Knowledge Graphs for Design of Experiments (DoE) for coatings research

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Abstract

Coating development requires navigating a large compositional and process space in which ingredient interactions are nonlinear, individual experiments are costly, and hard-won formulation knowledge is rarely reused across campaigns. Design of Experiments (DoE) offers statistical efficiency by reducing the number of experiments and efficiently identifying significant factors and their interactions. Yet, adoption in the paint and coating industry remains low, constrained by expertise barriers and the absence of machine-readable infrastructure for encoding domain knowledge and experiment planning logic. This paper presents a vision for a knowledge-graph–driven framework for intelligent, staged experiment planning in coatings research. We present a formal model of the coating design space and discuss how ontology-based knowledge representation can support DoE selection. This paper presents only the fragments of coatings domain model required to characterize experiment design problems for coatings research and map them to a DoE method selection ontology that captures design procedures, campaign-stage logic, and transition criteria. Semantic Web Rule Language (SWRL) can be used to define rules that automatically infer the appropriate design strategy, i.e., deciding which stages and methods are needed, from a structured problem description. Annotating each recommendation with a traceable inference chain provides explainability to the system. A potential four-component architecture is presented for a knowledge-based DoE assistant for experiment designers. A user interface serializes problem inputs and experimental results as RDF triples in a Web Ontology Language (OWL) ontology, thereby constructing a knowledge graph. A reasoning engine executes ontology and rule-based inference to recommend suitable experimental methods. An orchestration agent retrieves these recommendations using SPARQL and generates an experiment plan. Following each experimental cycle, a post-experiment analysis component updates the knowledge graph and triggers transitions to subsequent stages. Finally, we discuss the advantages of a knowledge-based DoE assistant.

Keywords

knowledge graphs, design of experiments, information modelling, coatings

1. Introduction

Coatings are thin functional layers applied to solid surfaces to protect, decorate, or confer specific properties. They appear across automotive, aerospace, construction, and healthcare: corrosion-protection primers extend the service life of structural steel by decades; UV-stable clear coats preserve automotive bodywork; anti-fouling coatings protect underwater surfaces of ships and boats. With a global market exceeding $170 billion annually [1], coatings are a critical enabling technology. A coating is not a single compound but an engineered mixture: the **binder** (polymer backbone) provides structural integrity, e.g., epoxy resins in primers, acrylics in topcoats; some binders require **crosslinkers**, which react with the resin to form a cured film network; **pigments** deliver color or active protection (zinc phosphate inhibits corrosion on steel); **solvents** control application viscosity and evaporate on drying and different types of **additives** provide different properties to a coating [2]. The final performance measured in terms of adhesion, gloss, corrosion resistance, pot life, film hardness, etc., depends on all the identities and proportions of the ingredients together with the preparation, application, and curing conditions [1].

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Developing a coating formulation requires searching a vast combinatorial design space constrained by formulation rules (e.g., weight fractions of all components in a mixture should sum to one), material compatibility, and a limited experimental budget. Ingredient interactions are strongly nonlinear: raising pigment loading simultaneously affects gloss, viscosity, and film integrity; adjusting crosslinker concentration couples hardness to pot life. With five or more variables, exhaustive testing is infeasible, and the traditional One-Factor-At-a-Time (OFAT) approach misses interactions and wastes budget [1, 3]. Because the cost of each trial can be high, budget waste can limit the scope of an experimental study.

Design of Experiments (DoE) addresses this by selecting a statistically powerful and minimal set of test conditions. Different DoE methods were developed to be used for different scenarios and objectives: Screening designs identify dominant variables; response surface methods build quantitative predictive models; mixture designs accommodate the constraint that ingredient proportions must sum to unity [1, 3, 4, 5].

DoE has been successfully applied to optimize the performance of fire-retardant coatings [6], characterize corrosion-protection systems [7], and accelerate the development of radiation-curable coatings [8]. As per a 2019 survey, only 15–20% of manufacturing engineers use DoE routinely [9, 10], as statistical expertise is scarce in chemistry curricula, OFAT culture persists, and there is no regulatory mandate comparable to that for pharmaceuticals [9, 11]. Hard-won knowledge consequently stays locked in individual experts and is rarely reused [12].

While DoE methods are well established, the knowledge required to select and configure them remains largely implicit in literature and expert experience. Information about formulation constraints, material interactions, substrate characteristics, and prior experimental outcomes is rarely represented in a form that computational systems can reason over [13, 12]. We envision that future experiment assistants should integrate formal domain knowledge with statistical DoE methods to recommend appropriate designs, incorporate prior knowledge, enforce formulation constraints, and explain their recommendations. Semantic Web technologies such as OWL ontologies, RDF knowledge graphs, and SPARQL provide a suitable foundation for representing and reasoning over this knowledge [14, 15, 12].

Contributions: This paper presents a vision for a knowledge-based DoE assistant for coating design. Specifically, we present: (i) a formal conceptual model of the coating design space and its mapping to a formal DoE problem representation; (ii) ontology-based models and mappings that connect coating design concepts with DoE concepts to enable knowledge-driven experiment planning; (iii) SWRL based reasoning for automatically recommending suitable experimental strategies from structured problem descriptions; (iv) a knowledge graph driven, human-in-loop architecture for an explainable DoE assistant that supports experiment planning, analysis, and iterative decision making; and (v) a research agenda for integrating coating domain knowledge as computable constraints into adaptive DoE methods. Section 2 surveys existing DoE approaches in coatings, Section 3 provides formal modal and ontology mapping, and Section 4 presents a potential system architecture.

2. Current experimental design landscape in coatings

Experimental design campaigns in coatings typically begin with an objective, such as understanding system behaviour or optimizing a formulation. Based on the objective and problem characteristics, the experimenter selects a suitable DoE method to design experiments. When the effects of many factors are unknown, a screening stage may first be used to eliminate insignificant variables before modelling or optimization. Although modelling and optimization often employ similar methods, the former aims to characterize the response across the design space, whereas the latter exploits prior knowledge or predictive models to search for improved solutions [5, 16]. In practice, experimenters usually select a familiar DoE method rather than explicitly reasoning about campaign stages and transitions [6]. Method selection and configuration require expertise in statistics, DoE methodology, and coating formulation. For example, Plackett–Burman designs estimate only main effects and therefore cannot identify interactions, despite interaction effects being common in coating formulations [17, 18]. Likewise, configuring fractional factorial designs requires choosing generator functions that determine the aliasing

structure and therefore which effects can be estimated independently [5]. Additional considerations, including categorical versus continuous factors, formulation constraints, and experiment budget, further complicate experiment planning.

DoE has been successfully applied to designing and optimization of different types of coatings like fire-retardant coatings, corrosion-resistant coatings, zinc-rich coatings, etc [6, 7, 16]. More recently, adaptive DoE methods have combined surrogate models with acquisition functions to guide expensive experiments, while self-driving laboratories automate synthesis, characterization, and experiment execution in closed-loop systems [19, 20]. However, these approaches primarily optimize experiment execution rather than reasoning about campaign strategy, stage transitions, or DoE method selection. Campaign-guidance systems proposed for specific coating systems remain application-specific [13, 20], while knowledge-based DoE recommendation systems developed in other engineering domains have not yet been extended to coatings [21, 22].

These limitations arise because experiment planning is inherently knowledge-intensive, requiring three complementary forms of reasoning. Constraint reasoning is needed to ensure that proposed experiments satisfy physical chemistry, manufacturing knowledge, and regulatory requirements, such as stoichiometric relationships, Volatile Organic Compound (VOC) limits, incompatible material combinations, and formulation heuristics [15, 13, 16]. Existing adaptive systems typically enforce such constraints only as post-processing filters rather than explicit knowledge used during planning. Campaign reasoning is required because experimental campaigns consist of multiple stages whose progression depends on accumulated knowledge, problem characteristics, and previous results. Decisions such as whether additional screening is required, when response modelling is sufficiently accurate, or which optimization strategy should be adopted remain largely dependent on expert judgement [12, 16]. Finally, explainable recommendations are essential for industrial adoption [23]. Unlike purely data-driven approaches, ontology-based reasoning can provide traceable inference chains linking every recommendation to the domain knowledge and logical rules that produced it [22].

Figure 1 contrasts conventional experimental workflows with the proposed knowledge-guided approach. In current practice, experimenters are responsible for selecting suitable DoE methods, interpreting results, determining stage transitions, and planning subsequent experiments. These decisions depend heavily on individual expertise and may lead to inefficient experimentation or incorrect conclusions when inappropriate methods are applied [18]. Instead, we propose representing both coating-domain knowledge and DoE knowledge in a machine-interpretable ontology that supports logical reasoning over constraints, campaign progression, and method selection, thereby providing explainable recommendations throughout the experimental campaign.

3. Formalizing coating design and experiment planning

As no unified ontology for the coatings domain currently exists, we first formalize the coating design problem to identify the concepts required for ontology-based experiment planning. These concepts form the basis of the proposed DoE method selection ontology shown in Fig. 2.

3.1. Formal problem definition

A coating experiment consists of preparing a formulation by combining raw materials through a sequence of manufacturing processes and measuring the resulting coating properties. Let I denote the set of candidate ingredients (e.g., binders, pigments, solvents, and additives), and let $w : I \to [0, 1]$ assign the weight fraction of each ingredient, subject to $\sum_{i \in I} w(i) = 1$, representing the mixture constraint central to coating formulations [12, 24]. Let P denote the set of manufacturing processes with configurable parameters, and let v assign values to those parameters. Assuming standardized preparation procedures, a coating sample is specified by $d = (I, w, P, v)$, and the set of all valid samples defines the coating design space D.

Let M denote the set of measurable response metrics. Each response is an unknown function $f_m : D \to \mathbb{R}$, whose evaluation requires a physical experiment. A design objective therefore consists of

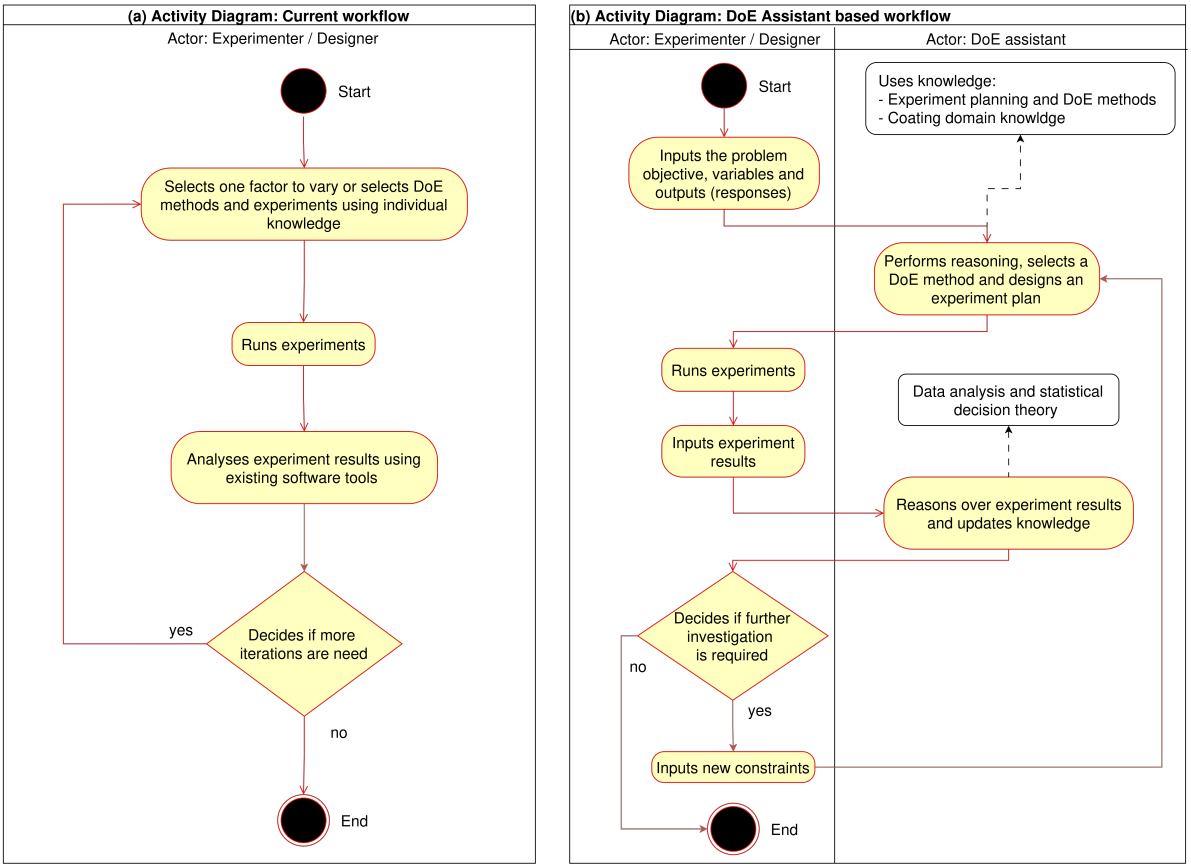


Figure 1: (a) shows the existing workflow, in which design decisions and inferences are based on the designer's knowledge and expertise. (b) shows the proposed workflow with the DoE assistant. Reasoning requiring statistical and domain knowledge is handled by the assistant, while the user specifies the design constraints and directs the investigation. The uncolored boxes indicate the knowledge required at each stage of the reasoning process.

optimizing one or more responses, e.g., $G = \{\text{Maximize(adhesion)}, \text{Minimize(cost)}\}$. Only a subset of variables is varied during experimentation. Let $I_e \subseteq I$ and $P_e \subseteq P$ denote the selected ingredients and process parameters. The active design variables $F = I_e \cup P_e$ form the experimental factors explored by the DoE campaign.

3.2. Ontology-based experiment planning

The formal model maps naturally to an OWL ontology (see Fig. 2). The core concepts are **Experiment Design Problem**, **Factor**, **Response**, and **Objective**. Factors represent independent variables, responses represent measurable performance metrics, and objectives describe the purpose of the campaign (e.g., modelling or optimization). An **Experiment Design Problem** captures the problem characteristics and prior knowledge required for automated DoE method selection.

SWRL rules [25] operate on problem instances to infer required campaign stages and candidate DoE methods. An example rule is shown below.

```
'Experiment Design Problem'(?p) ^ hasObjective(?p, Modelling) ^
varyingFactorCount(?p, ?d) ^ swrlb:greaterThan(?d,5) ^ hasExperimentBudget(?p, ?b)
^ swrlb:lessThan(?b, 32) -> requiresStage(?p, 'Screening Stage') ^
suggestedMethod(?p, 'Plackett--Burman Design') ^ suggestedMethod(?p,
'Fractional Factorial Design')
```

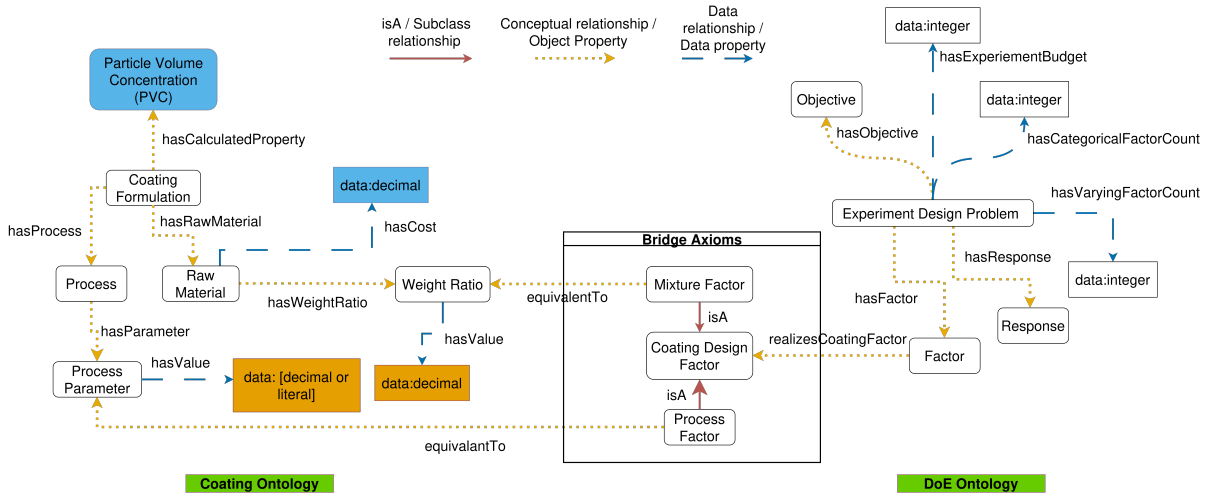


Figure 2: The figure illustrates the DoE ontology and the Coating domain ontology connected using bridge axioms. Red arrows denote *isA* (subclass) relationships, while yellow and blue arrows represent object and datatype properties, respectively. Orange boxes indicate knowledge already present in the DoE knowledge graph (Factor values), whereas blue boxes represent additional domain knowledge made accessible through the bridge axioms. Such knowledge can be cost of ingredients used or some meta-properties of formulation connected to factors or responses. This semantic linkage enables the DoE assistant to reason over coating-domain information without merging the two ontologies.

Under a limited experimental budget, this rule infers that problems with more than five varying factors require a screening stage and recommends Plackett–Burman and Fractional Factorial designs as candidate methods [9, 5]. Because recommendations are derived from explicit logical rules, the reasoning process remains transparent and explainable.

The proposed ontology is designed to integrate with a future coatings ontology through bridge axioms rather than merging the ontologies [26, 27]. This mapping links generic DoE concepts to coating-domain entities, enabling reasoning over formulation constraints, material properties, manufacturing information, and performance metrics.

During execution, the user's problem is represented as an **Experiment Design Problem** linked to the coatings ontology. A SPARQL CONSTRUCT query populates the required properties, SWRL rules infer campaign stages and candidate DoE methods, and the ontology is updated after each experimental stage with newly acquired knowledge, enabling reasoning over subsequent stages of the experimental campaign.

4. Potential architecture and workflow

Knowledge-graph–driven orchestration patterns have been demonstrated in self-driving laboratory platforms [28] and digital lab management tools [29]. The presented design adapts them for staged, human-in-the-loop DoE. The main components of our 4-component architecture are (see Fig. 3):

User Interface collects campaign information, including factor names, types, ranges, responses, objectives, and known constraints. These inputs are serialized as RDF triples conforming to the DoE and coatings ontologies and uploaded to the knowledge graph using SPARQL Update or direct Python API calls.

Reasoning Engine performs OWL DL and SWRL reasoning over the knowledge graph, classifying factors, responses, and **Experiment Design Problem** individuals. When a new problem is added, SWRL rules infer `requiredStage` and `suggestedMethod` triples. After experimental results are entered through the user interface, the Reasoning Engine updates the response values. The orchestration agent runs the appropriate data analysis workflow for the selected design and adds the results in the KG.

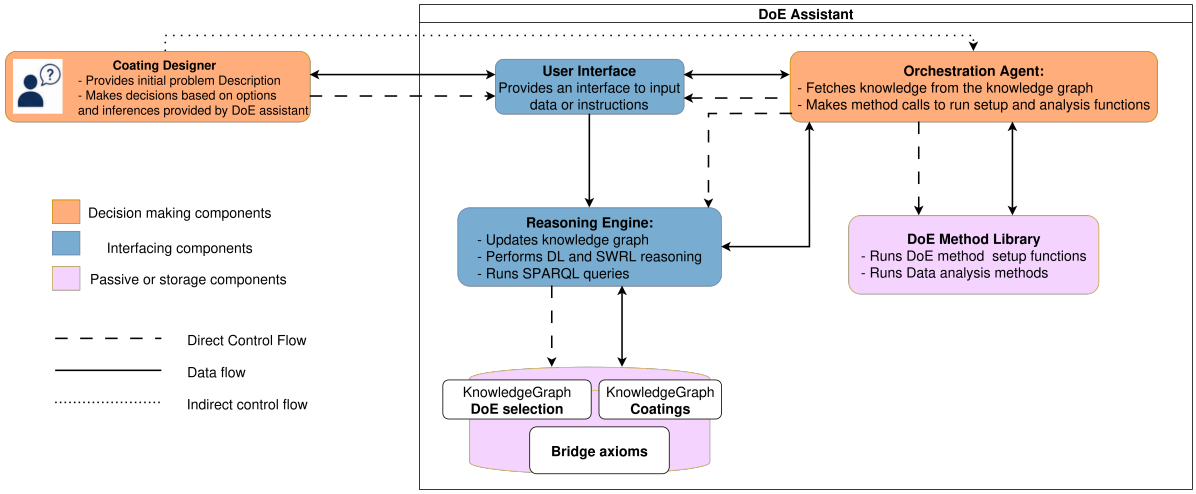


Figure 3: DoE Assistant Architecture: Coating Designer interacts with the Orchestration Agent through a user interface. Responsibility for experimental design decisions is shared between the **Coating Designer** and the **Orchestration Agent**. The designer makes high-level decisions, such as selecting campaign objectives or choosing among recommended experimental strategies, while the Orchestration Agent makes knowledge-driven decisions based on information stored in the knowledge graph. The **Reasoning Engine** provides an interface between the linked knowledge graph and the Orchestration Agent, performing OWL and SWRL reasoning to infer recommended DoE stages and methods. The **DoE Method Library** contains functions for generating experimental designs, performing statistical analysis, and updating the knowledge graph with experimental results. Throughout the campaign, the Coating Designer guides the experimental direction by selecting from the alternatives proposed by the agent. In contrast, the agent continuously reasons over both the user's decisions and the knowledge graph to recommend subsequent stages and experimental designs.

These results can then be used by reasoning engine to derive facts such as `significantFactorCount` and `interactsWith` relationships before performing reasoning to suggest designs for the next stage.

Orchestration Agent retrieves the inferred `suggestedMethod`, corresponding design family, and configuration parameters (e.g., number of runs, factor ranges, and centre-point count) from the knowledge graph using SPARQL queries. The best method is selected using budget and problem constraints and user preferences. The agent then invokes the corresponding Python function in the DoE library, generates the experimental design, updates the knowledge graph, and returns the design matrix to the user interface. Following each round of experimentation, the agent retrieves the updated `requiredStage` and `suggestedMethod` values to guide the next stage of the campaign. The Orchestration Agent can be implemented as a rule-based Python program and extended with large language model (LLM).

DoE Method Library consists of Python functions that generate experimental designs, perform statistical analysis, construct surrogate models, and execute adaptive DoE methods. The Orchestration Agent invokes these functions to configure and execute the experimental campaign. It also maintains a trace of the campaign by recording newly inferred axioms and user decisions, providing a complete trace of the reasoning process.

4.1. Advantages of DoE tool

The use of knowledge graphs for DoE method selection and semantic integration of experimental requirements and results makes the proposed system both **extensible** and **flexible**. New domain knowledge, DoE methods, and reasoning rules can be incorporated by extending the ontologies without modifying the system architecture. **Explainability** is provided by maintaining a complete record of inferred axioms, user decisions, and reasoning steps throughout the experimental campaign. The knowledge graph can also serve as a structured **context graph** for LLMs, enabling them to reason over formally represented domain knowledge while keeping their recommendations traceable and

explainable. This could allow LLMs to assist experimenters in selecting promising initial regions of the design space.
The framework can also derive mixture properties such as pigment volume concentration (PVC) (see Fig. 2) and solid volume content from formulation data using external functions.These properties are frequently used as design variables for coatings [13]. Finally, **automatic constraint verification** can be used to help identify infeasible experiments before execution.

5. Conclusion

This paper surveys current experiment design strategies for coatings research and argues that coating design is an inherently knowledge-intensive problem. Although significant advances have been made in laboratory automation, surrogate modelling, and DoE methods, comparatively little attention has been given to knowledge-based reasoning for campaign-level experiment design. To address this gap, we outline a knowledge graph-based framework that combines conceptual modelling, ontology reasoning, and an architecture for a DoE assistant. Such a system has the potential to provide explainable, extensible, and efficient support for experiment planning, execution, and analysis in coating design.

6. Declaration on Generative AI

During the preparation of this work, the author(s) used ChatGPT(OpenAI) and Grammarly to perform grammar and spelling checks and make the language clear and concise. GenAI Usage Taxonomy: Language editing and text refinement. After using the GenAI tool/service, the authors reviewed and edited the content as needed and take full responsibility for the publication's content

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