox update, the application of $\theta$ to $\mathcal{A}$, written $\theta\mathcal{A}$, returns the ABox $\mathcal{A}'$ where
$\mathcal{A}' = \mathcal{A} \cup \{\succ (rf0a01, cb0a03)\}$. Let $\mathcal{M}$ be an interpretation that satisfies $\mathcal{A}$ w.r.t.

$\mathcal{T}$ ($\mathcal{M}$ is said to be a model of $\mathcal{A}$ w.r.t. $\mathcal{T}$). In order to compute the consistency of the updated ABox $\mathcal{A}'$, the existence of a model $\mathcal{M}'$ of $\mathcal{A}'$ w.r.t. to $\mathcal{T}$ has to be checked. Given the semantics of the cardinality constraint in $\mathcal{T}$, the example shows that a similar model does not exists: the insertion of $\succ\ (rf0a01, cb0a03)$ produces the violation of the *at most* cardinality constraint in $\mathcal{T}$.

The above example can be generalized in order to define an algorithmic procedure that check consistency of an ABox update w.r.t. to an invariant TBox for compounding. The algorithm is aimed at checking consistency of updates that consist in insertion and deletion of mereological individual assertions (i.e. the assertions involving $\prec$ and $\succ$ roles). This assumption covers all the relevant cases of ABox updates of our model for chemical compound formulation. In order to achieve the generalization, we define the notions of *compounding TBox* and of *compounding ABox*.

A TBox $\mathcal{T}$ is said to be a *compounding TBox* iff it contains a set of axioms with the following syntactic form:

$$
\begin{aligned}
\mathtt{C}_{COMP} \equiv\ & \mathtt{Compound} \sqcap\ (= 1 \succ .\mathtt{C}_{SYS_1}) \\
& \dots \\
& \sqcap\ (= 1 \succ .\mathtt{C}_{SYS_n}) \\
& \sqcap\ ((\geq 0 \succ .\mathtt{C}_{SYS_{n+1}}) \sqcap (\leq 1 \succ .\mathtt{C}_{SYS_{n+1}})) \\
& \dots \\
& \sqcap\ ((\geq 0 \succ .\mathtt{C}_{SYS_{n+m}}) \sqcap (\leq 1 \succ .\mathtt{C}_{SYS_{n+m}})) \\
\mathtt{C}_{SYS} \equiv\ & \mathtt{System} \sqcap ((\geq min_1 \succ .\mathtt{C}_{ING_1}) \sqcap (\leq max_1 \succ .\mathtt{C}_{ING_1})) \\
& \dots \\
& ((\geq min_n \succ .\mathtt{C}_{ING_n}) \sqcap (\leq max_n \succ .\mathtt{C}_{ING_n})) \\
\mathtt{C}_{ING} \equiv\ & \mathtt{GroundElement} \sqcap\ (= 1 \prec .\mathtt{C}_{SYS_j}) \\
& \sqcap\ (f_1.\mathtt{C}_1) \sqcap \dots \sqcap\ (f_s.\mathtt{C}_s)
\end{aligned}
$$

In the above formula schema, $C_{COMP}, C_{SYS}, C_{ING_1}, \dots, C_{ING_n}$ are concept names for compounds, systems and ingredients respectively, and $min_j, max_j$ are variable for integers with $min_j \leq max_j$ for $1 \leq j \leq n$. The scheme can be instantiated in a number of different cardinality constraint axioms, fixing the quantity $min_j$, and $max_j$ of a specific set of ingredient $C_{ING_1}, \dots, C_{ING_n}$ a given functional system $C_{SYS_i}$ must contain.

For all the systems $\mathtt{C}_{SYS_i}$ that are relevant for a given compounding problem, and all the available chemicals $\mathtt{C}_{ING_i}$, let $\mathcal{A}$ be an ABox containing assertions of the following forms:

$$
\begin{aligned}
& \mathtt{C}_{COMP}(\mathtt{compound}), \mathtt{C}_{SYS_i}(\mathtt{sys}),\ \mathtt{C}_{ING_1}(\mathtt{ing}_{1_1}), \dots, \mathtt{C}_{ING_1}(\mathtt{ing}_{1_j}) \\
& \qquad\qquad \dots \\
& \qquad\qquad \mathtt{C}_{ING_n}(\mathtt{ing}_{n_1}), \dots, \mathtt{C}_{ING_n}(\mathtt{ing}_{n_{j'}})
\end{aligned}
$$

where `sys` and `ing` are variable names for individuals. The assertions in $\mathcal{A}$ define *what are* the available systems and chemicals that could be parts of the compound. Given a specific compounding domain, we assume that all the ABoxes involved in the process contain an identical set of such assertions. During the compounding process, the system can take a quantity increase for an ingredient in the compound, or a substitution of an

ingredient with a different one of the same family, but it cannot generate new chemicals from scratch. Therefore, the ABoxes differ only with respect to the compound formulations they describe. An ABox $\mathcal{A}$ is said to be a *compounding ABox* iff it contains a suitable set of axioms with the above syntactic form, plus a set of axioms like: $\succ (\mathtt{compound}, \mathtt{sys})$, and $\succ (\mathtt{sys}, \mathtt{ing})$ for all systems and ingredients that participate to a given compound.

Given a compounding TBox $\mathcal{T}$ and a compounding ABox $\mathcal{A}$, and an interpretation $\mathcal{I} = \langle \Delta, \cdot^{\mathcal{I}} \rangle$ that is a model of $\mathcal{A}$ w.r.t. $\mathcal{T}$, the algorithm computes if the application of an increase transformation action $\theta$ generates an updated ABox $\mathcal{A}'$ that is consistent w.r.t. $\mathcal{T}$[4].

**INPUT**: (i) a TBox $\mathcal{T}$, an ABox $\mathcal{A}$, an interpretation $\mathcal{I}$ such that $\mathcal{I} \models \mathcal{A}$ and $\mathcal{I} \models \mathcal{T}$; (ii) an Increase Transformation Action $\theta$.

**OUTPUT**: a satisfiable knowledge base $\mathcal{K} = \langle \mathcal{T}, \mathcal{A}' \rangle$, where $A' = \theta A$, or **ERROR**.

1. **If** $\theta$ is an *Increase Transformation Action* and $\theta A = A'$, $A' = A \cup \{\succ (\mathtt{sys}, \mathtt{ing}_{j_n})\}$, for some system $\mathtt{sys}$ and ingredient $\mathtt{ing}_{j_n}$ of the family $j$, with $\{C_{SYS}(sys), ING_j(ing_j)\} \subset A$ **then**
2. **for each** $m$, $\alpha := \succ (\mathtt{sys}, \mathtt{ing}_{j_m})$, with $\alpha \subset A$, $n \neq m$ and $\beta := \mathtt{C}_{SYS} \sqsubseteq \mathtt{System} \sqcap ((\geq min_j \succ .\mathtt{C}_{ING_j}) \sqcap (\leq max_j \succ .\mathtt{C}_{ING_j}))$, with $\beta \subset \mathcal{T}$
3. **if** $countOccurrence(\alpha, A) = a$ and $a \geq min_j$ and $a \leq max_j$ **then** $\mathcal{K} = \langle \mathcal{T}, \mathcal{A}' \rangle$ is satisfiable **else ERROR**.

## 5 Concluding remarks and future work

The number of results about reasoning techniques and algorithms for ontology updating is still poor, and the update of ontological KBs remains a promising and challenging field of research [10–12]. Our work exploited the notion of model of an ABox, once the intensional level of the knowledge base has been specified. This means that, given an ABox, the consistency check is always performed with respect to a TBox that we assumed to be invariant. Even if the result of [11] for $\mathcal{ALC}$, is naturally inherited by $\mathcal{SIQ}$, we tried to define an algorithmic procedure to perform reasoning, e.g. the consistency check for updated ABoxes w.r.t. a TBox, outside the logic itself.

In the context of the P-Truck Project, a specific experimental campaign has been devised and encouraging results have been obtained from the application of several search algorithms (namely A*, IDA*, Iterative Expansion and Branch and Bound) to a state space defined and implemented according to the present knowledge model. The algorithm for the consistency check of the ABox updates, has produced a significantly reduction of the expansion rate of the space, and an automatic system has been developed and tested on a significant number of prototypical chemical compounding problems (e.g. the problem of increasing the Tread Tear Resistance, the problem of increasing the Rolling Resistance, together with a reduction of the Wet Handling, and the maintenance of all the remaining performances) [13]. Future developments of our work are aimed at a complete generalization of the introduced computational model, in order to define an ABox updating algorithm for arbitrary DL-based mereological KBs.

[4] We proceeded in a similarly way for reduction and substitution transformation actions.

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