Advanced Engineering Informatics 36 (2018) 163–177

Contents lists available at ScienceDirect

Advanced Engineering Informatics

journal homepage: www.elsevier.com/locate/aei

Full length article

Systematic design space exploration using a template-based ontological method

Ru Wang[a], Anand Balu Nellippallil[b], Guoxin Wang[c,*], Yan Yan[d], Janet K. Allen[e], Farrokh Mistree[f]

[a] Beijing Institute of Technology, Rm 337, No. 1 Teaching Building, No. 5 Zhongguancun South Street, Haidian District, Beijing 100081, China
[b] University of Oklahoma, 202 W. Boyd St., Suite 219, Norman, OK 73019, United States
[c] Beijing Institute of Technology, Rm 343, No. 1 Teaching Building, No. 5 Zhongguancun South Street, Haidian District, Beijing 100081, China
[d] Beijing Institute of Technology, No. 5 Zhongguancun South Street, Haidian District, Beijing 100081, China
[e] University of Oklahoma, 202 W. Boyd St., Suite 116, Norman, OK 73019, United States
[f] University of Oklahoma, 865 Asp Avenue, Felgar Hall, Rm. 306, Norman, OK 73019, United States

ARTICLE INFO

Keywords:
Ontology
Decision-based design
Design space exploration
Process template
Reuse

ABSTRACT

The realization of complex engineered systems using models that are typically incomplete, inaccurate and not of equal fidelity requires the understanding and prediction of process behavior in design. This necessitates the need for extending designer's abilities in making design decisions that are robust, flexible and modifiable particularly in the early stages of design. To address this requirement, we propose in this paper, an ontology for design space exploration and a template-based ontological method that supports systematic design space exploration ensuring the determination of the right combination of design information that meets the different goals and requirements set for a process chain. Using the proposed method, a designer is able to (1) systematically adjust the design space in due time to manage the risks of errors accumulating and propagating during the design of different stages of the process chain, (2) improve the ability to communicate and understand the interactions between design information in the process chain. We achieve the said through (1) procedure for design space exploration is identified to determine the sequence of activities needed for the systematic exploration of design space under uncertainty; (2) the decision-based design information flow is archived using the design space exploration process template and represented by utilizing frame-based ontology to facilitate the management of re-usable information. We demonstrate the efficacy of this template-based ontological method for design space exploration by carrying out the design of a multi-stage hot rod rolling system in steel manufacturing process chain.

1. Frame of reference

Due to the limited information in the early stages of design, the designer has to deal with different types of uncertainty. The presence of incomplete, inaccurate and infidel models for complex engineering systems also adds to this uncertainty [1]. Design Space Exploration (DSE) refers to the activities of exploring (discovering and evaluating) design alternatives or space of potential design candidates before implementation during the system development [2]. Since the design is mainly a knowledge-driven process, it is possible to represent the inherent knowledge of many design problem through some hierarchical associative relationships, which will provide the guidance of the instantiation process for the problem-solving [3]. Several challenges have involved the management of complexity and uncertainty associated with the DSE in the model-based realization of complex engineered systems [4]. Two major ones are: (1) the challenge of creating knowledge about the complex engineered systems and; (2) the challenge of capturing and reusing tacit knowledge, building the ability to learn from data and cases, and developing knowledge-based methods for guided assistance in decision-making.

Design productivity can be enhanced by both increasing design knowledge in the early stages of designs and maintaining design freedom throughout the design process [5]. There have been propositions that aimed to computationally support designers in the exploration of conceptual design space [6]. Such as Chong et al. [7] define a conceptual design space and its framework to organize design knowledge objects and inter-relationships, then a tailored heuristic algorithm is employed for the determination of a satisficing solution graph [6]. Instead of the traditional optimization, the paradigm of DSE is used to evaluate "what-if" scenarios and trade-off studies. Some research

---

* Corresponding author.
E-mail addresses: haitang.56@163.com (R. Wang), anand.balu@ou.edu (A.B. Nellippallil), wangguoxin@bit.edu.cn (G. Wang), yanyan331@bit.edu.cn (Y. Yan), janet.allen@ou.edu (J.K. Allen), farrokh.mistree@ou.edu (F. Mistree).

https://doi.org/10.1016/j.aei.2018.03.006
Received 9 October 2017; Received in revised form 20 March 2018; Accepted 24 March 2018
1474-0346/

results put forward from the decision-based design perspective, e.g., RCEM [8], IDEM [9], which facilitate a broader design space exploration using the compromise Decision Support Problem (cDSP). Meanwhile, as traditional an optimization commercial software system, iSIGHT has grown to be a design exploration environment by integrating some methods, techniques, and modules to reflect that shift [10].

However, there is still a lack of effective means to capture, reuse, and represent tacit knowledge in the exploration process of design space in response to the second challenge above, which requires various types of design information to be assembled to form a representation of the context [11]. The contribution of this work is providing effective decision support for a designer to achieve the trade-off between identified multiple conflicting design goals, as well as manage the risk of errors. Therefore, to achieve a context environment for the exploration processes in designing complex engineered systems, a good understanding of predicting process behavior is paramount. Achieving this purpose using decision-based design perspective necessitates a systematic, flexible, and adaptive designing decision workflows involved. The decision-based design results associated with these workflows should be relatively insensitive to the uncertainties involved. The design results should also be flexible enough to accommodate any risk of errors that may accumulate along the decision workflows. To address above demands, we present in this paper an ontology for design space exploration and a template-based ontological method that supports systematic design space exploration in the model-based realization of complex engineered systems.

The remainder of this paper is organized as follows. In Section 2, we describe the foundation for this work – the Decision Support Problem (DSP) and its applicability in providing insight to designers for managing complexity and uncertainty. We also address the utility of ontology-based knowledge modeling in facilitating efficiency and effectiveness in the applications of DSPs. In Section 3, we propose a template-based method for computationally modeling the processes of DSE in response to the defined requirements, which includes a systematic procedure, design space adjustment, and a template scheme. In Section 4, we develop an ontology that represents the underlying knowledge related to the DSE process template, as well as the instantiation approach in keeping with the model of DSE process template. The efficacy of this method is illustrated by using an example associated with the design of a multi-stage hot rod rolling system in Section 5, and we end with the closing remarks in Section 6.

2. Foundations

2.1. Decision support problem construct

Due to the complexity and uncertainty associated with complex systems with emergent behavior, the model-based realization of complex engineering systems is characterized by models that are typically incomplete, inaccurate and not of equal fidelity especially in the early stages of design [4]. From the perspective of decision-based design, the primary role of designers is to make robust design decisions given the uncertainties associated with the system and models. Mistree et al. [12] present the compromise Decision Support Problem (cDSP) as a decision construct to aid designers in carrying out trade-offs among multiple conflicting goals. Using the cDSP model *satisficing* solutions for the desired system performance are sought rather than optimum solutions that are valid only in the narrow range of conditions. The generic mathematical formulation of the cDSP construct is shown in Fig. 1. A PEI-X (Phase-Event-Information - X) diagram is proposed to represent the decision workflows, which is defined as various sequences of computational tasks related decision-making.

Robustness refers to mitigating the consequences of variability to variations in engineering design, which means the ability to tolerate perturbations from some noise source. Many researchers have focused on the methods and applications for robust design in engineering design, Taguchi being the first to provide initial insight into the robust design and its principles which are widely advocated by both industry and academia. Despite this, there are some limitations to the Taguchi approach, the details of which are available in [1]. The design decisions in the earlier stages of design have a profound impact on the performance and quality of the final product. Chen et al. [8] formulate a robust design problem as a decision model using the cDSP construct. Building on this work, they present the Robust Concept Exploration Method (RCEM) and its applications [5]. These works are foundational in addressing the incorporation of robustness in the early stages of design. Based on these foundational work, several integrated computational methods are proposed to explore the design space by utilizing the cDSP construct [13–15]. Such as Nellippallil et al. [16] present a goal-oriented, inverse decision-based design method to achieve the vertical and horizontal integration of models for a multi-stage hot rod rolling system. In this work, they employ well-established empirical models, response surface models generated from simulation experiments as well as the cDSP construct supported by the Concept Exploration Framework (CEF). We will be addressing this work in the following sections.

2.2. Ontology-based knowledge modeling

The formalization and representation of knowledge have received strong attention in the last decades, especially in the context of knowledge-intensive system engineering [17,18], product lifecycle management [19], knowledge management [20,21], and artificial intelligence-based solutions [22,23]. As an idea of a design solution, “design concept” means a designer’s knowledge of process behaviors in design [24]. Thus design is also regarded as a structured reflection process [25], whereby a designer stepwise handles a problem via the developing and evaluating of a design concept. As a specification of a conceptualization, ontology provides a common vocabulary for the representation of domain-specific knowledge [26]. The two key elements of an ontology are concepts and relations, which facilitate the capturing and reusing in-context design knowledge with an integrated representation model [20,24].

Ontology has a great potential impact on the designing of engineering system [27]. The applications of ontology in design engineering have three major categories [28]: (1) concept interoperability [17–19]; (1) annotation of design information, sharing, and retrieval [20–22]; (3) product design configuration [23], which benefit from the following characteristics:

- Flexibility - knowledge is defined in terms of an ontology instead of “hardcoding” within the platform.
- Intelligent behavior - knowledge can be derived from the factual knowledge explicitly represented in the ontologies.
- Semantic interoperability - semantics of the (possibly several) languages used by the platform’s external parties can be defined by a set of interrelated ontologies.
- Expressiveness - context information is represented using a formal representation language, which enables to check the consistency of the models automatically.

In the past work, ontologies for representing the knowledge in cDSP template [29], a selection DSP (sDSP) template [30], and a hierarchy DSP template [31] are presented to facilitate efficiency and effectiveness in design, respectively. A PEI-X ontology for meta-design process hierarchies [32] is proposed, which can capture, represent and document the knowledge for supporting the re-usability of information in the decision workflows. Here, we focus on the integration of vertical information in the decision workflows.

Given

An alternative to be improved, domain dependent assumptions

n	number of system variables
q	inequality constraints
p + q	number of system constraints
m	number of system goals
$g_i(X)$	system constraint function
$f_k(d_i)$	function of deviation variables to be minimized

Find

X_i	System variables	i = 1, …, n
d_i^+, d_i^-	Deviation Variables	i = 1, …, m

Satisfy

System constraints (linear, nonlinear)

$g_i(X) = 0$ i = 1, …, p

$g_i(X) \geq 0$ i = p+1, …, p+q

System goals (linear, nonlinear)

$A_i(X) + d_i^- - d_i^+ = G_i$ i = 1, …, m

Bounds

$X_i^{min} \leq X_i \leq X_i^{max}$ i = 1, …, n

$d_i^+, d_i^- \geq 0;\ d_i^+ \cdot d_i^- = 0$

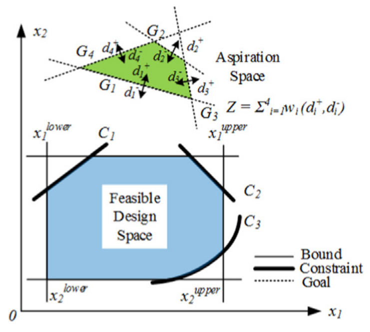
Minimize

Deviation Function:

Archimedean: $Z = \Sigma_{i=1}^{m} w_i(d_i^-, d_i^+)$

Preemptive: $Z = [f_i(d_i^-, d_i^+), \ldots, f_k(d_i^-, d_i^+)]$ i = 1, …, m

(a)



(b)

Fig. 1. Mathematical formulation of the cDSP construct [12].

3. Modeling the processes of design space exploration

In this section, according to requirements for DSE defined for the model-based realization of engineered systems, a template-based method for computationally modeling the processes of exploration is proposed, which includes a systematic procedure for DSE, design space adjustment, and a DSE template scheme.

3.1. Requirements for design space exploration

The management of complexity and uncertainty during the processes of DSE is required to be considered in the model-based realization of engineered systems. Kang et al. [2] suggest that an effective DSE framework needs to consist of the following ingredients: (1) a suitable representation of the design space, (2) an effective exploration method, (3) machine-assisted techniques for analyzing. For the conceptual design space, Chong and Chen [6] give a methodology that guides designers in the processes of DSE. Here, we extend the exploration process to the subsequent design phase where design space can be quantified. To further ensure the validity of design, we identify the following requirements:

- **Support Decision-Centric Robust Design**

Decision-Based Design (DBD) helps bridge the gap between a physical world and model world [33] and emphasizes the core role of human designers as decision-makers in the computer design environment. It is widely accepted that design is viewed as decision-making processes, which is a matter of making rational decisions on the available alternatives that satisfy one's preference [34,35]. Robust decision-making involves a particular set of methods aimed to help human designers identify potential robust strategies under conditions of complexity and uncertainty. As one embodiment of DBD, DSPs provide domain-specific mathematical models built as structured templates, which can be used to formulate a suitable representation of the design space.

- **Support Understanding and Predicting of Process Behavior**

To support different decision-making needs, the exploration processes of design space need to provide several levels of aggregation. So it can allow the analysis, evaluation, and synthesis, as well as the definition to be done (each task to be performed) at different levels of detail using methods that guide a sequence of tasks from one level of abstraction to the next lower level. Computer Aided Engineering (CAE) tools, can enhance the efficiency and facilitate the accomplishment of the tasks. Thus, from the perspective of model-based realization of engineered systems [36,37], the application of processes, methods, and tools in the exploration of design space necessitates an environment that can integrate the associated information and provide improved communications to support human designers in understanding and predict the process behavior in DSE.

- **Support Interaction and Visualization**

In a computer environment, the model-based realization of engineered systems cannot be done without the information flows that facilitate the ability to interact with models. Due to the complex characteristics of the engineered systems, the hierarchy of design processes needs to organize and manage the information flows to support vertical and horizontal integration. Therefore, a method for supporting integrated information flows across different dimensions and stages of the design process is essential. Meanwhile, visualization is also indispensable to support effective decision-making in the exploration processes of design space.

3.2. Procedure for design space exploration

In this paper, a systematic exploration processes for design space that support decision-centric robust design is proposed to identify design alternatives and generate *satisficing* solutions for the specific design problem. The exploration is inspired by RCEM [8] and CEF [16]. The frame of DSE is a logical sequence of activities performed to achieve a particular objective, as shown in Fig. 2.

Step 0: Data Input/Output - *Input A and Output H in* Fig. 2

The application of DSE procedure begins with the designer identifying design requirements for the current design event that provides data-entry from a static problem statement or dynamic data (e.g., sensors data of operation) for DSE. Moreover, it ends up with identifying design solution regions or points that satisfy the requirements identified for supporting the designer to make comprehensive decisions. Design requirements necessitate taking account of the possibly

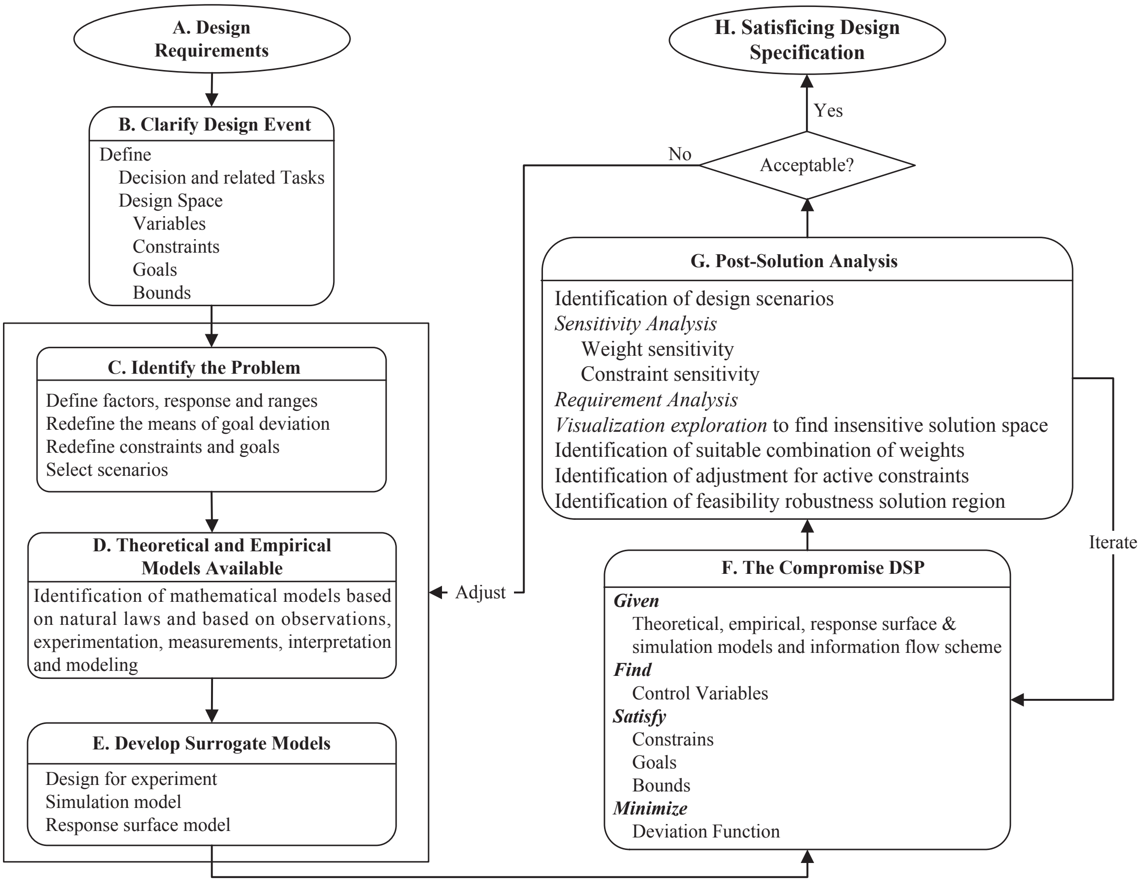


Fig. 2. Procedure for design space exploration.

conflicting wants of the various stakeholders because an effective product attribute deployment incorporates the needs of both the consumers and producers in decision-making which facilitates the conceptualization of design alternatives and constraints [38].

Step 1: Pre-Process - *Processor B in* Fig. 2

The partitioning a problem and planning the processes of decisions using generic discipline-independent modeling are presented in DSPs, namely meta-design [39]. PEI-X (Phase-Event-Information - X) diagram is used to model the design processes from a perspective of event-based time. To ensure whether appropriate *Support Problems* are available to solving via the computer-based design and analysis of design space, it requires further refinement of the complexity of the identified problem, that is, clarify the design event by defining the decisions and related tasks. The information associated with design space (i.e., variables, constraints, goals, and bounds) is gathered from various sources to make ready for a specific problem modeling.

Step 2: Problem Modeling - *Processor C, D, and E in* Fig. 2

To determine the initial design space and provide a combination of design information as the inputs for the cDSP model, the designer needs to perform three task processes (*Processor C, D,* and *E*) to model the specified problem via the mathematical formulations. First, identify significant design parameters in the specific design problem. They are classified as control factors ($\mathbf{x}$, design variables that designers can control), noise factors ($\mathbf{z}$, design variables that designers cannot control) and responses ($\mathbf{y}$, performance measures identified as goals), in parallel with the identification of their ranges. Then, define the functional relationship (f) between factors and responses, namely $\mathbf{y} = f(\mathbf{x})$. In *Processor C,* some available theoretical and empirical mathematical models based on the existing knowledge of natural laws or experiments/modeling in literature are identified and reused. In case some of them are not available or if there is a need to develop reduced order models to reduce the size of the problem, which requires designers to develop surrogate/reduced order models for the problem formulated. Statistical techniques (e.g., statistical design of experiments and response surface method) are widely used in engineering design to address these concerns [40], which is to develop a model of the model (meta-model) via building approximations of the computer analysis codes to yield insight into the functional relationship between $\mathbf{x}$ and $\mathbf{y}$. As shown in Fig. 3, a generic procedure of response surface modeling is summarized and provided to generate prediction function $g(x)$ approximating the true response surface function $f(x)$ via integrating base steps and support tools.

In the development processes of surrogate models, some candidate parameters and the boundaries (i.e., factors, responses, and ranges) are defined as the inputs based on the existing knowledge. They characterize the design space for the identified problem as well as factor levels used in simulations for Design of Experiments (DoE). The *Simulation Program* as a “slot” for inserting Finite Element Analysis (FEA) and other simulation programs is used to run the experiments designed. To generate data set for creating response surface models, two stages of sequential experimentation constitute the base steps for building approximations of computer analyses, namely screening, and model building. More detailed study of response surfaces modeling is provided in [41]. *Point Generator* and *Experiments Analyzer* are used to design and evaluate the essential experiments and their results [8].

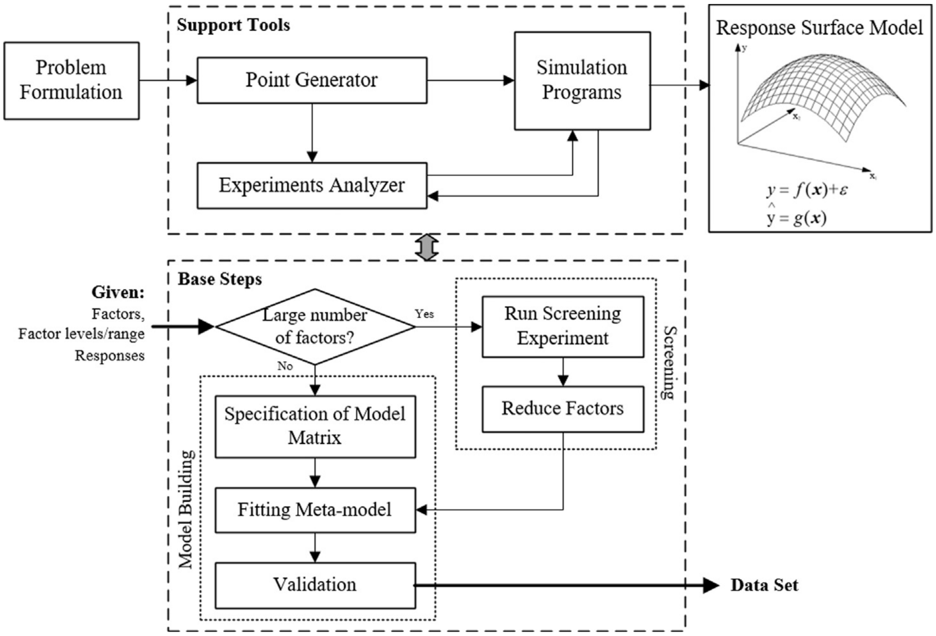


Fig. 3. Generic procedure for response surface modeling.

Step 3: Compromise DSP - *Processor F in* Fig. 2

The core step of DSE is the *compromise Decision Support Problem* (cDSP), which is a means to synthesize information for designing with multiple goals under uncertainty [42]. A given combination of design information generated from the specific problem model identified are communicated to the *Processor F*, namely cDSP, which is capable of handling constraints, bounds and multiple objectives and minimize deviation function, ultimately find the design variable values to satisfy a set of conflicting goals. The selection of two types of deviation function ($Z = [f_1(d_i^-,d_i^+),...,f_k(d_i^-,d_i^+)]$), Preemptive Formulation; $Z = \sum_i^W (d_i^- + d_i^+)$, Archimedean Formulation) depends on whether a designer has sufficient information and knowledge to indicate the priority of the different objectives. Various design preference P_i associated with weights W_i to the corresponding design goals G_i are defined as different design scenarios to explore the solution space via a great amount of iteration of the developed cDSP model. To solve the cDSP model, a tailored computational tool known as DSIDES has been developed incorporating Adaptive Linear Programming (ALP) algorithm [12], and a user-specified input file consisting of data file defining the size of design space, and user supplied FORTRAN routines (monitoring of the solution process) are required to create, formulate and execute the problem.

Step 4: Post-Solution Analysis - *Processor G in* Fig. 2

The notion of a multi-objective approach based on the cDSP formulation originates in an understanding of the problem defined by different performance criteria, which is appropriate in design under various uncertainties because it offers a “satisficing range” solution rather than an “optimizing point” solution. Instead of finding the best single-point solution (optimization philosophy), the satisficing philosophy focuses on keeping the flexibility and modifiable for each design stage solution, particularly in the early stages of design. Through the definition of deviation functions, the designer in post-solution analysis explores the possibility of design weight combination that guarantees a “satisficing range” of solutions to trade-off the multiple conflicting objectives. In Fig. 4, the desired solution is implemented by exploring the design preferences for analyzing the sensitivity of design weights of system goals. Different design scenarios are created and grouped in ‘scenarios experiments’ according to the designer’s interests. These scenarios are exercised to explore the design space. The generated results of the solution are visualized and analyzed via the comparison charts and ternary plots to bring insight for decision makers. In the comparison chart, the change trend of goal deviation in different design scenarios is a graphics display. In the ternary plot, the values inside the color contours of the plot are the deviation associated with each system goal or the actual attained values of goals for each scenario. The color bar next to the triangles indicates the changes of values. After the sensitivity analysis, some satisfying solution points are identified and recommended as the value of design or operating set points from the feasible design space that meets the multiple design objectives.

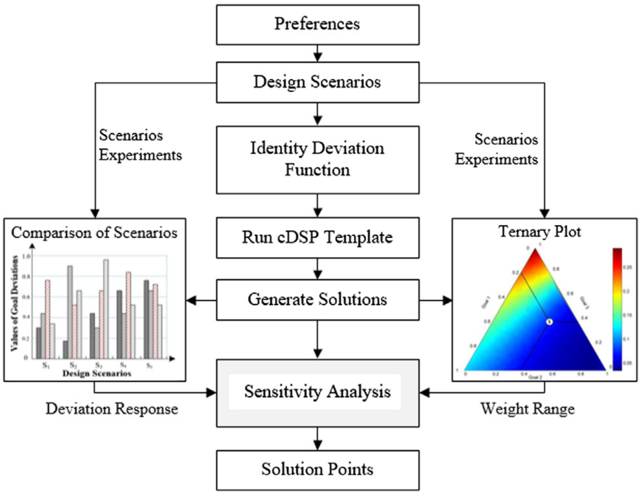


Fig. 4. Procedure for design preference exploration.

In the exploration processes, the designer can get the deviation response in different design scenarios and find a “satisficing range” solution by the superimposed plot in a single ternary plot to meet all the system goals. In the case that there exists a common region for all the goals simultaneously, the designer can define weight range that satisfies all the goals from the superimposed plot, then identify values of the solution including goals and system variables. Another case is when such a common regions do not exist [43]. In such a situation, there is an essential to modify the target value of system goals assigned in the cDSP to lower the deviations and thereby enhance the overlap possible, or even reformulate the constraints/goals to adjust the feasible design space. Both of those two cases will be discussed in the following sections. After the weight sensitivity analysis, some solution points selected in the satisficing range are recommended to the designers. Then, the designers have to make trade-offs among the conflicting goals and make a decision to choose one solution point as input to the next stage according to their empirical knowledge and preference.

3.3. Design space adjustment

Taking into account the interdependencies between different design events in design processes, the exploration processes of the design space should also have better modifiability and robustness to mitigate the risk of design errors caused by other design stage issues (e.g., processing error). In the cDSP model, the system constraints/goals are the functions of system variables, namely, $f(x_i)$ and $g(x_i)$, which can get a response according to the minimization of deviation variables under different design scenarios. Thus, the rest influential factors in a design space, namely the design constraints/goals/variables, also need to be further analyzed to check for feasibility robustness. In this paper, we consider four possibilities scenarios that happen in the design space changes, as shown in Fig. 5. These four scenarios can be explored by the designer for identifying a common satisficing region depending on the requirements of the design space currently generated/problem under consideration.

In Fig. 5, the Scenario I, II, and III adjust target values associated with goals or ranges of the variables, goals, and constraints in the initial design space, respectively. Generally, in practice, the modifications are based on the designer's empirical knowledge and corresponding comparison of the initial design results. Therefore, a detailed response analysis will increase the confidence of the designer in decision-making. For Scenario III, the extra capacity of design space depending on the constraints is determined by the identification of adjustments for active constraints [13], which reduces the risk of boundary solution with zero tolerance becomes infeasible in the face of variations. Thus, it is necessary to analyze the constraint sensitivity for determining those constraints that need to be modified by adding extra capacity. For Scenario IV, the designer considers the newer requirements from the side of constraints or system variables in addition to the system goals to make a decision. These "additional requirements" when incorporated would change the design space thereby allowing the designer to make a confident design decision. The Scenario IV happened in the designing of the multi-stage steel manufacturing process [16] is further addressed in this paper in Section 5.3. The appearance of those four scenarios depends on the specific design problem and the settings of the initial design space.

3.4. Modular process template for DSE

In the computational environment, modular-based design methods will enhance design flexibility and improve the design efficiency. So, a modular-based process template model for design space exploration is developed to achieve the capabilities of reusability and executability. The main contents of DSE process template include the three sub-templates: *Problem Model* (PM), *compromise Decision Support Problem* (cDSP), and *Post-Solution Analysis* (PSA). The PM sub-template has two modules: *Theoretical and Empirical Model* and *Surrogate Model*. The PSA sub-template has five modules: *Weight Sensitivity Analysis* (WSA), *Constraint Sensitivity Analysis* (CSA), *Additional Requirement Analysis* (ARA), *SSE_Experiment* (Solution Space Exploration Experiment), and *Deviation Response*. The detailed modules of the cDSP template are explained in [29]. The functions of each module are described in detail in Section 4.

In Fig. 6, the DSE process template is expressed as a structure similar

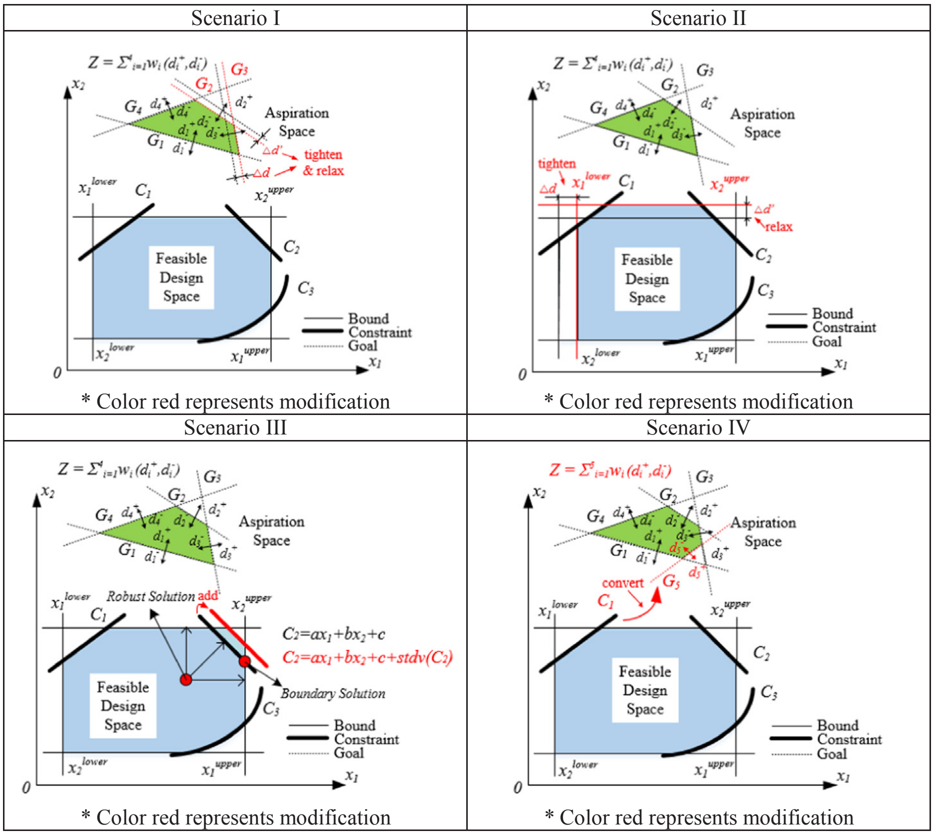


Fig. 5. Four possible scenarios for the design space adjustment.

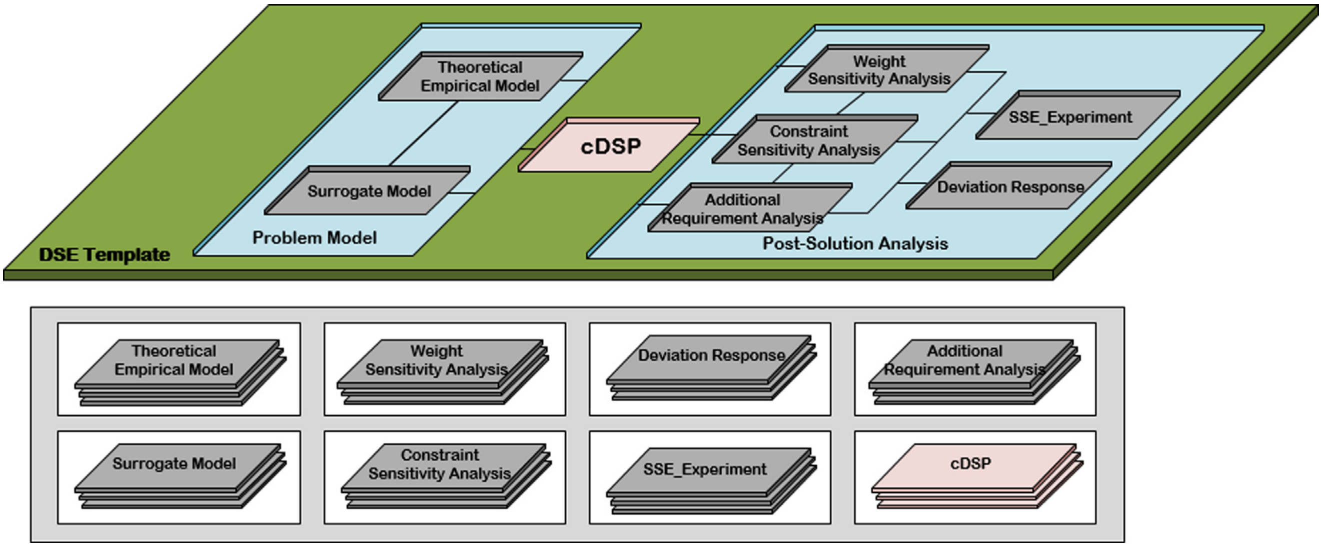


Fig. 6. The DSE process template.

to a printed board assembly having some electronic components. The elements (modules), like the theoretical and empirical model, deviation response, etc., are represented by "chips" and the procedure introduced in Section 3.2, is represented by the "breadboard." Due to the modular structure, the DSE process template includes three reuse scenarios:

(1) Reuse the "breadboard." The procedure for design space exploration corresponding to the "breadboard" is reused in the instantiation of any problem by populating specific information on the board.
(2) Reuse the "chips." Specific information (e.g., *Surrogate Model*) corresponding to the "chips" is reused in any different instantiation of a problem for the exploration process template.
(3) Reuse the assembly. An instantiated DSE process template with specific information corresponding to the "chips" is reused, where some "chips" (e.g., *SEE_Experiment*) are modified whereas others stay unchanged.

The modular DSE process template provides the ability to capture and reuse the information of DSE, which increase the confidence of designer's decision-making and give them insight into making comprehensive decisions, particularly in the early stages of design.

4. Ontology development for design space exploration process template

To further satisfy the requirements of DSE presented in Section 3.1, a frame-based ontology for DSE process template is developed to support the management of re-usability information and enhance the designer's understanding of process behavior. In this section, the classes and slots that constitute a frame-based ontology are formally defined, as well as the instantiation of exploration processes using the ontology is presented in keeping with the DSE process template model.

4.1. Definition of class and Slot

In the DSE process template, the "chips" embedded in the "breadboard" constitute the main structure of the ontology. The concepts in the DSE process template are explicitly defined as `Classes`, like *DSE_Template*, *PM_Template*, *PSA_Template*, etc. Some additional associated `Classes`, like *ResponseSurface, Response, Factor*, etc., are identified to capture the re-usability information of DSE, which also increase the semantic richness and integrity of the DSE process template ontology. The detailed definitions of the `Classes` are shown in Table 1.

Meanwhile, the semantic relationships between `Classes` are captured using `Slots`. There are two types of `Slots` - data slots and object slots. Data slots are used to link classes to end data (e.g., *weightRange* links the *WS_Analysis* to capture a value of weight range), while object slots are used to link classes to other classes (e.g., *hasWSA* links *PSA_Template* to *WS_Analysis*) or to themselves. Based on the exploration processes and the DSE process template structure, the data slots and object slots of the ontology are defined as shown in Tables 2 and 3, respectively. Some slots that reuse other ontologies will not be described here, like *name, value, image*, etc.

4.2. Instantiation of exploration using DSE process template ontology

According to the procedure for DSE defined in Section 3.2, the DSE process template is assembled by three sub-templates: PM template, cDSP template, and PSA template, as shown in Fig. 7. Before instantiating the DSE process template, the designer needs to clarify the corresponding design event defined in the PEI-X diagram process, which is useful for the designer to determine the relevant design information and knowledge involved in the design problem that is addressed. In this paper, we focus on creating and populating the PM template and the PSA template, the instantiation procedure for them are listed below.

(1) **Create *PM_Template* `Instance`.** Based on the input instances of `Classes` *Information* and *GeneralDesign_ Knowledge* that are defined in the design event, create and populate the *TheoreticalEmpiricalModel* `Instance`. When some existing TEM instances are not available, it needs to create *SurrogateModel* `Instance` arises, that is, creating predictive *Factor* and *Response* `Instances` and embed them into *RSM* (Response Surface Model) `Instance` based on the developed DoE. The newly created template instance of the surrogate model will be stored as new knowledge to achieve subsequent reuse.
(2) **Create *PSA_Template* `Instance`.** The PSA template can be equipped with three modules, i.e., weight sensitivity analysis, constraint sensitivity analysis, and additional requirement analysis, which are combined based on the needs of the specific problem and populated into the `Slots` of PSA template instance. The `Instance` of WSA is a basic module used to support the designer to determine the desired solution region. The input `Slot` of WSA module is the

Table 1
Classes of DSE process template ontology.

Class	Definition
DSE_Template	A formulation that integrates all the associated template modules and represents the information structure of DSE processes
PM_Template	A sub-template that integrates all the associated modules and represents the information structure for a specific problem
PSA_Template	A sub-template that integrates all the associated modules and represents the information structure of solution space exploration
TheoreticalEmpiricalModel	A module that integrates all the related information of mathematical model for initial design space
SurrogateModel	A module that integrates all the related information of surrogate model and experimental design
WS_Analysis	A module that integrates all the related information of weight analysis to define a satisficing range solution to all the system goals
CS_Analysis	A module that integrates all the related information of constraint analysis to define an extra capacity of design space
AR_Analysis	A module that integrates all the related information of additional requirement analysis to define a common range solution
SSE_Experiment	A module that represents a set of design scenarios corresponding to the associated goal weight
DeviationResponse	A module that represents a set of goal deviation corresponding to the associated design scenario
ResponseSurface	A module that integrates all the related information of surrogate model using response surface methodology
Response	A class represents a mathematical model for performance measures
Factor	A class represents input variables corresponds to a specific process
GoalWeight	A class represents the designers' interest in the associated system goal
GoalDesponse	A class represents the achieved value of the associated system goal in a specific design scenario
ConstraintResponse	A class represents the achieved value of the associated constraint in a specific design scenario, including "*Active Constraint*" and "Inactivate Constraint"
VariableResponse	A class that represents the achieved value of the associated system variable in a specific design scenario
DesignScenario	A class that represents a set of preference value corresponds to the associated design weight
FactorValue	A class that represents the value of a specific factor corresponds to the associated factor level
FactorLevel	A class that represents the value of a factor level identified by the designers
Preference	A class that represents the value of preference corresponds to the associated system goal in a specific design scenario
SolutionPoint	A class that represents the value of a point in the specific satisficing range solution
TernaryPlot	A class that represents the visualizing information of desired and sensitive regions of solution space

Table 2
Data slots of DSE process template ontology.

Class	Definition	Type
lowest_SSE	The value of the lowest sum of squares error (highest R^2) used to be fitting the regression model of response	Float
factorVaule	The value of a specific factor corresponds to the associated factor level, and it is used in simulations of DoE	Float
dataPoint	A set of goal deviation values associated a specific system goal, and it used to generate the ternary plot	Float
resluts_of_SSE	A set of values (system variables and goals) for solution points that satisfy all the design requirements and goals	Float
extraCapactiy	A value of standard deviation that is added to the active constraints with zero or limited capacity	Float
achievedValue	A value that can be achieved in response to the result of minimizing the deviation function	Float
preferenceValue	A set of preference values for a specific design scenario and experiment of solution space exploration	Float
acceptableValue	A value of the minimum target for requirements that can be accepted or approved	Float
deviationValue	A set of response values that is a normalized treatment to generate the ternary plot	Float
weightRange	The range value of weight for an associated goal which satisfies all the system goals	Interval
simulationPrograms	The (path of) code execution that is used to run the simulation programs of designed experiments	String
modelMatrix	The (path of) model matrix that represents the treatment combinations corresponding to the type of DoE	String
typesOfFittingModel	The types of fitting model that represents a regression meta-model	Symbol
validationRSM	The verification results of response surface model	String

Table 3
Object slots of DSE process template ontology.

Class	Definition	Type
hasPM	Specifies the *PM_Template* instance of *DSE_Template*	Instance
hasPSA	Specifies the *PSA_Template* instance of *DSE_Template*	Instance
is_Solved	Specifies the *cDSP_Template* instance of *DSE_Template*	Instance
hasSM	Specifies the *SurrogateModel* instance of *PM_Template*	Instance
hasTEM	Specifies the *TheoreticalEmpiricalModel* instance of *PM_Template*	Instance
hasFactor	Specifies the *Factor* instance of *ResponseSurface*	Instance
hasResponse	Specifies the *Response* instance of *ResponseSurface*	Instance
functionOf	Specifies the *Factor* instance of *Response*	Instance
associatedFactor	Specifies the *Factor* instance of *FactorValue*	Instance
toFactorLevel	Specifies the *FactorLevel* instance of *FactorValue*	Instance
hasWSA	Specifies the *WS_Analysis* instance of *PSA_Template*	Instance
hasCSA	Specifies the *CS_Analysis* instance of *PSA_Template*	Instance
hasARA	Specifies the *AR_Analysis* instance of *PSA_Template*	Instance
constraintResponse	Specifies the *ConstraintResponse* instance of *CS_Analysis*	Instance
associatedVariable	Specifies the *Variable* instance of *AR_Analysis* and *SolutionPoint*	Instance
associatedGoal	Specifies the *Goal* instance of *TernaryPlot, GoalDeviation, GoalWeight,* and *SolutionPoint*	Instance
associatedConstraint	Specifies the *Constraint* instance of *AR_Analysis* and *ConstraintResponse*	Instance
associatedWeight	Specifies the *GoalWeight* instance of *Preference*	Instance
toScenario	Specifies the *DesignScenario* instance	Instance
preferenceValue	Specifies the *Preference* instance of *DesignScenario*	Instance

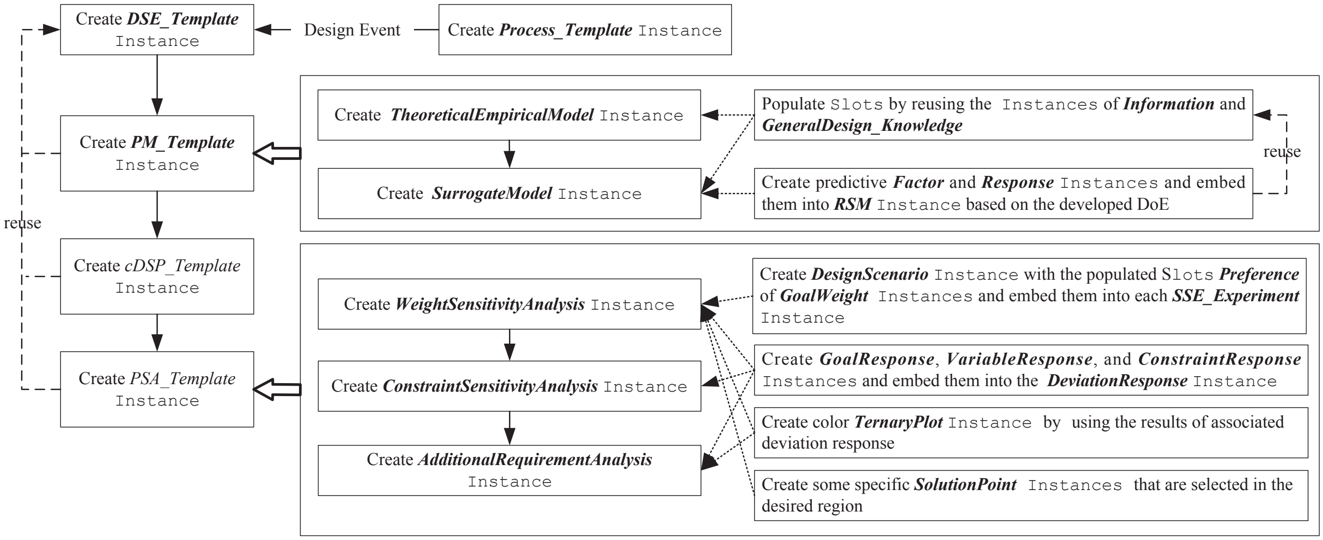


Fig. 7. Instantiation procedure of the DSE process template.

experiment of solution space exploration (*SSE_Experiment*), and the output `Slots` are *TernaryPlot* and *DeviationResponse* sub-modules used to bring insight for the designer in decision-making. At the beginning of post-solution analysis, the *DesignScenario* `Instance` with the populated `slots` *Preference* of *GoalWeight* `Instances` is created and embedded into each *SSE_Experiment* `Instance`. The results of the cDSP template are captured by the instances of `Classes` *GoalResponse*, *VariableResponse*, and *ConstraintResponse*. Meanwhile, these various types of response instances are populated into the *DeviationResponse* `Instance`. The `Instance` of color *TernaryPlot* for each system goal is created by using the results of associated goal deviation response and populated into the WSA module, then based on these ternary plots, a common region that satisfies all the system goals is generated by the formation of the superimposed ternary plot.

In some special problem cases, for example, no common region in the initial design solution space, the designer needs to carry out a detailed post-solution analysis to increase the understanding of the design response and the confidence in the prediction. Therefore, the `Instances` of CSA module and ARA module are created to capture the re-usability of information in the design space adjustment for a satisfying range. In the CSA module, the extra capacity of design space is identified to adjust the active constraints. While, in the ARA module, the variables/constraints are further analyzed as an additional requirement for the system goals, and the *TernaryPlot* `Instance` for each variable/constraint is created by using the results of associated variable/constraint deviation response. All the information from WSA, CSA, and ARA modules that are embedded into PSA template instance contributes to determining the desired solutions from which some specific *SolutionPoint* `Instances` are selected to support the designer to identify the design set points.

According to the scenarios defined in Section 3.3, the modified information based on the deviation response can be documented by the different instance versions. Such as, the target for requirements that can be accepted or approved, the acceptable value is modified based on the designer's experience knowledge or preference to get a satisficing common region. The adjusted acceptable value is captured by the different versions of the *TernaryPlot* `Instance`, which is embedded into the corresponding WSA, CSA, and ARA modules.

5. Test example

In this section, the utility of DSE process template ontology is illustrated via the design problem of an automotive gear manufacturing process - a complex system design that calls for a series of decisions to be made. As a key transmission element of automotive, gear is made of various grades of carburized steels. Due to the increasing demand for lightweight in the automotive sector, steel manufacturers urgently require the rapid development of newer grades of advanced high strength steels in response to the competition from other materials, especially some emerging materials with performance. Some model-based methods for the realization of engineered materials, products, and associated manufacturing processes are presented to couple the material processing-structure-property-performance spaces [44]. The manufacturing processes of automotive gear involve several different stages, in this paper, we primarily focus on the hot rod rolling process stage.

5.1. Designing of hot rod rolling (HRR) process chain

The products of steel manufacture processes include rod, bar, sheet, which involve a series of unit operations like continuous casting, reheating, rolling, cooling, etc. Nellippallil et al. [16] define vertical and horizontal integration for hot rod rolling process chain problem and showcase the information flows in Fig. 8. For horizontal integration, it means the integration of different unit operations having sequential

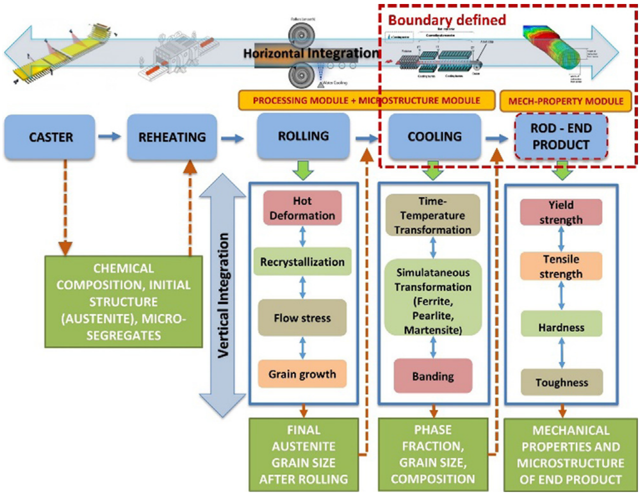
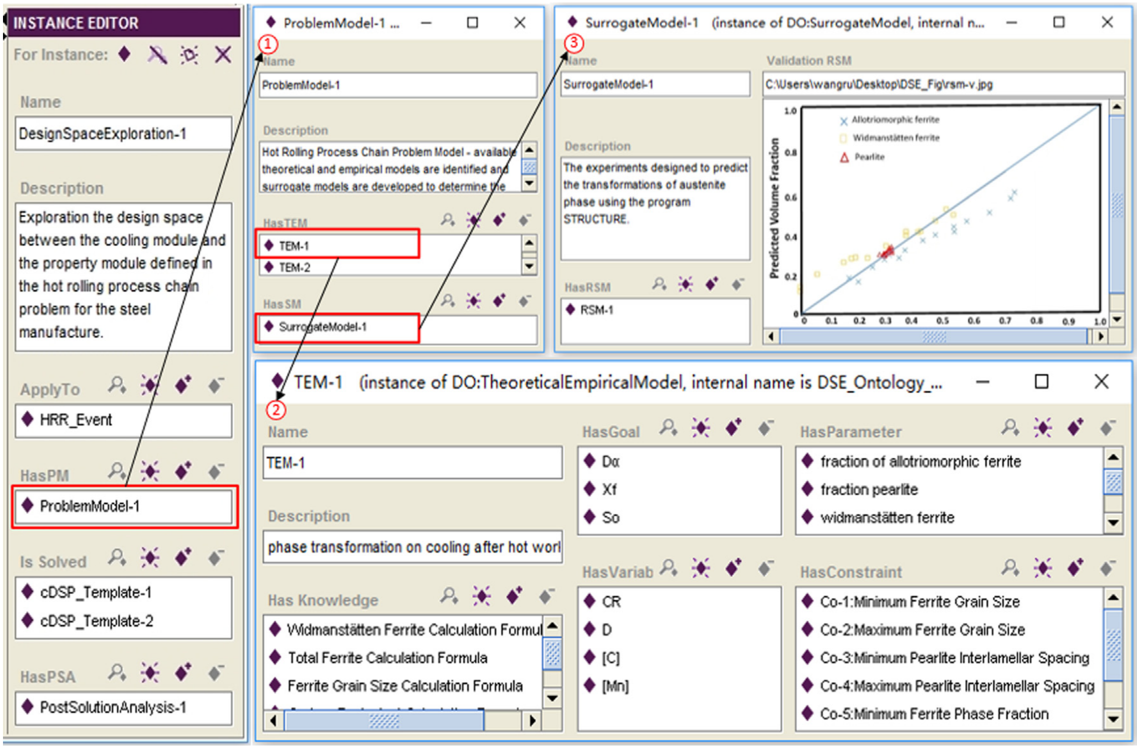


Fig. 8. Integration of models with information flow in hot rod rolling process chain [16].


INSTANCE EDITOR
For Instance:
Name: DesignSpaceExploration-1
Description: Exploration the design space between the cooling module and the property module defined in the hot rolling process chain problem for the steel manufacture.
ApplyTo: HRR_Event
HasPM: ProblemModel-1
Is Solved: cDSP_Template-1, cDSP_Template-2
HasPSA: PostSolutionAnalysis-1

① ProblemModel-1 ...
Name: ProblemModel-1
Description: Hot Rolling Process Chain Problem Model - available theoretical and empirical models are identified and surrogate models are developed to determine the
HasTEM: TEM-1, TEM-2
HasSM: SurrogateModel-1

③ SurrogateModel-1 (instance of DO:SurrogateModel, internal n...
Name: SurrogateModel-1
Validation RSM: C:\Users\wangru\Desktop\DSE_Fig\rsm-v.jpg
Description: The experiments designed to predict the transformations of austenite phase using the program STRUCTURE.
HasRSM: RSM-1

② TEM-1 (instance of DO:TheoreticalEmpiricalModel, internal name is DSE_Ontology_...
Name: TEM-1
Description: phase transformation on cooling after hot worl
Has Knowledge: Widmanstätten Ferrite Calculation Formul, Total Ferrite Calculation Formula, Ferrite Grain Size Calculation Formula
HasGoal: Dα, Xf, So
HasVariab: CR, D, [C], [Mn]
HasParameter: fraction of allotriomorphic ferrite, fraction pearlite, widmanstätten ferrite
HasConstraint: Co-1:Minimum Ferrite Grain Size, Co-2:Maximum Ferrite Grain Size, Co-3:Minimum Pearlite Interlamellar Spacing, Co-4:Maximum Pearlite Interlamellar Spacing, Co-5:Minimum Ferrite Phase Fraction

Fig. 9. Instances of the PM template embedded in DSE process template.

information flows (material) to produce the final product. There needs some information in detail regarding the individual processes happening at different length scales for each unit operation to achieve horizontal integration. It is achieved by carrying out modeling of material behaviors at different scales within a unit operation and integrating the information generated. This is defined as the vertical integration of models within a unit process/operation. Vertical integration allows the designer identify the information to be communicated from one unit operations to next thereby allowing to achieve the horizontal integration of the entire manufacturing process chain. The vertical and horizontal integration of models further allows the designer to carry out the integrated decision-based design exploration of the manufacturing process chain to realize the end product.

In the hot rod rolling process, the designer has to deal with large amount information (e.g., process parameters, constraints, bounds, etc) that raises the complexity of designing. Hence the requirement of defining a boundary and framing the right problem is critical. The designer has to precisely control the process variables to obtain the desired mechanical properties and microstructure for the rod and to achieve this model coupling at different scales is required. To illustrate the re-usability of information during the design space exploration processes using the DSE process template, we are framing a boundary within the problem defined by Nellippallil et al. [16]. Our focus in this work is to demonstrate how a designer can capture, represent, and document re-usable information using the hot rod rolling problem and thereby support the process designers to make decisions by considering robustness in design.

5.2. Populating a basic DSE process template Instance

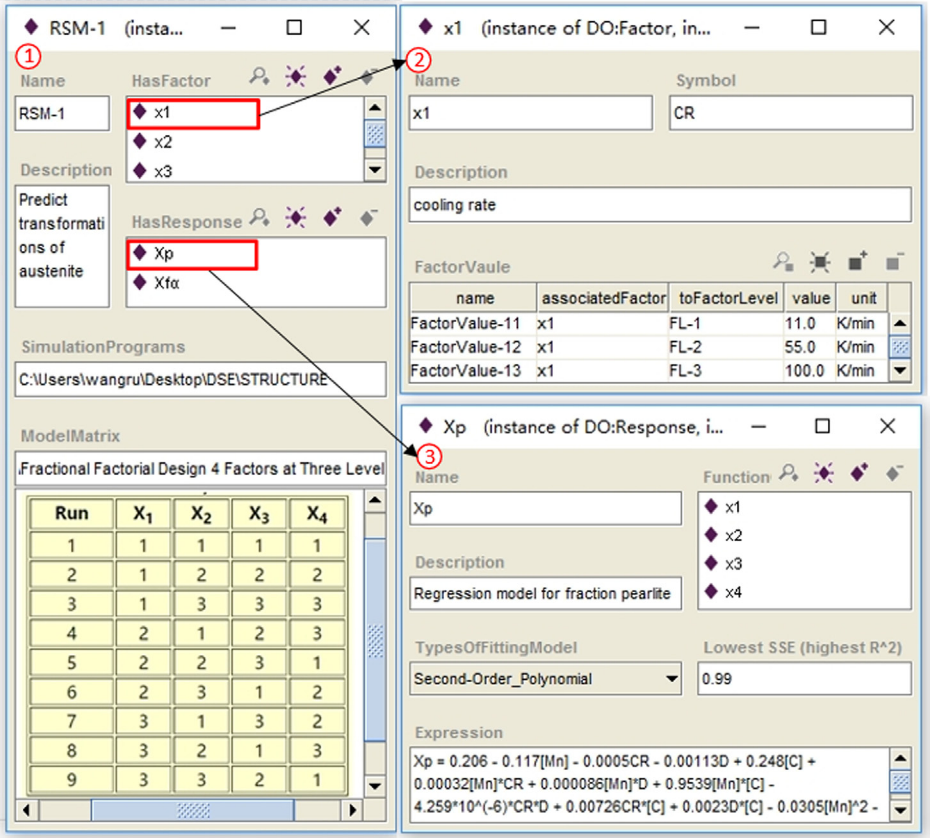
According to the procedure for DSE mentioned in Section 3.2 and the instantiation approach for DSE process template mentioned in Section 4.2, a basic DSE process template instance is created, and the populated sub-templates for problem model and post-solution analysis are illustrated by using the cooling module process stage of hot rod rolling problem.

5.2.1. Create and populate process template for problem model

The purposes of the problem model template are to allow the designer to determine the initial design space and then providing a combination of design information as the inputs for the cDSP model. In other words, the process designer needs to initially determine the basic elements of the design space when he creates the exploration processes. We showcase the same using Fig. 9. For the hot rod rolling process chain problem addressed in this paper, see the embedded `Instance` "ProblemModel-1" presented in the window "①" of Fig. 9. The inputs to the problem module are the chemical composition (e.g., the carbon concentration [C], the manganese concentration after rolling [Mn]), final austenite grain size after rolling (D), the cooling conditions, i.e., cooling rate (CR). The outputs are the mechanical properties of end product, i.e., yield strength (YS), tensile strength (TS), and hardness (HV) for the rod, which dependent on the final microstructure after cooling like the ferrite grain size after cooling (FGS, D_α), the phase fractions of ferrite (X_f) and pearlite ($1-X_f$), the pearlite interlamellar spacing (S_0) and the composition variables like silicon ([Si]), nitrogen ([N]), phosphorous (P), manganese ([Mn]).

According to the boundary within the problem described in Section 5.1, the problem of cooling module and property module in HRR is addressed via two compromise Decision Support Problem (cDSP) mathematical constructs based on the design set points of the steel manufacture processes. Therefore, the process designer populates two theoretical and empirical model (TEM) modules for providing a combination of design information as the inputs for the cDSP models, i.e., "TEM-1" and "TEM-2". As shown in Fig. 9, the design information that constitutes the module includes: "system goal," "constraint," "system variable," "design parameter," and "existing knowledge" about the available functional relationships. The detailed of these information instances are given in [16]. For example, the "TSM-1" embedded in the `Instance` "ProblemModel-1" is presented in the window "②" of Fig. 9.

In the hot rod rolling problem addressed, there is a need to design an experiment for predicting the transformations of the austenite phase. Depending on the cooling criteria, the phase transformations that happens during cooling after hot working converts the austenite phase



Name: RSM-1

HasFactor: x1, x2, x3

Description: Predict transformations of austenite

HasResponse: Xp, Xfα

SimulationPrograms: C:\Users\wangru\Desktop\DSE\STRUCTURE

ModelMatrix: Fractional Factorial Design 4 Factors at Three Level

Run	X_1	X_2	X_3	X_4
1	1	1	1	1
2	1	2	2	2
3	1	3	3	3
4	2	1	2	3
5	2	2	3	1
6	2	3	1	2
7	3	1	3	2
8	3	2	1	3
9	3	3	2	1

Name: x1

Symbol: CR

Description: cooling rate

FactorVaule

name	associatedFactor	toFactorLevel	value	unit
FactorValue-11	x1	FL-1	11.0	K/min
FactorValue-12	x1	FL-2	55.0	K/min
FactorValue-13	x1	FL-3	100.0	K/min

Name: Xp

Function: x1, x2, x3, x4

Description: Regression model for fraction pearlite

TypesOfFittingModel: Second-Order_Polynomial

Lowest SSE (highest R^2): 0.99

Expression:
Xp = 0.206 - 0.117[Mn] - 0.0005CR - 0.00113D + 0.248[C] +
0.00032[Mn]*CR + 0.000086[Mn]*D + 0.9539[Mn]*[C] -
4.259*10^(-6)*CR*D + 0.00726CR*[C] + 0.0023D*[C] - 0.0305[Mn]^2 -

Fig. 10. Instance of the RSM model.

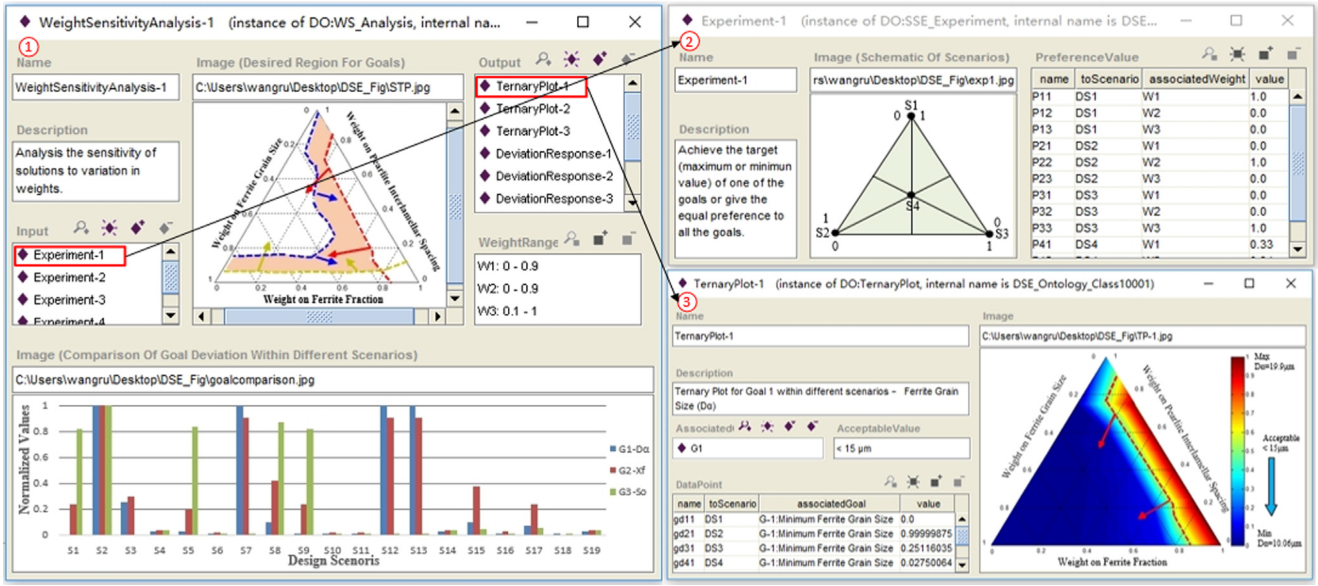
to different steel phases like allotriomorphic ferrite, pearlite, widmanstätten ferrite, bainite, and martensite, etc. [45]. There is a requirement to predict these transformed phases to manage the banding phenomena that happens in the microstructure. A meta-modeling approach is used to develop surrogate models for the different phases of steel that is transformed, as shown the window "③" in Fig. 9. In this case, we assume that the transformations of austenite only happen to ferrite and pearlite phases. In the window "①" of Fig. 10, a three-level fractional factorial design is carried out to develop response surface models for the transformation of austenite to ferrite and pearlite via the embedded `Instance` of "RSM-1". Four factors are identified for the design of experiments to develop the responses for the phases since their huge influence on austenite transformations and the formation of banded microstructures [46]. The factor values corresponding to the relevant factor levels for the simulations are identified, see the window "②" of Fig. 10. The simulation runs are performed using simulation programs to obtain the input-output correlations so that the cDSP for the problem can be formulated based on the specific problem. For example, in the problem addressed in [43], the simulation program used is the finite element software ABAQUS in which a finite element model for hot rod rolling is developed to predict the oval to round geometry conversion during rolling. Here, we carry out the experimental runs to predict the steel phases using the 'STRUCTURE' program based on the data and tools available in [45]. The input and output data sets are used to estimate the parameter values of the meta-model using least squares. Typically, a regression meta-model belongs to one of the three classes: (1) main effects model (a first-order polynomial), (2) main effects + interaction effects (a first-order polynomial augmented with two-factor interactions), (3) quadratic model with quantitative factors (a second order polynomial including purely quadratic). In the window "③" of Fig. 10, the regression model developed for fraction pearlite X_p with the lowest sum of squares error R^2 value of 0.99 is given, and it is generated by fitting a second order polynomial type function.

5.2.2. *Create and populate template for post solution analysis*

Based on the given combination of design information that is generated from the specific problem model shown in Fig. 9, two cDSP templates are formulated, which are used to find the values of the design variables that satisfy a set of conflicting goals, such as minimizing D_α, S_0 for the microstructure space after cooling and maximizing YS, TS for the end mechanical properties of rod. The detailed information of the cDSP formulations are available in [16], and the description on creating and populating the cDSP template is illustrated in [29]. In this paper, we focus on the keeping flexibility in identifying design solutions under uncertainty, and the process designer still needs to exploring various design preferences to guarantee a "satisficing range" solution and trade-off the conflicting multiple objectives. The information of sensitivity analysis and deviation response in the exploration process is captured via the `Slots` of *PSA_Template*.

In Fig. 11, the weight sensitivity analysis is carried out first to obtain the desired solutions that satisfy high priority goals. Here, the deviation function is identified as *Archimedean* formulation so that the process designer can explore as many scenarios as possible by assigning various combinations of weights to the associated system goals. In this case, the process designer creates four types of exploration experiments that are captured by the `Slots` "Input" in "WeightSensitivityAnalysis-1" (see the window "①" in Fig. 11) for the "cDSP_Template-1". It is used to determine the microstructure factors after rolling and operating set points for cooling that satisfies the requirements identified (i.e., system goals D_α, X_f, and S_0 are defined by system variables CR, D, [C], and [Mn]).

As shown in Fig. 12, design scenarios 1–4 in "Experiment-1" is a situation where the designer's interest is to achieve the target of one of the system goals (S1, S2, and S3) or gives equal preference to all the goals considered (S4). The design scenarios 5–7 are in "Experiment-2" where two goals are given equal preference, while the third goal is not given any preference. The design scenarios 8–13 are in "Experiment-3"



WeightSensitivityAnalysis-1 (instance of DO:WS_Analysis, internal na...

①

Name: WeightSensitivityAnalysis-1

Image (Desired Region For Goals): C:\Users\wangru\Desktop\DSE_Fig\STP.jpg

Output:
- TernaryPlot-1
- TernaryPlot-2
- TernaryPlot-3
- DeviationResponse-1
- DeviationResponse-2
- DeviationResponse-3

Description: Analysis the sensitivity of solutions to variation in weights.

Input:
- Experiment-1
- Experiment-2
- Experiment-3
- Experiment-4

WeightRange:
W1: 0 - 0.9
W2: 0 - 0.9
W3: 0.1 - 1

Image (Comparison Of Goal Deviation Within Different Scenarios): C:\Users\wangru\Desktop\DSE_Fig\goalcomparison.jpg

Experiment-1 (instance of DO:SSE_Experiment, internal name is DSE...

②

Name: Experiment-1

Image (Schematic Of Scenarios): rs\wangru\Desktop\DSE_Fig\exp1.jpg

Description: Achieve the target (maximum or minimun value) of one of the goals or give the equal preference to all the goals.

PreferenceValue

name	toScenario	associatedWeight	value
P11	DS1	W1	1.0
P12	DS1	W2	0.0
P13	DS1	W3	0.0
P21	DS2	W1	0.0
P22	DS2	W2	1.0
P23	DS2	W3	0.0
P31	DS3	W1	0.0
P32	DS3	W2	0.0
P33	DS3	W3	1.0
P41	DS4	W1	0.33

TernaryPlot-1 (instance of DO:TernaryPlot, internal name is DSE_Ontology_Class10001)

③

Name: TernaryPlot-1

Image: C:\Users\wangru\Desktop\DSE_Fig\TP-1.jpg

Description: Ternary Plot for Goal 1 within different scenarios - Ferrite Grain Size (Dα)

Associated: G1

AcceptableValue: < 15 μm

DataPoint

name	toScenario	associatedGoal	value
gd11	DS1	G-1:Minimum Ferrite Grain Size	0.0
gd21	DS2	G-1:Minimum Ferrite Grain Size	0.99999875
gd31	DS3	G-1:Minimum Ferrite Grain Size	0.25116035
gd41	DS4	G-1:Minimum Ferrite Grain Size	0.02750064

Fig. 11. Instance of weight sensitivity analysis for cooling module.

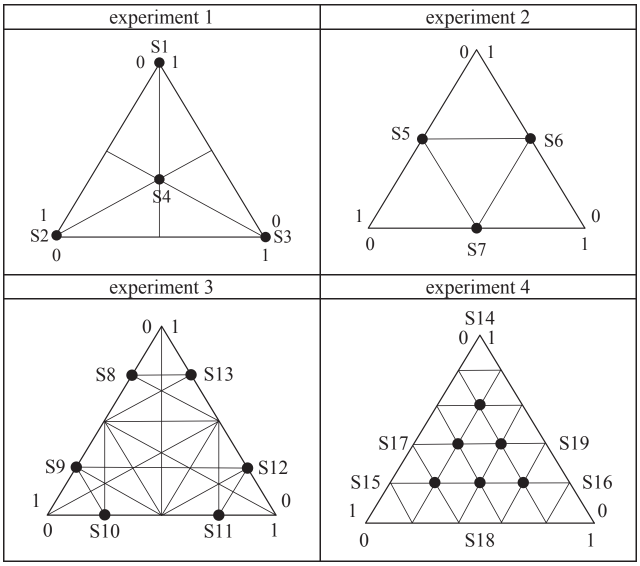


Fig. 12. Experiment scenarios for solution space exploration.

where the designer gives greater preference to one goal, a lesser preference to the second goal and zero preference to the third goal; design scenarios 14–19 are in “Experiment-4” where all the goals are given preferences with two of them being the same preference. The preference value for each goal weight in design scenario is captured, see the window “②” in Fig. 11.

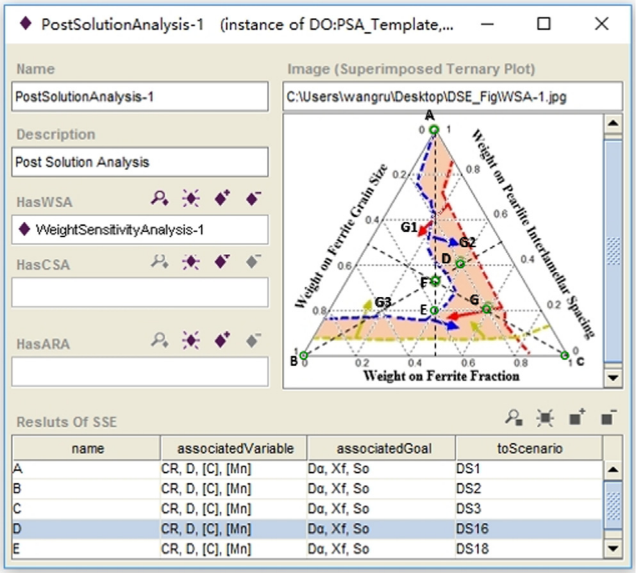
The cDSP template formulated is exercised for different design scenarios by running the tool DSIDES. The cDSP models are executed which is used to minimize the deviation function and offer the corresponding values of system variables. Then, the deviation variables of system goals which represent the degree by which achieved value is off the target are captured in the window “③” of Fig. 11. Ternary plots for each goal are generated to visualize and explore the solution space based on those sets of deviation variables. Such as the solution space for “G1” (minimizing ferrite grain size D_α) is shown in Fig. 11, the process designer can find the minimum achieved value of D_α using the current configuration information of cDSP template is 10.06 μm, which satisfies the acceptable value from the existing empirical knowledge 15 μm. We can see the contour region identified by the red dashed lines satisfy the design requirements for “G1”. The similar ternary plots for all the system goals are populated in the `Slots` “Output” of `Instance` “WeightSensitivityAnalysis-1”. Based on those data of design sets, all the goals in one superimposed plot is created to identify a common region that meets all the goals and adds confidence to the designer's decision-making, as shown the pink area in the window “①” of Fig. 11. Meanwhile, the weight ranges associated with the common region are also defined and, any combination of those weights that sums up to one guarantee a desired solution for the designer. To increase the designer's understanding of the solution space, the bar chart that represents the comparison of goal deviation within different design scenarios is created. In this bar chart formed, the shorter bar indicates a better design point/solution as the solution’s deviation from the target defined is less in that situation. By observing and analyzing the superimposed region for the problem discussed, it is possible to predict that some satisfactory solution points may occur in the following design scenarios: S6, S10, S11, S16, and S18. The process designer only needs to carry out design trade-offs based on the specific requirements and select the final design among those satisfactory solution points.

To further explain this process, we pick seven points to fully compare the good and bad of solutions within the different scenarios both from the common region identified, boundary, and outside, as shown in Fig. 13. The information of design points is populated in the `Slots` “Results_SSE” (results of solution space exploration) of `Instance` “PostSolutionAnalysis-1”. The detailed results of the selected points are listed in Table 4.

In Table 4, we observe that solution points A, B, and C satisfy the associated goals respectively, i.e., minimum ferrite grain size (D_α), maximum ferrite fractions (X_f), and minimum pearlite interlamellar spacing (S_0). Compared to other design points E, F, and G, the point D that lies in the common region identified and corresponds to design scenarios S16 satisfies all the conflicting goals in the best possible manner. Thus, the point D is selected as the recommended solution to the subsequent process stage. This information will be passed to next cDSP models formulated for subsequent manufacturing operations thereby achieving the horizontal integration of manufacturing process chain.

5.3. Populating a special DSE process template Instance

In Section 5.2, a basic DSE process template instance is created by instantiating the PM template and the PSA template, and the re-



◆ PostSolutionAnalysis-1 (instance of DO:PSA_Template,...

Name: PostSolutionAnalysis-1

Image (Superimposed Ternary Plot): C:\Users\wangru\Desktop\DSE_Fig\WSA-1.jpg

Description: Post Solution Analysis

HasWSA: ◆ WeightSensitivityAnalysis-1

HasCSA:

HasARA:

Resluts Of SSE

name	associatedVariable	associatedGoal	toScenario
A	CR, D, [C], [Mn]	Dα, Xf, So	DS1
B	CR, D, [C], [Mn]	Dα, Xf, So	DS2
C	CR, D, [C], [Mn]	Dα, Xf, So	DS3
D	CR, D, [C], [Mn]	Dα, Xf, So	DS16
E	CR, D, [C], [Mn]	Dα, Xf, So	DS18

Fig. 13. Instance of PSA template for cooling module.

Table 4
Comparison results for the selected points.

Sol. Pt	D_α	X_f	S_0, µm	CR, K/min	D, µm	[C], %	[Mn], %
A	12.5	0.684	**0.149**	11	30	0.19	1.02
B	**10.06**	0.681	0.176	99.9	30	0.18	0.7
C	19.9	**0.714**	0.182	11	74.2	0.18	0.7
D	*10.74*	*0.681*	*0.151*	*44.4*	*30*	*0.18*	*0.94*
E	10.33	0.673	0.151	70.3	30	0.18	0.93
F	10.33	0.673	0.151	70.1	30	0.18	0.93
G	11.05	0.687	0.151	33.06	30	0.18	0.95

usability information of design space exploration for the cooling module in HRR is populated. In that case, there exists a common region that satisfies all the goals simultaneously in the processes of post-solution analysis. The process designer has sufficient confidence to identify the design set points from the desired solutions identified for cooling that meet the target microstructure requirements defined. In this section, another case that here there doesn't any exists a common region is discussed via instantiating a special DSE process template.

In the HRR problem defined in Section 5.1, the subsequent process stage after microstructure correlation calculation (cooling module) is the property module for predicting the mechanical properties. Here the mechanical property system goals for the rod (end product) are identified as yield strength (*YS*), tensile strength (*TS*), and hardness (*HV*), the theoretical and empirical models of property module (TEM-2 `Instance`) is populated into the PM template instance as shown in Fig. 9, which allows the designer/user to determine the design elements (e.g., goal, constraint, variable) and the mathematical models involved in the cDSP model (cDSP_Template-2 `Instance`) that is used to solve the property module above. Similar to the exploration processes explained in the previous section, the basic module of PSA template "WeightSensitivityAnalysis-2" `Instance` is created, and its output `Slots` are populated based on the results of cDSP_ Template-2 `Instance` by carrying out the experiment scenarios for solution space exploration (see Table 4). According to the ternary plots for each system goal (mechanical properties of the rod) created by using the results of associated goal deviation response, a superimposed ternary plot is generated to support the designer to determine the desired solution region that satisfies the requirements, as shown in Fig. 14.

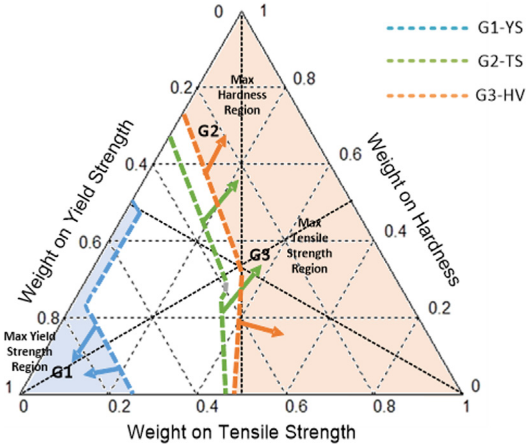
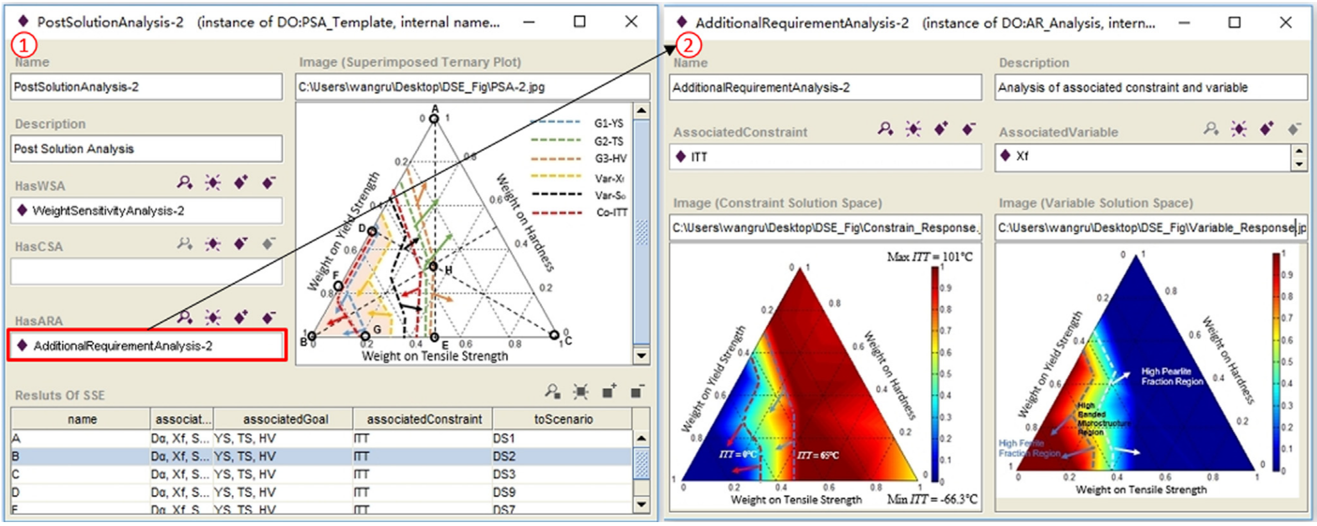


Fig. 14. Superimposed ternary plot.

In the superimposed ternary plot, the blue contour region identified by the blue dashed lines satisfies the system goal - 1 of maximizing yield strength and the maximum yield strength achieved is 320.6 MPa when the weight assigned to yield strength goal is 1.0. The pink contour region identified by the orange and green dashed lines simultaneously satisfy the system goals of maximizing tensile strength and hardness. The target values of tensile strength and hardness are achieved when the weight of their associated goals tends to 1. The maximum value achieved value for tensile strength is 750 MPa and for hardness is 170. In Fig. 14, we observe that there does not exist a common region that satisfies all the system goals even if the designer adjusts the acceptable value of the target. In this situation, the process designer has to consider some additional requirements for adjusting the initial design space and use the information associated to make a design decision. The information associated with system variables and constraints associated with the problem under study, when incorporated into the solution space exploration scheme along with the system goals will/could provide the designer with information that can then be used to make a design decision in such situations. We explain the same for the HRR problem in the following section.

In the HRR problem, other important design requirements affect the mechanical properties of the product, such as the material's impact toughness and the banded microstructure after cooling. As a measure's impact toughness, the impact transition temperature (*ITT*) denotes the boundary between brittle and ductile failure when subjected to impact loads, and it is identified as a constraint in the initial design space. Meanwhile, the management of banded microstructure after cooling is studied by considering the ferrite fraction (X_f), and pearlite fraction (S_0) obtained after cooling, are identified as system variables in the "TEM-2" instance and a system goal in the previous process stage (i.e., cooling module), respectively. In the post-solution analysis for mechanical properties module, the `Slot` of additional requirement analysis needs to be populated after the instantiation of "WeightSensitivityAnalysis-2". In Fig. 15, the "AdditionalRequirementAnalysis-2" `Instance` is created based on the deviation responses for the system variable (ferrite fraction) and the constraint (impact transition temperature) identified for this problem. The ternary plots for the achieved solution space for the constraint (impact transition temperature (*ITT*)) and the system variable (ferrite fraction (X_f)) with respect to the change in weights assigned to the system goals defined by yield strength (*YS*), tensile strength (*TS*), and hardness (*HV*) are shown in the window "②" of Fig. 15.

In the constraint solution space, the contour region identified by the red dashed lines are where the impact transition temperature is minimum, the red dashed line corresponds to an *ITT* of 0 °C. In the variable solution space, the gray and white dashed lines define the contour regions of higher ferrite fractions and higher pearlite fractions, and the intermediate region is the highly banded microstructure having both ferrite and pearlite. Comparing both the plots we observe that the achieved value of increases (65–100 °C) as the pearlite fraction



PostSolutionAnalysis-2 (instance of DO:PSA_Template, internal name...

Name: PostSolutionAnalysis-2

Image (Superimposed Ternary Plot): C:\Users\wangru\Desktop\DSE_Fig\PSA-2.jpg

Description: Post Solution Analysis

HasWSA: WeightSensitivityAnalysis-2

HasCSA:

HasARA: AdditionalRequirementAnalysis-2

Resluts Of SSE

name	associat...	associatedGoal	associatedConstraint	toScenario
A	Dα, Xf, S...	YS, TS, HV	ITT	DS1
B	Dα, Xf, S...	YS, TS, HV	ITT	DS2
C	Dα, Xf, S...	YS, TS, HV	ITT	DS3
D	Dα, Xf, S...	YS, TS, HV	ITT	DS9
E	Dα, Xf, S...	YS, TS, HV	ITT	DS7

AdditionalRequirementAnalysis-2 (instance of DO:AR_Analysis, intern...

Name: AdditionalRequirementAnalysis-2

Description: Analysis of associated constraint and variable

AssociatedConstraint: ITT

AssociatedVariable: Xf

Image (Constraint Solution Space): C:\Users\wangru\Desktop\DSE_Fig\Constrain_Response.

Image (Variable Solution Space): C:\Users\wangru\Desktop\DSE_Fig\Variable_Response.jp

Fig. 15. Instance of PSA template for mechanical properties module.

increases which is not at all acceptable in practice design. Thus, we define a green dashed line that corresponds to an *ITT* of 65 °C. Here, the wish is to achieve a minimum value of and a maximum value of ferrite fraction thereby managing the banding of the microstructure. All these additional requirements and system goals are identified in the superimposed ternary plot (shown the window “①” in Fig. 15) to support the process designer in carrying out trade-off and thus make a decision. The pink contour region with high ferrite fraction is identified in a compromised manner. In this region, both yield strength and impact transition temperature requirements are met while compromising on the requirements on tensile strength and hardness. Again, some special design points are selected to further illustrate this process, see the window “②” in Fig. 15. Finally, the solution point B having the highest ferrite fraction and maximum yield strength is recommended as the solution of interest.

5.4. Summary and discussion

Using the cooling module and the mechanical properties module identified in HRR process chain, we instantiate a DSE process template by populating the re-usability of information in the design space exploration processes. According to the DSE process template construct, the PM template for HRR problem is created and provides a combination of design information as the inputs for the cDSP template, which is used to minimize deviation function for satisfying a set of conflicting goals. The PSA template is also created and populated via the exploration processes of design preference in different experiment scenarios to keep the flexibility and robustness of each process stage. As a basic module of PSA template, the WSA instance is populated and supports the designer to determine the desired solution region. Meanwhile, to increase the designer’s confidence, the modules CSA and ARA also need to be created based on the specific problem identified. Meanwhile, it should be noted that the ontology enables reusability via the assembly of the “breadboard” and the “chips” as well as independent the “breadboard” and the “chips” due to the module construct during the instantiating of DSE process template. It maps to the three reuse scenarios of DSE process template presented in Section 3.4.

Since the engineering design problems always include rigid constraints and bounds on the system variables, most of the decisions that are quantified using analysis-based “hard” and insight-based “soft” information can be modeled as a multiobjective, nonlinear optimization problem. Instead of the traditional “goal programming” to indicate the search for an “optimal”, we prefer to suggest a designer find “satisfying” solutions, which facilitates a broader design space exploration and maintaining design freedom. We assert that it is possible, based on the qualitative relationship (i.e., the qualitative ratio of hard-to-soft information) to define any of the processes in design. The limitation is that at the beginning of the design (e.g., the conceptual design), that is, the quantitative ratio is very small, the designers have to rely on their judgment and experience. Thus some heuristic-based conceptual design approaches have been presented to facilitate exploration of product design concepts. However, the selection decisions of concepts can also be converted into the cDSP construct and implemented the design space exploration, if the attributes of the design concept are quantified effectively.

6. Closure

Model-based realization of complex engineered systems involves managing information associated with models that are typically incomplete, inaccurate and not of equal fidelity. Designing such systems, therefore, demands the designers to carry out rapid and systematic exploration of design space to identify solutions that are relatively insensitive to the uncertainties associated. To address this requirement, we propose in this paper, the ontology for design space exploration and a template-based ontological method that supports systematic design space exploration in the model-based realization of complex engineered systems.

In the proposed method, we demonstrate the computational formulation and execution of the processes of Design Space Exploration (DSE). The systematic exploration of design space involves a procedure for DSE, design space adjustment, and a DSE template scheme. The DSE process template and the method proposed helps a designer in determining the right combination of design information that meets the different goals and requirements set for a process chain, and also adjust the design space to achieve solutions that are robust and flexible enough to manage any risk of error propagation in continuous multi-stage design. Using the ontology developed and the proposed method, a designer is able to (1) systematically adjust the design space in due time to manage the risks of errors accumulating and propagating during the design of different stages of a process chain, (2) improve the ability to communicate and understand the interactions between design information in the process chain.

We demonstrate the efficacy of DSE process template ontology by carrying out the decision-based design of a multi-stage hot rod rolling system in a steel manufacturing process chain. Using this industry-inspired example problem, we illustrate the utility of ternary plot feature in Post-Solution Analysis (PSA) template to explore the design space.

The microstructure space solutions that satisfy the conflicting mechanical property goals in the best possible manner for the rod produced are identified by carrying out design trade-offs. The template-based ontological method for design space exploration facilitates the understanding and prediction of process behavior in design via extending designer's abilities and supporting them to make decisions with the features of robustness, flexibility, and modifiability, particularly in the early stages of design.

Acknowledgment

Ru Wang gratefully acknowledges the funding (Grant 1320012351601) received from the Beijing Institute of Technology Postgraduate Internationalization Project to visit the System Realization Laboratory at the University of Oklahoma. Yan Yan and Guoxin Wang gratefully acknowledge NSFC (Grant 51375049) and the National Ministries Projects of China (Grant JCKY2014602B007). Janet K. Allen and Farrokh Mistree gratefully acknowledge the John and Mary Moore Chair and the L.A. Comp Chair at the University of Oklahoma. This paper is an outcome of the International Systems Realization Partnership between the Institute for Industrial Engineering @ The Beijing Institute of Technology, The Systems Realization Laboratory @ The University of Oklahoma and the Design Engineering Laboratory @ Purdue.

References

[1] J.K. Allen, C. Seepersad, H. Choi, F. Mistree, Robust design for multiscale and multidisciplinary applications, J. Mech. Des. 128 (2006) 832–843.
[2] E. Kang, E. Jackson, W. Schulte, An Approach for Effective Design Space Exploration, Monterey Workshop, Springer, 2010, pp. 33–54.
[3] A.J. Dentsoras, Problem-dependent search for optimal parameter instantiation order in design spaces, Adv. Eng. Inform. 23 (2009) 474–482.
[4] J.K. Allen, J. Panchal, F. Mistree, A.K. Singh, B. Gautham, Uncertainty management in the integrated realization of materials and components, Proceedings of the 3rd World Congress on Integrated Computational Materials Engineering (ICME 2015), John Wiley & Sons, Inc., 2015, pp. 339–346.
[5] W. Chen, J.K. Allen, F. Mistree, A robust concept exploration method for enhancing productivity in concurrent systems design, Concurrent Eng. 5 (1997) 203–217.
[6] Y.T. Chong, C.H. Chen, K.F. Leong, A heuristic-based approach to conceptual design, Res. Eng. Des. 20 (2009) 97–116.
[7] Y.T. Chong, C.H. Chen, K.F. Leong, Human-centric product conceptualization using a design space framework, Adv. Eng. Inform. 23 (2009) 149–156.
[8] W. Chen, J.K. Allen, D.N. Mavris, F. Mistree, A concept exploration method for determining robust top-level specifications, Eng. Optim.+ A35, 26 (1996) 137–158.
[9] H. Choi, D.L. McDowell, J.K. Allen, D. Rosen, F. Mistree, An inductive design exploration method for robust multiscale materials design, J. Mech. Des. 130 (2008) 031402.
[10] P.N. Koch, J.P. Evans, D. Powell, Interdigitation for effective design space exploration using iSIGHT, Struct. Multidiscipl. Optim. 23 (2002) 111–126.
[11] D.J. Cook, J.C. Augusto, V.R. Jakkula, Ambient intelligence: Technologies, applications, and opportunities, Pervasive Mobile Comput. 5 (2009) 277–298.
[12] F. Mistree, O.F. Hughes, B. Bras, Compromise decision support problem and the adaptive linear programming algorithm, Prog. Astronaut. Aeronaut. 150 (1993) 251 251-251.
[13] M. Sabeghi, W. Smith, J.K. Allen, F. Mistree, Solution space exploration in model-based realization of engineered systems, in: ASME 2015 International Design Engineering Technical Conferences and Computers and Information in Engineering Conference, American Society of Mechanical Engineers, 2015, pp. V02AT03A015.
[14] R. Shukla, N.H. Kulkarni, B. Gautham, A.K. Singh, F. Mistree, J.K. Allen, J.H. Panchal, Design exploration of engineered materials, products, and associated manufacturing processes, JOM J. Minerals Metals Mater. Soc. 67 (2015) 94–107.
[15] A.B. Nellippallil, K.N. Song, C.-H. Goh, P. Zagade, B. Gautham, J.K. Allen, F. Mistree, A. Goal-Oriented, Sequential, inverse design method for the horizontal integration of a multistage hot rod rolling system, J. Mech. Des. 139 (2017) 031403.
[16] A.B. Nellippallil, J.K. Allen, F. Mistree, R. Vignesh, B.P. Gautham, A.K. Singh, A Goal-Oriented, Inverse decision-based design method to achieve the vertical and horizontal integration of models in a hot-rod rolling process chain, in: ASME Design Automation Conference Cleveland, Ohio, USA, 2017, pp. V02BT03A003.
[17] M. Yoshioka, Y. Umeda, H. Takeda, Y. Shimomura, Y. Nomaguchi, T. Tomiyama, Physical concept ontology for the knowledge intensive engineering framework, Adv. Eng. Inform. 18 (2004) 95–113.
[18] C. Bock, X.F. Zha, H.W. Suh, J.H. Lee, Ontological product modeling for collaborative design, Adv. Eng. Inform. 24 (2010) 510–524.
[19] H. Panetto, M. Dassisti, A. Tursi, ONTO-PDM: Product-driven ONTOlogy for product data management interoperability within manufacturing process environment, Adv. Eng. Inform. 26 (2012) 334–348.
[20] G. Peng, H. Wang, H. Zhang, Y. Zhao, A.L. Johnson, A collaborative system for capturing and reusing in-context design knowledge with an integrated representation model, Adv. Eng. Inform. 33 (2017) 314–329.
[21] S.C.J. Lim, Y. Liu, W.B. Lee, A methodology for building a semantically annotated multi-faceted ontology for product family modelling, Adv. Eng. Inform. 25 (2011) 147–161.
[22] D. Mun, K. Ramani, Knowledge-based part similarity measurement utilizing ontology and multi-criteria decision making technique, Adv. Eng. Inform. 25 (2011) 119–130.
[23] E. Gruhier, F. Demoly, O. Dutartre, S. Abboudi, S. Gomes, A formal ontology-based spatiotemporal mereotopology for integrated product design and assembly sequence planning, Adv. Eng. Inform. 29 (2015) 495–512.
[24] Y. Nomaguchi, K. Fujita, Knowledge representation framework for interactive capture and management of reflection process in product concepts development, Adv. Eng. Inform. 27 (2013) 537–554.
[25] I.M.M.J. Reymen, D.K. Hammer, P.A. Kroes, J.E. van Aken, C.H. Dorst, M.F.T. Bax, T. Basten, A domain-independent descriptive design model and its application to structured reflection on design processes, Res. Eng. Des. 16 (2006) 147–173.
[26] N.F. Noy, D.L. McGuinness, Ontology Development 101: A Guide to Creating Your First Ontology, Stanford Knowledge Systems Laboratory Technical Report KSL-01-05 and Stanford Medical Informatics Technical Report SMI-2001-0880, Stanford, CA, 2001.
[27] M.J. Darlington, S.J. Culley, Investigating Ontology Development for Engineering Design Support, Elsevier Science Publishers B. V., 2008.
[28] Y. Liu, S. Lim, Using Ontology for Design Information and Knowledge Management: A Critical Review, Global Product Development, Springer, 2011, pp. 427–433.
[29] Z. Ming, Y. Yan, G. Wang, J.H. Panchal, C.-H. Goh, J.K. Allen, F. Mistree, Ontology-based executable design decision template representation and reuse, Artif. Intell. Eng. Des. Manuf. (AIEDAM) 30 (2016) 390–405.
[30] Z. Ming, G. Wang, Y. Yan, J.K. Allen, F. Mistree, An ontology for reusable and executable decision templates, J. Comput. Inform. Sci. Eng. 17 (2016) 031008-031008-13.
[31] Z. Ming, Y. Yan, G. Wang, J.H. Panchal, C.H. Goh, J.K. Allen, F. Mistree, Ontology-based representation of design decision hierarchies, J. Comput. Inform. Sci. Eng. 18 (2016) 011001-011001-12.
[32] R. Wang, G. Wang, Y. Yan, M. Sabeghi, Z. Ming, J.K. Allen, F. Mistree, Ontology-based representation of meta-design in designing decision workflows, in: ASME 2017 International Design Engineering Technical Conferences and Computers and Information in Engineering Conference, American Society of Mechanical Engineers, 2017, pp. V001T02A056.
[33] W.F. Smith, J. Milisavljevic, M. Sabeghi, J.K. Allen, F. Mistree, The realization of engineered systems with considerations of complexity, in: ASME 2015 International Design Engineering Technical Conferences and Computers and Information in Engineering Conference, American Society of Mechanical Engineers, 2015, pp. V007T006A019.
[34] C.L. Bloebaum, A.-M.R. McGowan, Design of complex engineered systems, J. Mech. Des. 132 (2010) 120201-120201-7.
[35] M. Tribus, Rational Descriptions, Decisions and Designs: Pergamon Unified Engineering Series, Elsevier, 2016.
[36] J.A. Estefan, Survey of model-based systems engineering (MBSE) methodologies, Incose MBSE Focus Group 25 (2007).
[37] P. Micouin, Model Based Systems Engineering: Fundamentals and Methods, John Wiley & Sons, 2014.
[38] C.J. Hoyle, W. Chen, Product attribute function deployment (PAFD) for decision-based conceptual design, IEEE Trans. Eng. Manage. 56 (2009) 271–284.
[39] F. Mistree, B. Bras, W.F. Smith, J. Allen, Modelling design processes: a conceptual, decision-based perspective, Int. J. Eng. Des. Autom. (1995).
[40] T.W. Simpson, J. Poplinski, P.N. Koch, J.K. Allen, Metamodels for computer-based engineering design: survey and recommendations, Eng. Comput. 17 (2001) 129–150.
[41] D.C. Montgomery, R.H. Myers, Response surface methodology: process and product optimization using designed experiments, Raymond H. Meyers, Douglas C. Montgomery, A Wiley-Interscience Publications, 1995.
[42] B. Bras, F. Mistree, Robust design using compromise decision support problems, Eng. Optim. 21 (1993) 213–239.
[43] A.B. Nellippallil, K.N. Song, C.-H. Goh, P. Zagade, B. Gautham, J.K. Allen, F. Mistree, A. Goal-Oriented, Sequential, inverse design method for the horizontal integration of a multi-stage hot rod rolling system, J. Mech. Des. 139 (2017) 031403-031403-16.
[44] A.B. Nellippallil, R. Vignesh, J.K. Allen, F. Mistree, B.P. Gautham, A.K. Singh, A decision-based design method to explore the solution space for microstructure after cooling stage to realize the end mechanical properties of hot rolled product, in: 4th World Congress on Integrated Computational Materials Engineering (ICME 2017) Ypsilanti, Michigan, USA, 2017, pp. 353–363.
[45] S. Jones, H. Bhadeshia, Kinetics of the simultaneous decomposition of austenite into several transformation products, Acta Mater. 45 (1997) 2911–2920.
[46] J. Robson, H. Bhadeshia, Modelling precipitation sequences in power plant steels Part 1–Kinetic theory, Mater. Sci. Technol. 13 (1997) 631–639.