Struct Multidisc Optim (2016) 54:1527–1541
DOI 10.1007/s00158-016-1493-3

INDUSTRIAL APPLICATION

A systematic approach for model refinement considering blind and recognized uncertainties in engineered product development

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Received: 20 December 2015 / Revised: 8 April 2016 / Accepted: 20 May 2016 / Published online: 2 June 2016

Abstract In recent years, virtual testing has played an increasingly important role in the design and evaluation of engineered products. However, it is challenging to build the highly accurate computational models for virtual testing. Blind and recognized uncertainties are often unintentionally incorporated. These uncertainties consequently decrease the predictive capability of the models. To this end, this paper proposes a systematic approach for model refinement that minimizes the impact of unrecognized blind and recognized epistemic uncertainties in computational modeling. The approach consists of three steps: model invalidity analysis (MIA), development of an invalidity reasoning tree (IRT), and invalidity sensitivity analysis (ISA). First, in the MIA, possible causes that lead to discrepancies between the experimental and simulation responses are identified through brainstorming. Next, the IRT is built using the affinity diagram. It sequentially lists and screens potential candidate issues for model refinement at the stages of conceptual, mathematical, and computational modeling. Finally, the ISA quantifies the effect of incorporating updates in the model to address potential candidate issues with the goal of reducing the impact of the blind and recognized uncertainties. The most critical candidates are determined by using a weighted decision matrix. To demonstrate the effectiveness of the proposed approach, a case study examining a smartphone liquid crystal display fracture is presented.

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Keywords Model refinement · Uncertainty characterization · Blind uncertainty · Recognized uncertainty · Virtual testing

1 Introduction

The role of "virtual testing" has been increasing throughout the product development process. Nevertheless, it is still challenging to build a highly accurate computational model that emulates the behavior of real products. To improve the accuracy of computational models and thus improve their predictive capability, model verification and validation (V&V) have received significant research attention. Pioneering papers and industry standards have outlined the concepts and definitions of model V&V (AIAA 1998; ASME 2006; Thacker et al. 2004). According to the ASME guide (ASME 2006), model verification is the process of determining whether a computational model accurately represents the underlying mathematical model and its solution, while model validation is the process of determining whether a computational model is an exact representation of the real world from the perspective of the intended uses of the model. In recent years, the model validation is not only the quantification of the accuracy of a computational model, but also the improvement of the accuracy of the numerical solutions provided by the computational model.

Key components of the model validation are model updating, validity check, and model refinement as shown in Fig. 1 (Youn et al. 2011). The model updating utilizes mathematical means to maximize the agreement between outputs from simulations and physical observations (Xiong et al. 2009). Subsequently, the validity check can be used to quantify the degree of the agreement, and determines whether or not the updated model is appropriate for predicting the performance of interest (POI) of the real system. Model validation ends if it is determined that the model is valid. If not,

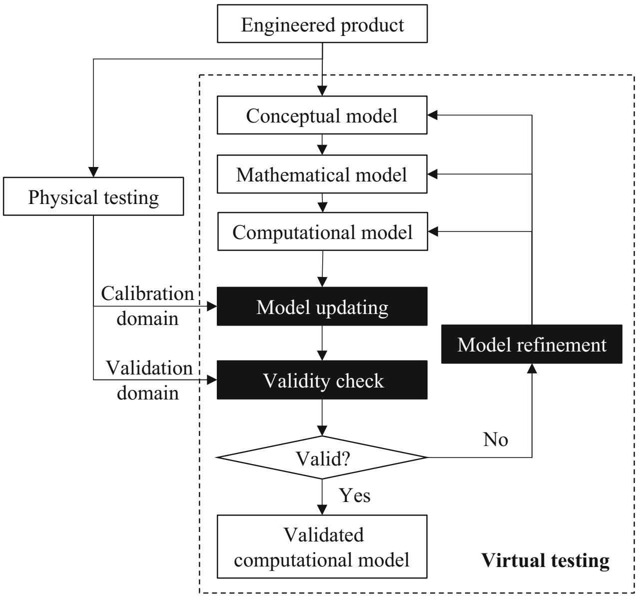


Fig. 1 Validation activities with model improvement (Youn et al. 2011)

improvement of the model can be performed to remove the major cause of the disagreement through "model refinement". The model refinement involves "changing the physical principles in modeling" or using other means to elaborate the invalid model (Xiong et al. 2009). For example, a model can be refined by revisiting the physical behavior of the engineered product and then changing the conceptual, mathematical, and computational models, accordingly. If a problem is found with the test, the test should be revised.

The model updating can be practical and useful. If it is done correctly, an accurate computational model with reliable predictive capability can be built in engineering product development. With this in mind, numerous studies have proposed systematic approaches on how to efficiently conduct model updating and validity checks. In the study by Oden et al. (2013), a virtual statistical validation process was proposed as an aid to the design of experiments for complex multiscale systems, such as elastomeric solids. Farrell et al. presented a Bayesian framework that addresses uncertainties in parameters, data, and model selection for coarse-grained models of atomistic systems (Farrell et al. 2015). Jung et al. proposed a model validation framework for virtual testing with limited experimental data, while model refinement was not addressed (Jung et al. 2015). Ferson et al. introduced a general metric for validity checks by comparing probability density functions (PDFs) from the simulation results with experimental data in the thermal challenge problem (Ferson et al. 2008). Lin et al. reviewed the state-of-the-art regarding validation metrics, pursuing the development of a unified one (Liu et al. 2011). Several metrics, such as confidence-interval based (Chen et al. 2004), Bayesian (Zhang and Mahadevan 2003), mean-based (Oberkampf and Barone 2006), and U-pooling methods (Ferson et al. 2008) have been developed to quantify the degree of agreement for the validity check. However, there has been little discussion about systematic approaches for model refinement. When an existing computational model turns out to be unacceptable during the validity check, current practice relies on personal experience (Xiong et al. 2009), which can delay the use of computational models for product development. Therefore, this paper attempts to develop a systematic approach for model refinement that includes model invalidity analysis, invalidity reasoning tree development, and invalidity sensitivity analysis.

Note that this study assumes that experimental results from testing are free from any error, although, in practice, failure of the validity check can be caused by errors in modeling, testing, or both. When results do not agree, the experiment may need to be revisited. Several well-known V&V papers (Hills and Leslie 2003; Oberkampf and Trucano 2002; Trucano et al. 2006) presented guidelines for designing and executing "validation" experiments in such a way that undesired random and bias errors can be reduced during model validation activities. This study focuses exclusively on modeling and assumes that experimental errors (e.g., blind uncertainty in experiments) are negligible. Correcting experimental errors is beyond the scope of this paper and should be examined in future work.

This paper is organized as follows. Section 2 overviews the types of uncertainties and their role in the model refinement activity of V&V. Section 3 presents the systematic approach for model refinement proposed in this study. In Section 4, a real-world problem predicting fracture failure of smartphone liquid crystal display (LCD) is used to demonstrate the effectiveness of the proposed approach.

2 Types of uncertainty considered in model verification and validation

It is generally accepted that uncertainty is divided into aleatory and epistemic uncertainty. Aleatory uncertainty is attributed to inherent randomness, e.g., variability in material property, geometric dimension, loading conditions, boundary conditions, and other physical properties (Oberkampf and Roy 2010). The inherent randomness implies deviations between samples in a population. It can exist spatially or temporally. For example, the exact value of a particular physical property of a product varies from site to site in space, or from moment to moment in time. Aleatory uncertainty is typically treated with probability theory. In principle, the randomness can be reduced with the improved control of a random process. However, if it is reduced, the nature of physical properties is fundamentally changed. When the inherent randomness is perfectly characterized with a sufficient amount of experimental data, the randomness cannot be reduced further.

Epistemic uncertainty refers to uncertainty owing to the lack of knowledge. The lack of knowledge about the system of interest can be associated with several modeling issues (e.g., physical process in a system, mathematical model form, and numerical solution approximation, etc.) (Oberkampf and Roy 2010). The degree of epistemic uncertainty can be reduced when additional information becomes available, while that of aleatory uncertainty cannot. Depending on the awareness of the existence, epistemic uncertainty is further divided into recognized (or acknowledged) uncertainty and blind (or unrecognized, unacknowledged) uncertainty (Ayyub 2001), as follows:

- Recognized uncertainty comes from conscious decision making. In building a computational model, this type of uncertainty can be ignored for practical reasons, or handled in various ways. Representative examples include (1) error caused by the use of limited significant digits, (2) assumptions or approximations in modeling, and (3) use of expert opinion in the absence of experimental data. Some mathematical theories were developed to quantify recognized uncertainty (Bai et al. 2013), including convex models, fuzzy sets, possibility theory, evidence theory, and random sets.
- Alternatively, blind uncertainty originates from being incognizant of incomplete knowledge or of the amount of knowledge needed to accurately model the system of interest. The most common reasons for blind uncertainty include mistakes, blunders, errors, and misunderstanding. A typical example of blind uncertainty in the development of engineered products is inadequate communication between individuals, for instance, between those providing expert opinion and those interpreting the information for input to the modeling. The predictive capability of a computational model can be degraded if this type of uncertainty is not properly addressed. Keeping the effect of blind uncertainty minimal is important to the success of model validation. According to Oberkampf and Roy (Oberkampf and Roy 2010), "there are no reliable methods for estimating or bounding the magnitude of blind uncertainties, their impact on a model, its simulation, or on the system's response." The critical nature of blind uncertainty (i.e., unknown unknowns) started to be recognized and studied first in fields of study other than model V&V, such as risk management of a LNG plant (Haugen and Vinnem 2015) examination of the swine flu (Aven 2015), molecular dynamic simulations (Romo and Grossfield 2014), project management (Ramasesh and Browning 2014), risk analysis in complex systems (Blockley 2013), and hypersonic flight (Bertin and Cummings 2003).

Theoretically, the impact of epistemic uncertainty can be reduced by adding knowledge. In practice, however, it is almost infeasible to determine what kind of knowledge needs be added to reduce epistemic uncertainty in the development of a high-fidelity computational model. For example, there are numerous recognized and blind uncertainties assumed in the development of a crash model of full vehicles. As shown in Fig. 2, two types of uncertainty-reducing activities can be considered: (1) recognized uncertainty can evolve to certainty or aleatory uncertainty and (2) blind uncertainty can evolve to certainty, aleatory uncertainty, or recognized uncertainty. Through this process, agreement between simulation responses and experimental results can be enhanced. If the validity check determines that a calibrated model is valid, the model can be used for product evaluation and design. Otherwise, the model should be improved. At this step, everything from conceptual modeling to computational modeling should be fundamentally reconsidered to make a more realistic model. To this end, the proposed model refinement approach aims to identify recognized and blind uncertainties and correct them through a series of activities.

3 A model refinement procedure

The ideal response of an engineered product (y_{true}) can be related to the response predicted from a simulation model (y_{pre}) as:

$$y_{\text{true}} = y_{\text{pre}}(x) + \varepsilon; \quad x \epsilon \Omega^l \tag{1}$$

where x is the known variable vector; and ε is the error between the ideal and simulation responses.

The ideal response of an engineered product (y_{true}) can be approximated to the experimental response (y_{exp}), when experimental errors are negligible:

$$y_{\text{true}} \approx y_{\text{exp}} \tag{2}$$

The response predicted from the simulation model can be identical to the one observed from an experiment by proper adjustment of an unknown variable vector.

$$y_{\text{exp}} = y_{\text{pre}}(x, \theta); \quad x \epsilon \Omega^l, y \epsilon \Omega^k \tag{3}$$

where θ is the unknown variable vector. In reality, however, both predicted and observed responses can be significantly different from the experimental responses due to the blind and recognized uncertainty. When they exist in the model, even after model calibration in the calibration domain, the predicted response may not emulate the experimental responses in the validation domain. Then, (3) becomes,

$$y_{\text{exp}} = \hat{y}_{\text{pre}}(x, \theta) + e; \quad x \epsilon \Omega^l, y \epsilon \Omega^k \tag{4}$$

where e is the error due to blind and recognized uncertainty; and $\hat{y}_{\text{pre}}$ is the responses from the invalid simulation model. To construct a valid model, the effect of the blind and recognized uncertainty must be removed or minimized.

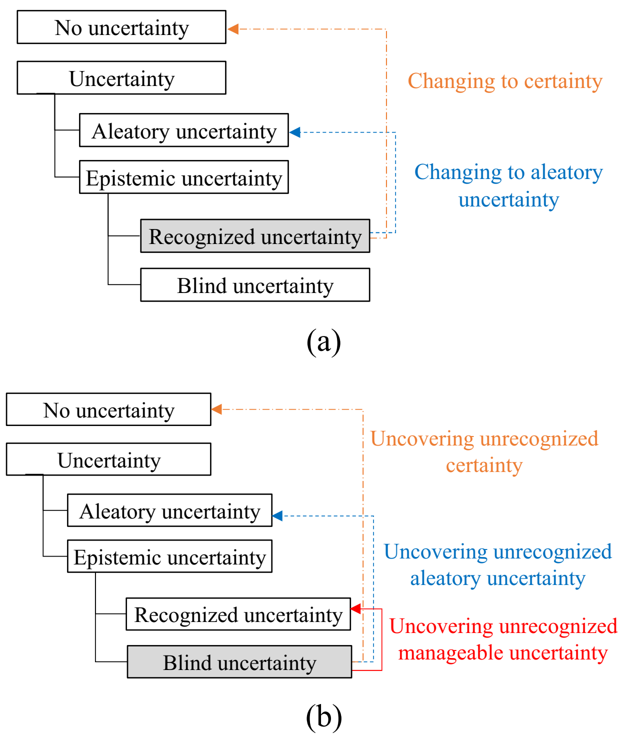


Fig. 2 Two types of uncertainty-reducing activities in model refinement: **a** minimizing the impact of recognized uncertainty and **b** uncovering blind uncertainty

Root causes for those uncertainties are various. Identifying root causes is not trivial since there are so many possible causes that lead to invalid modeling. It is challenging to build an accurate computational model when it turns out that a calibrated model is invalid. As a computational model becomes more complex to increase accuracy, there is more chance of mistakes, blunders, and errors that eventually lead to decreased accuracy. This underscores the need to develop a systematic approach. By identifying the root causes of model invalidity, uncertainties can be addressed. This can enhance the predictive capability of the computational model. To this end, this section presents a procedure for model refinement. The three core steps are: (1) model invalidity analysis, (2) development of an invalidity reasoning tree, and (3) invalidity sensitivity analysis.

3.1 Model invalidity analysis

Failure in the validity check implies that blind and recognized uncertainties in a calibrated computational model have significant impact on the predictive capability of the model. An invalid computational model should be refined. As a first step, model invalidity analysis (MIA) is used to identify possible causes of deficient knowledge. Here, we employ a brainstorming approach for MIA.

Brainstorming is defined as a solution-finding technique that generates ideas in a nonthreatening atmosphere. In MIA, the objective of brainstorming is to produce the greatest number of possible invalidity causes for the blind and recognized uncertainties. The group for brainstorming consists of simulation (and/or validation) engineers, design engineers, and test engineers. Simulation engineers not only include personnel in charge of refinement of the simulation model of interest, but also include individuals with expertise in modeling of similar products. It is helpful to have a moderator to direct brainstorming activities. The brainstorming activity for MIA starts with a clear, specific written statement of the issue. At this stage, background information should be provided to the group, including (1) the simulation model and experiments, (2) a comparison of simulation and experimental results, (3) critical factors identified in designing, modeling, and testing, (4) known limitations of the existing simulation model, (5) a review of simulation development history, and (6) benchmarking of similar simulation models. Next, the group is given a few minutes to collect their own thoughts. A moderator should provide individual participants ample opportunity to express their ideas and make contributions. No questions, discussion, or criticism of ideas are allowed, to encourage the collective creativity of the group. When ideas are exhausted, the brainstorming session can stop. The final outcome of the brainstorming is an affinity diagram.

The affinity diagram identifies inherent similarities between multiple ideas suggested from the brainstorming activity. It aims at grouping ideas, thoughts, and opinions into major categories. Through the process of building the affinity diagram, new ideas may occur to the participants and poor ideas can be abandoned. At the same time, the level of understanding about individual ideas can be also enhanced. The building of an affinity diagram starts by recording ideas on sticky memo notes or file cards. The notes (or cards) are randomly placed on a board. Next, each note is explained by the team member who suggested the idea and is subsequently discussed by all team members. After group discussion, a note is related to other notes that have similar ideas. When a note keeps being moved between two categories due to its similarity, another note that duplicates the original note is prepared so that the idea can be placed in both categories. If a note is determined to be worthless for further consideration, it is moved to the category of "irrelevant" and separated from other notes, but not discarded. In this way, none of ideas suggested in brainstorming are lost. Table 1 shows an example of an affinity diagram developed to uncover blind uncertainty in an invalid computational model created for a liquid crystal display (LCD) module of a smartphone. In the affinity diagram, three possible causes in materials, constraint, and boundary conditions are listed, while two non-critical items are also shown. The affinity diagram is the final outcome of MIA.

Table 1 Affinity diagram for the MIA of an LCD module in a smartphone

Material behavior
The use of a linear model is not proper to model the stress–strain curve of sheets and plates of the LCD module.
Constraint
The tied contact condition between the LCD chassis and LCD panel does not reflect reality.
Loading condition
The load path of the LCD module in the three-point bending tests is not considered properly.
Irrelevant
The thickness of the layers in the LCD module is not incorporated correctly.
The details of the LED lights are not modeled sufficiently.

3.2 Development of an invalidity reasoning tree

In the previous section, possible invalidity causes were identified. This section presents a tool called the invalidity reasoning tree (IRT) to identify potential candidates for model refinement. As shown in Fig. 3, the IRT searches for potential candidates for refinement in conjunction with possible causes identified in the affinity diagram of MIA. Potential candidates are identified by sequentially reviewing items in the conceptual, mathematical, and computational modeling. The final outcome of the IRT activity is a specific plan for model refinement.

3.2.1 Using an IRT for conceptual modeling

The conceptual model is defined as the ideal representation of the behavior of a real physical system. In conceptual modeling, assumptions are inevitable in order to simplify the physical behavior found in the real world. When the model is shown to be invalid, the conceptual modeling should be checked first. For refinement of an invalid model, we have provided here a checklist with seven specification categories to be considered.

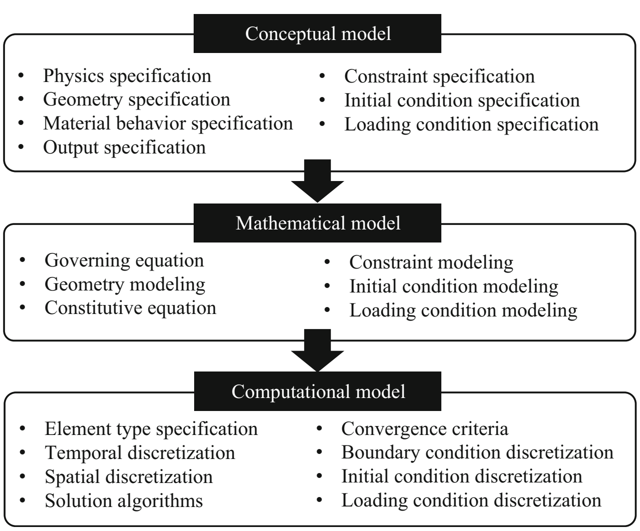


Fig. 3 Checklist for building the invalidity reasoning tree

(1) Physics – The complexity of the actual physical behavior of a real-world system should be sufficiently incorporated in the specification of the physics in the model. As an example, a model must be refined by turning a single-disciplinary problem (e.g., structural analysis) into a multi-disciplinary problem (e.g., structural analysis coupled with fluid dynamics analysis) provided that fluid–structure interaction is no longer ignorable.

(2) Geometry – More detailed features of the product's geometry may need to be included. The degree of simplification for small holes or fillets of a chassis can be critical in calculating the stress intensity factor.

(3) Material behavior – Blind and recognized uncertainties in modeling material behaviors can be a possible source for producing an invalid model. A linear model (e.g., elastic) can be substituted for a nonlinear one (e.g., plastic and viscoplastic) to describe material behaviors.

(4) Output – Simulation outputs are the response of a computational model with given inputs. The selection of an inappropriate output can lead to undesired consequences. For example, the use of maximum stress in calculating solder joint fatigue life can force the process to rely on a stress-based life model rather than using an energy-density-based life model.

(5) Constraints – Sufficient details in constraints have to be incorporated in the model. For example, in structural analysis, the stiffness or damping coefficients of welds are commonly assumed to be equivalent to the parent metal, thus ignoring residual stress. Excessive simplifications of constraints should be avoided for joints, welds, bonds, contacts, and friction conditions.

(6) Initial and loading conditions – Initial values for displacement, velocity, and acceleration must be carefully revisited. Distributed loads over a space are commonly replaced with a lumped load at a single point. This simplification should be checked with care.

3.2.2 Using the IRT for mathematical modeling

During the stage of mathematical modeling, building of the IRT is primarily aimed at correcting inadequate equations and incorrect mathematical statements. The revision of equations and statements begins by fully understanding any wrong specifications and/or incorrect assumptions identified in the conceptual modeling. The specifications modified in the conceptual modeling are translated into equations and mathematical statements at this stage. The user should also check whether input values in equations are correct. The mathematical modeling step in Fig. 3 lists the items to be considered during this step, including:

(1) Governing equation – A new governing equation can be considered to reflect the physics of the actual system of interest, based on the assumptions used in developing the conceptual model. Relevant partial or ordinary differential forms identified by examining the invalid model should be considered to remove blind and recognized uncertainty.
(2) Geometry modeling – The geometry of a system should be formulated into equations with a proper functional form. As an example, drawing functions such as a simple straight line or curve (e.g., Hermite and B-spline) must be carefully reselected if the use of a drawing function is expected to produce an unacceptable amount of errors.
(3) Constitutive equation – The use of a more relevant constitutive equation can be considered to better define the relationship between physical quantities. For example, a nonlinear curve can be substituted for a linear curve based on Hooke's law to define the force-displacement relation of elastomers subjected to elevated temperatures.
(4) Constraint, initial and loading condition modeling – If the conceptual modeling includes modification of constraints, as well as initial and loading conditions, the conceptual model specifications should be translated into appropriate mathematical model specifications.

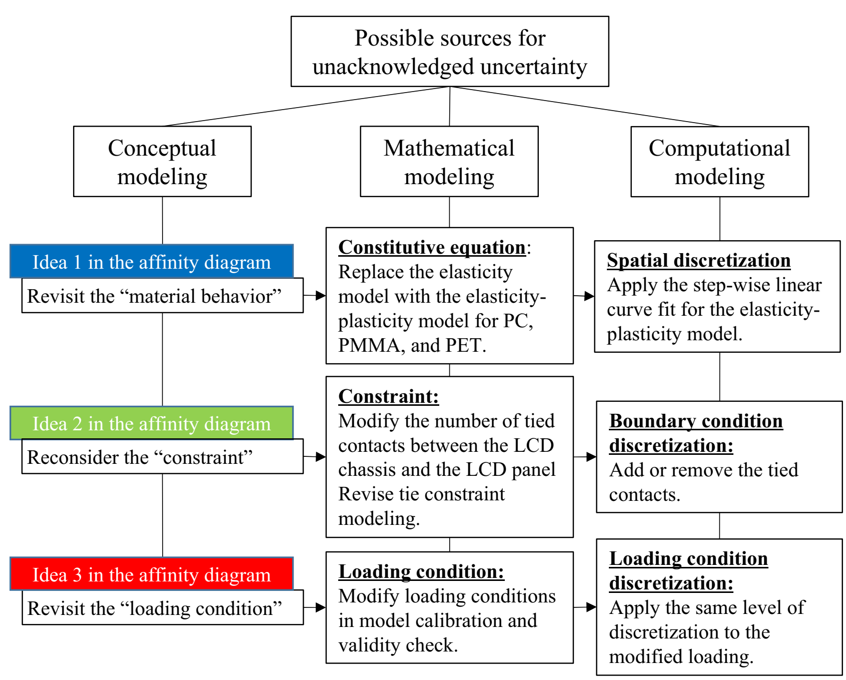
3.2.3 Using the IRT for computational modeling

A computational model is the numerical implementation of a mathematical model. As shown in Fig. 3, the last step in building the IRT is to review the checklist for computational modeling: element type, temporal and spatial discretization, initial and loading conditions, and convergence criteria. In this step, the level of temporal and spatial discretization for governing equations can be improved by considering the tradeoffs between computational cost and anticipated accuracy. Initial and loading conditions can be updated, if necessary. Convergence criteria and solution algorithms can also be checked.

Figure 4 presents an example of an IRT for the case study of the liquid crystal display (LCD) of a smartphone. The process started by identifying the invalidity causes related to the blind uncertainty. Then, potential candidates were screened during the three processes of model development: conceptual, mathematical, and computational modeling. In the conceptual modeling, it was found that the materials and constraints were the potential candidates, which were related to the ideas in the affinity diagram developed during the brainstorming activity. The IRT – when used for mathematical modeling – identified potential candidates for model refinement, which were the constitutive equation, constraints, and loading conditions. After reviewing them carefully, improved inputs to address these candidate issues enabled improvements in the computational modeling of the LCD module.

Used in this manner, the IRT technique provides a step-by-step procedure to discover potential candidates for model refinement by revising an invalid computational model. The

Fig. 4 IRT for model refinement – the case study of the LCD module



purpose is to enhance the prediction accuracy of the computational model in a systematic manner, while minimizing the time and effort required for model refinement.

3.3 Invalidity sensitivity analysis

The IRT lists model refinement candidates related to possible invalidity causes. However, it is not practical to address all of the candidate issues due to limited resources (e.g., time and budget). Thus, the degree of significance of model refinement candidates needs to be evaluated. The most critical candidates should be addressed during the model refinement phase, whereas insignificant candidates can be ignored. In this section, to achieve this goal, we introduce a technique for invalidity sensitivity analysis based on the weighted decision matrix method, which quantitatively assesses the degree of importance of each potential candidate.

The decision matrix was originally developed to evaluate competing design concepts (Dieter and Schimidt 2009). We devised a modified decision matrix-based approach to select the most significant candidates for model refinement. Building a decision matrix starts with defining various criteria and determining their weight values. To achieve this, three methods can be used: direct assignment, an objective tree, or an analytic hierarchy process (AHP) (Forman and Gass 2001). In this study, the objective tree method is employed since it balances the objectivity and the computational cost. By building an objective tree in accordance with the hierarchy, a better decision can be made for assigning weight values since the comparisons are made at the same level in the hierarchy. Figure 5 presents an example of a hierarchical objective tree. Figure 5a depicts the tree hierarchy that defines the criteria in evaluating the impact of potential candidates for model refinement. At the first level, two criteria including performance improvement and additional cost incurrence were considered. In a similar manner, at the second level, four criteria were assigned. Figure 5b weighs the criteria in order of importance to determine the most significant candidates for the model refinement activity. At the first level, a larger weight (i.e., 0.7) was assigned to the performance criterion than that (i.e., 0.3) of the cost since the degree in the improvement of the model validity is the most critical. It should be noted that determining weight values for criteria is an inexact process, although the sum of weighting values should be one at each level. To reduce the arbitrariness further, the AHP can be considered with the expense of high computational costs. The weights for individual criteria are determined by multiplying the weights at each of the hierarchical levels. As an example, the weight for the computational cost is 0.28 (= $O_1 \times O_{12} \times O_{121}$). The second step, building of the decision matrix, is to assign scores for potential candidates. Scores are assigned based on what degree of improvement is achieved. They can be quantitatively determined using the leave-one-out method (Kocaguneli and Menzies 2013), expert evaluation (Li and Li 2009), or sensitivity analysis (Fu 2008). As the final step in building the decision matrix, the weighted sums of the scores of all candidates are calculated. The candidates having the highest weighted sum are considered for model refinement.

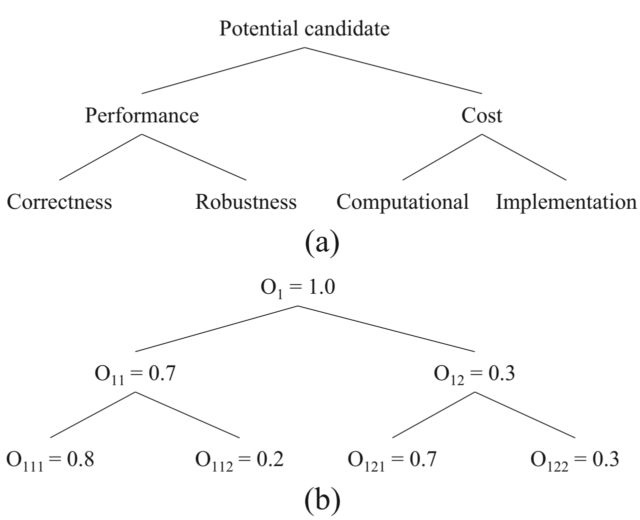


Fig. 5 An example of an objective tree for invalidity sensitivity analysis: **a** to define selection criteria for model refinement candidates and **b** with weight values

Table 2 presents an example of a decision matrix developed to select model refinement candidates for the computational model of LCD modules (our case study). The criteria and their weights from Fig. 5 were put into the first and second columns. When an invalid computational model is revised by incorporating each candidate, a corresponding score is assigned. For example, the score of Candidate 1 was assigned to "five" for "Correctness" because the validity check metric in model validation was significantly improved after updating the model. On the other hand, the score of Candidate 2 was assigned to "one" when a negligible change was found after updating the model. In this way, the ratings are calculated. The sum of the ratings for Candidate 1 is the highest, followed by Candidate 3. Considering the impact of potential candidates on the success in the validity check, final candidates are determined.

Upon completion of the model refinement process, the model is calibrated using the experimental data in the calibration domain, as shown in Fig. 1. The statistical model calibration determines unknown model variables in a computational model to maximize the agreement between the simulation and experimental results. A validity check is then conducted for the calibrated model. This check determines whether the calibrated model appropriately predicts the performance of the engineered product. If it is concluded that the calibrated model is valid, the model refinement procedures are terminated, and blind and recognized uncertainties are considered to have been identified and their impact is minimized. Otherwise, the model

Table 2 Weighted decision matrix to select model refinement candidates for the computational model of the LCD module

Criteria	Weight	Unit	Candidate 1: material model change			Candidate 2: contact condition change			Candidate 3: domain redefinition		
			Magnitude	Score*	Rating	Magnitude	Score*	Rating	Magnitude	Score*	Rating
Correctness	0.56	P-value	0.498	5	2.80	0.001	1	0.56	0.165	2	1.12
Robustness	0.14	Experience	Satisfactory	3	0.42	Satisfactory	3	0.42	Satisfactory	3	0.42
Computational cost	0.21	Hour	+10	2	0.42	0	5	1.05	0	5	1.05
Implementation cost	0.09	Hour	+3	2	0.18	+0.5	3	0.27	+0.5	3	0.27
Sum of rating				3.82			2.30			2.86	

* A five-point scale is used; excellent (5), good (4), satisfactory (3), tolerable (2), and inadequate (1)

refinement procedure must be revisited until a valid model is obtained.

4 Case study: refining a computational model for a smartphone LCD module

Fracture failure of smartphones is a primary concern of manufacturers as smartphones are designed to be larger and thinner to meet customer expectations. In the current competitive market, ensuring the reliability of a smartphone against glass fracture failure is of great importance. To accomplish this goal, the industry heavily relies on both virtual testing and physical testing.

Figure 6 shows the LCD module for smartphones, and includes depictions of: (a) the actual specimen, (b) a computational model, and (c) the multi-layer structure of the model. The LCD module consists of a chassis, mold, multilayer sheets, LED backlight unit, polarizers, and LCD panels. The LCD panels have a sandwich-like structure with liquid crystal filled between two glass plates. As presented in Fig. 6c, simulation engineers in the industry built a high-fidelity computational model that consists of 22 electronic components with careful consideration of contact conditions between individual layers. The number of nodes and elements of the computational model is 449,477 and 403,893, respectively. The degree of freedom is over 1.5 million.

During the development of a computational model for smartphones, the simulation engineers wanted to ensure the predictive capability of the computational model for the smartphone LCD module subjected to drop and shock loadings. Statistical model validation was adopted for this purpose. However, even after the model was calibrated, it turned out that the computational model failed to predict the experimental results under different loading conditions. This necessitated further improvement of the original model, as outlined in our case study. This section starts with the description of the problem we encountered and, subsequently, presents the use of the proposed model refinement approach to resolve the problem.

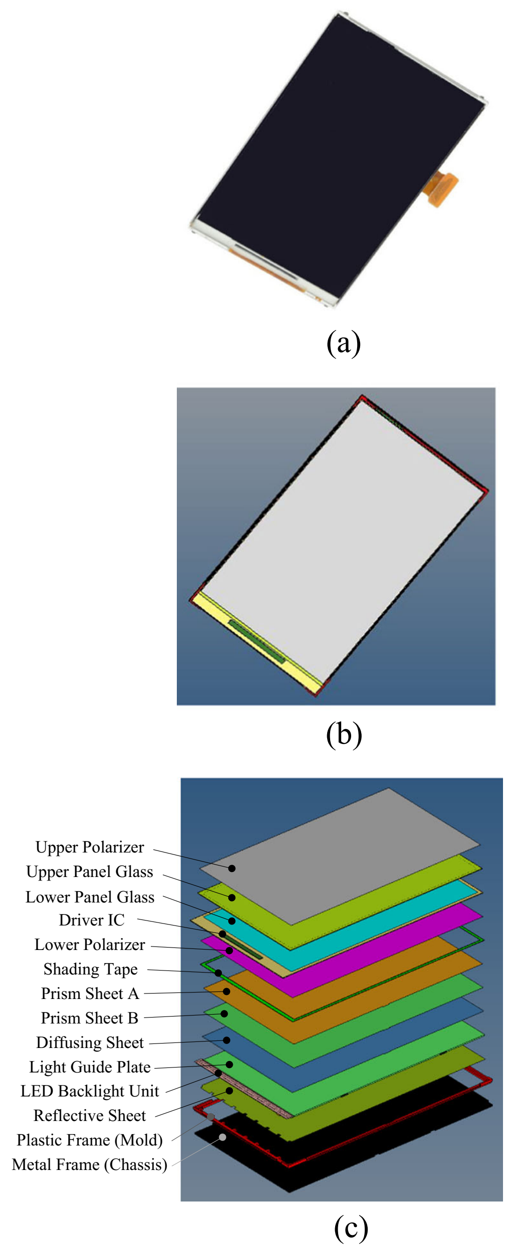


Fig. 6 Thin film transistor (TFT) – liquid crystal display (LCD) module: **a** actual specimen **b** computational model **c** multi-layer structure of the model

4.1 Problem description

An overview of the model validation activities for the smartphone LCD fracture problem is shown in Fig. 7. Model validation was planned by employing a top-down approach: (1) model decomposition planning, (2) statistical model calibration planning, and (3) experiment planning for model variable characterization. With close collaboration between experts from academia and industry, the smartphone system was broken down into with the hierarchy of the LCD module (i.e., subsystem) and the LCD panel (i.e., component). For computational modeling, as the model complexity increases, the uncertainty found in the computational model also inevitably increases. Through expert knowledge and sensitivity analysis, four variables (among many) were found to be unknown. At the component level, two unknown variables were identified: the Young's moduli of the glass (E_g) and the polarizer in the y-axis direction (E_{PY}). The cellphone manufacturer purchases the LCD panels from multiple first-tier suppliers. The suppliers examine the quality of the glass when they receive the glass from second-tier suppliers. However, the first-tier suppliers only check if the Young's modulus of the glass meets or exceeds the requirement. We were not able to receive the exact value of the Young's modulus of the glass from the first-tier suppliers. Therefore, we decided to put it as an unknown variable after discussing it with test and simulation engineers in the cellphone manufacturer. At the subsystem level, two unknown variables were identified: yield strength of the chassis (S_c) and its thickness (t).

A three-point bending test was suggested to emulate potential fracture modes of the LCD panel and the LCD module. The displacements in the three-point bending test were treated as the input, while the failure forces were considered to be the response. The tests with the alignments of Top-X and Top-Y were designed for model calibration, while the test with the alignment of Bottom-X was to check the validity.[1] The alignment of Bottom-Y was not considered because this is the most resistant to fracture. Three-point bending tests were conducted ten times in total for each alignment. A commercial software package, LS-DYNA 971, was used to find a solution of the computational model.

Validation planning was followed by validation execution, which was performed using a bottom-up approach. At the component level, the statistical distribution of the two unknown variables was assumed to follow a lognormal distribution since they cannot have a negative value. The model calibration determined the distribution parameters of the two unknown variables: E_g ~ lognormal (72.13, 2.86) and

[1] The "Top" (or "Bottom") indicates that the driver IC in the LCD panel or the LCD module faces upwards (or downwards). The "X" (or "Y") implies that the LCD panel or the LCD module is aligned to the x- (or y-) direction of the jig.

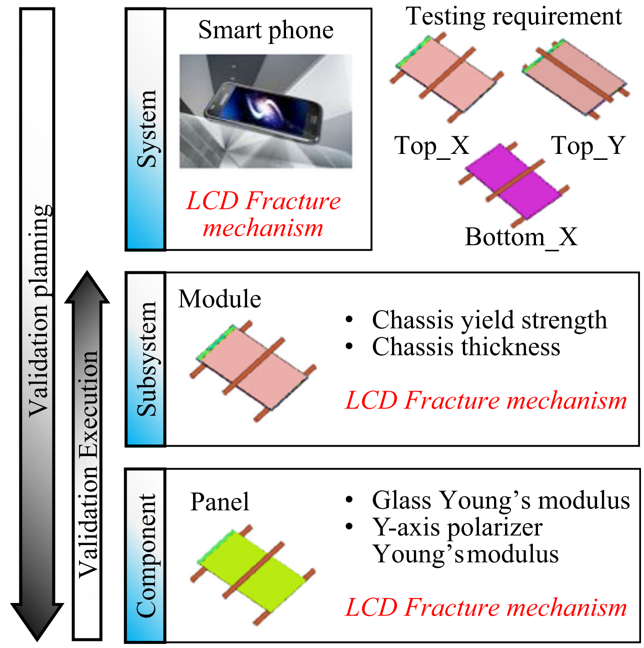


Fig. 7 Overview of model validation activities for the LCD fracture problem

E_{PY}~lognormal (3.40, 1.29). As shown in Fig. 8a, b, a good agreement was observed between the results from the simulation and experiments in the calibration domain. In the validation domain, a good agreement was observed from visual inspection. To quantify the degree of the agreement, the area metric was employed (Ferson et al. 2008). Physically, the area metric measures the mismatch between two curves, i.e., cumulative distribution function of computational responses and empirical distribution function of experimental data. When epistemic uncertainty due to insufficient experimental data is incorporated in the original concept of the area metric, a modified area metrics is defined:

$$D = \int_{-\infty}^{+\infty} |G(x) - u_i| dx \tag{5}$$

where G (x) is the CDF of a uniform distribution; u_i is the transformation of every datum x_i into the CDF of responses from a computational model ($u_i = F$ (x_i)). The modified area metric can be useful in validity check. If a value of the metric (D) is smaller than a threshold ($D_{m,\alpha}$; m is the size of experimental data; α is the significance level), a computational model is determined to be valid. Otherwise, invalid. For more details about how to calculate the threshold, see the study by Jung et al. (2015). As shown in Fig. 9, the area metric of 0.0732 was smaller than the threshold (0.1805 with the number of experimental data of 10 and the significance level of 0.05). Therefore, it was concluded that the calibrated model at the component level was valid.

At the subsystem level, other unknown variables (i.e., chassis yield strength and chassis thickness) in the LCD module

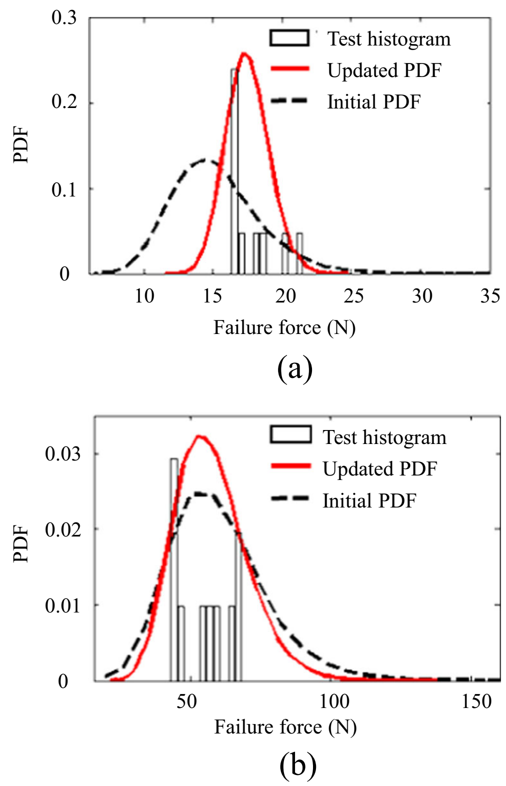


Fig. 8 At the component level, the responses of the initial and updated models are compared. Results are shown from the three-point bending test **a** with the alignment of Top-X; **b** with the alignment of Top-Y

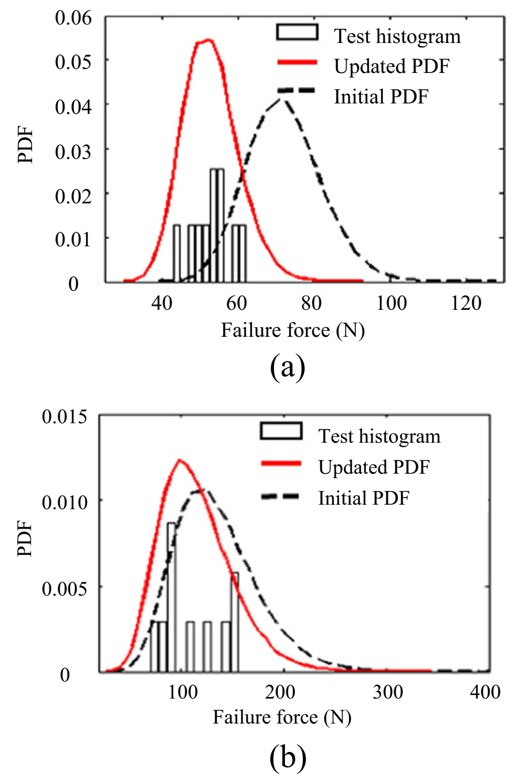


Fig. 10 At the subsystem level, the responses of the initial and updated models are compared to the results from the three-point bending test **a** with the alignment of Top-X; **b** with the alignment of Top-Y

were calibrated. The statistical distributions of S_c and t were assumed to follow lognormal and normal distributions. The initial values used for the unknown variables were: S_c~lognormal (6.617, 0.0772) and $t \sim N$ (0.2, 0.0156). The variables calibrated at the component level (E_g and E_{PY}) were incorporated in the model as the known variables. After model calibration, the simulation response had a good agreement with the experimental results, as shown in Fig. 10. However, in the validation domain, it was found that the computational model failed to predict the actual failure force measured by experiments (see Fig. 11). In Fig. 12, the value of the modified area metric was 0.4705, whereas the threshold was 0.1805 for the sample size of 10 and the significance level of 0.05. The P-value that corresponds to the metric value of 0.4705 was 0.001, which is almost negligible. Therefore, the small P-value indicated that the model was invalid, even after model calibration. From the quantitative result of the modified area metric – as well as the qualitative result of the visual inspection of the PDF and the histogram – it was concluded that the calibrated model was invalid in the validation domain. In light of the above observations, the model warranted refinement so that the computational model could be used to predict the fracture failure of the LCD module in real applications.

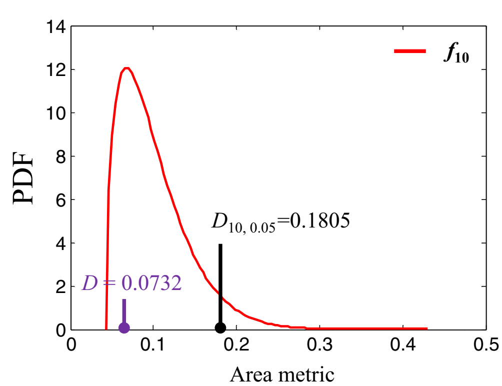


Fig. 9 The validity check shows the calibrated model is valid ($D < D_{10,\,0.05}$)

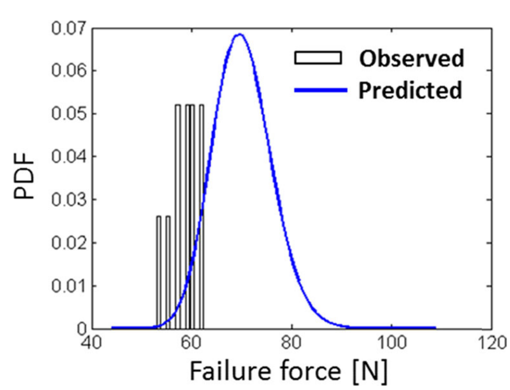


Fig. 11 Comparison of the PDF from the calibrated model with experimental results in the validation domain for the LCD module

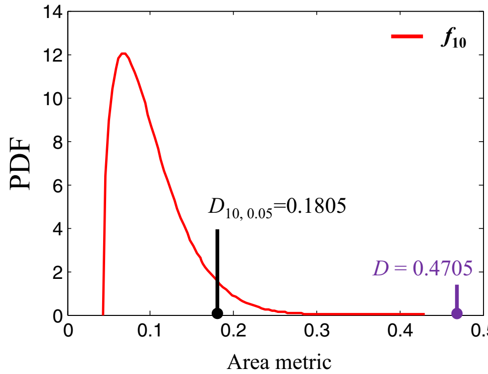


Fig. 12 The validity check shows the calibrated model is invalid ($D > D_{10,\,0.05}$)

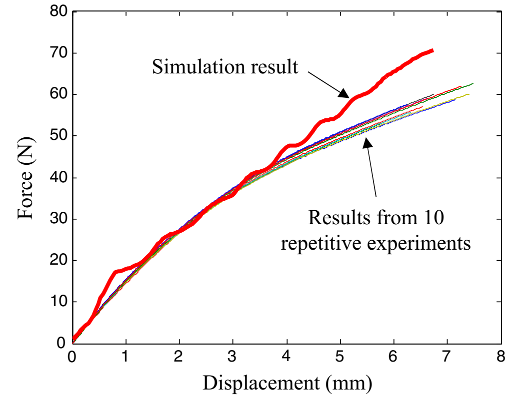


Fig. 13 Force-displacement curve obtained from three-point bending tests and its simulation

4.2 Model refinement: model invalidity analysis

The goal of the proposed model refinement approach was to find and remove blind and recognized uncertainties in the invalid computational model and, ultimately, to maximize the model's predictive capability in the design domain. As discussed in Section 3, the model refinement approach consists of three main components: MIA, IRT, and ISA. MIA is designed to identify possible causes that lead to failure of the validity check.

In this case study, multiple possible causes were suggested by simulation engineers from the CAE (Computer-Aided Engineering) team, test engineers from the Q&A (Quality & Assurance) team, experts from academia, and Ph.D.-level students. The ideas proposed from the brainstorming included: (1) invalid modeling of material behavior, (2) inappropriate boundary conditions between the LCD chassis and the LCD panel, (3) careless selection of loading conditions for model calibration and validation, (4) wrong thickness values for individual layers, and (5) insufficient details for modeling the LED lights.

First, the use of a linear model for plastic materials was suspected to be a dominant cause. As mentioned in Section 3.1, the background information of the computational model was revisited in the brainstorming: comparison of simulation and experimental results. As shown in Fig. 13, the computational model produced a curve that does not emulate the actual force-displacement curve from the experiments. After passing the point around the displacement of 3.5 mm, they do not follow a similar trajectory any more. The gap between the two curves becomes large as the displacement increases. This gave a clue that the LCD module in the computational model was not properly modeled and that blind uncertainty may be affecting the modeling of the physical behavior of materials.

Second, it was speculated that the tied contact condition utilized improper constraints between the LCD chassis and the LCD panel. We attempted to find any "known limitations of the existing simulation model," as specified in Section 3.1. It was well known that the LCD panel and other components were assembled through various bonding technologies, such as ultraviolet (UV)-curable resin and optical-clear-adhesive (OCA) tape. Nevertheless, the bonding strength of the bonds has large uncertainty. The spatial distribution of actual bonding strength cannot be modeled accurately, while the tied contact where the six degrees of freedom are constrained is widely accepted in computational modeling. Insufficient constraints can make the computational model of the LCD module behave differently from reality in the three-point bending tests. Therefore, it was suggested that another blind uncertainty was the insufficient constraints related to tying the plates in the LCD panel.

Third, it was proposed that the load path of the LCD module in the three-point bending test was not considered properly. We focused on the guidance in Section 3.1: "critical factors in designing, modeling, and testing." Suppose that three-point bending tests of LCD modules were conducted along the alignment Top-X, Top-Y, and Bottom-X. As shown in Fig. 14, the load path observed from the tests with the Top-X and Top-Y alignments is different from that with the Bottom-X alignment. With the Top-X and Top-Y alignment, the mechanical load is directly applied to the glass layer and transferred to the other parts due to the different stiffness of the layer materials of the LCD module. For example, the glass in the LCD panel is stiff, whereas the chassis is complaint. Due to this reason, with the Bottom-X alignment, a computational model calibrated with the Top X and Top Y alignments was invalid since the effect of different load paths was not reflected in the calibration of the computational model. Consequently, the simulation results may have exhibited an incorrect magnitude of stress on the failure site. Therefore, it was suspected that the blind uncertainty of unrecognizing the different load path in experiments was neglected in the computational modeling.

Through the group discussion in building the affinity diagram, two ideas were determined to be irrelevant. The final outcome of the MIA, i.e., the affinity diagram, is shown in Fig. 15.

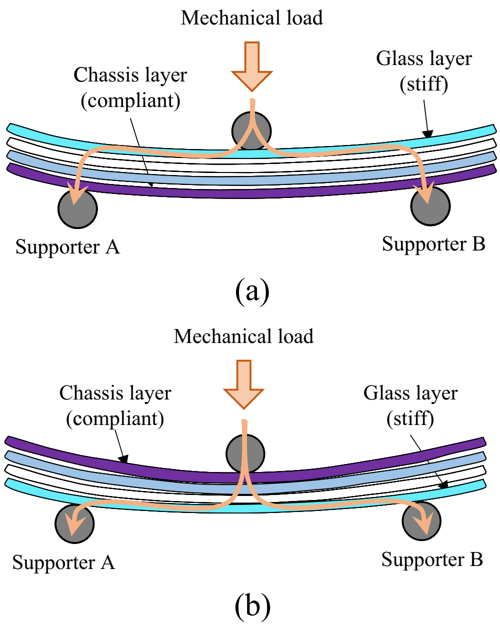


Fig. 14 LCD panel for the three-point bending test: **a** load path when testing with the alignment Top-X and **b** load path when testing with the alignment Bottom-X

4.3 Model refinement: development of the invalidity reasoning tree

The IRT is used to identify what should be corrected in a computational model to remove blind and recognized uncertainty. In the previous section, three possible causes (Ideas 1, 2, and 3) of blind uncertainty were identified. As shown in Fig. 4, the three ideas were sequentially revisited during the stages of conceptual, mathematical, and computational modeling. During the stage of conceptual modeling, first, material behavior specifications in the LCD module were revisited, followed by the reconsideration of the constraint and loading condition specifications.

To correct potential blind uncertainty at the stage of mathematical modeling, the specifications were updated. First, the material behavior was updated by substituting an elastic–plastic model (i.e., stepwise linear curve fit) for the elastic model (i.e., linear curve fit) in the selected materials of the module. These materials are polycarbonate (PC), polymethyl methacrylate (PMMA), and polyesters (PET). Their material properties are very sensitive to environmental temperature. The strain–stress curves of these materials can be approximated to be linear at low temperature such as 4 °C whereas they tend to have more plasticity at room temperature, such as 27 °C (Callister 2003). The details are shown in Fig. 16. The yield strengths of PC, PMMA, and PET are 40.5, 42.6, and 55.0 MPa, respectively. Their tangent moduli are 64.6, 74.4, and 60.0 MPa, respectively. The use of the elasticity-plasticity model was valid in this study since the experimental work was conducted under laboratory conditions.

Second, the number of tied contacts between the LCD chassis and the LCD panel was increased. The LCD panel is mounted on the LCD chassis with epoxy adhesive. Additional tied contacts were modeled to the bonding area between the chassis and the panel in such a way that the six degrees of the freedom of the bonding area were constrained.

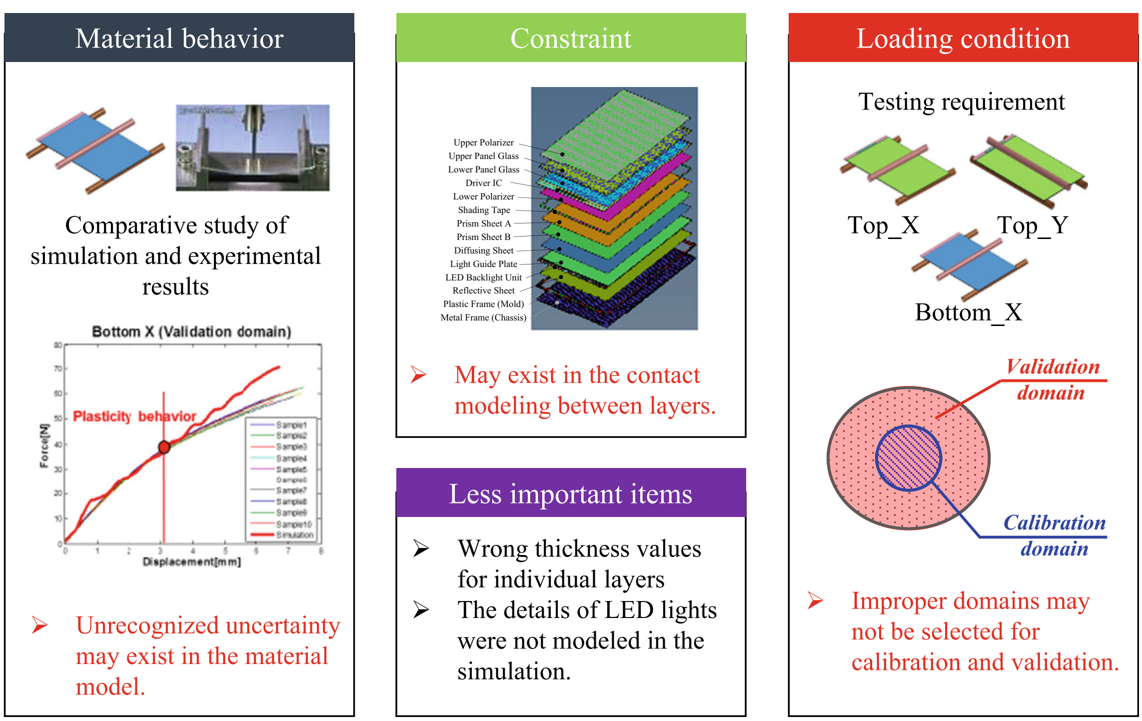


Fig. 15 Affinity diagram from brainstorming that defines possible invalidity causes

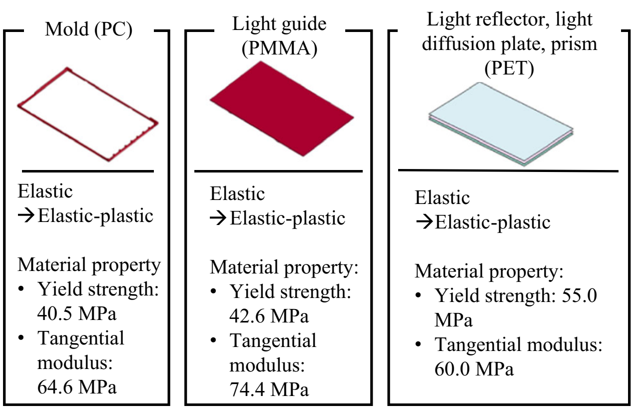


Fig. 16 Comparison of sensitivity for three candidate materials in the revision of material modeling

Last, the domains for model calibration and model validation were redefined. The Top-X and Bottom-X alignments were selected for model calibration, whereas the Top-Y alignment was selected for model validation. This change was expected to reflect the actual load path in the computational model.

The checklist at the stage of computational modeling shown in Fig. 3 was verified, including: (1) spatial discretization of the elasticity-plasticity model, (2) boundary condition discretization of the tied contacts, (3) loading condition discretization. After building the IRT, the three potential candidates were prepared with specific instructions for model refinement.

4.4 Model refinement: invalidity sensitivity analysis

The potential candidates for model refinement were selected as: material model change, constraint change, and loading condition redefinition. As presented in Table 2, an ISA with the three candidates was conducted to examine the impact of the identified candidates. As described in Section 3.3, the weights are determined by the objective tree method (also see Fig. 5). The score for each criterion was determined by a five-point scale for the magnitude of the unit. For example, the validity of the model was improved from 0.001 to 0.498 in terms of P-value after model refinement with Candidate 1, whereas no improvement was found with the employment of Candidate 2. Therefore, the score for Candidate 1 for the "correctness" criterion was assigned to be 5 ("excellent"), whereas that for Candidate 2 was 1 ("inadequate"). It is worth noting that Candidate 1 is related to the change of material models for the three materials. Through detailed investigation, the yield strength of the PC and PMMA were shown to have significant impact on the variability of the output response, while that of the PET does not, as shown in Table 3. Therefore, it was confirmed that the change of the material models from the elastic to the elastic–plastic is relevant for PC and PMMA. As another example, incorporating Candidate 1 incurred additional 10 hours of "computational time" since the use of the elastic–plastic material model in the refined model required longer computational time. The addition of 10 hours was evaluated to be tolerable whose score was 2 ("tolerable"). Implementing additional tie contacts (Candidate 2) and changing the domain (Candidate 3) did not add any computational time. Therefore, the scores were assigned to be 5. It was identified that Candidate 1 has the most significant impact for improving model validity, followed by Candidate 3 and then Candidate 2. The sum of the rating for Candidate 2 is below those of Candidates 1 and 3. Therefore, we determined to incorporate only the two relevant candidates (1 and 3) for model refinement.

The computational model was refined using the information from MIA, IRT, and ISA. As discussed in Section 4.1, at the component level, the two unknown variables (i.e., Young's moduli of the glass and polarizer in the y-axis direction) already calibrated and validated. Then, at the subsystem level, model calibration was executed to adjust the variability of another two unknown variables (i.e., yield strength of the chassis and its thickness). A good agreement between simulation responses and experimental results was observed in the calibration domain, as shown in Fig. 17. The optimal values of the unknown variables were determined to be $S_c \sim$lognormal (5.415, 0.0547) and $t \sim N$ (0.2, 0.00244). In the validation domain, the PDF predicted by the refined model showed a good agreement with the experimental results. Subsequently, a validity check was performed to determine whether the model was valid. As shown in Fig. 18, the area metric (i.e., 0.0805) was smaller than the threshold (i.e., 0.1805) with the sample size of 10 and significance level of 5 %. The P-value for the area metric of 0.0805 is 0.612. When compared to the results in Fig. 12, the P-value that shows the validity of the model was improved from 0.1 % to 61.2 %. Therefore, it was concluded that the model is valid for future use. The response of the three-point bending test can be virtually assessed using the computational model, which helps ensure the reliability of the LCD panel against fracture failure.

Table 3 Invalidity sensitivity analysis for three candidate materials

Material (X_i)	Y (X_i); Newton	Y ($X_i+\Delta X_i$); Newton	ΔX_i; *MPa*	Sensitivity; [Y ($X_i+\Delta X_i$)-Y (X_i)]/ΔX_i
PC (X_1)	72.95	72.27	0.405	−1.679
PMMA (X_2)	72.95	72.36	0.426	1.385
PET (X_3)	72.95	72.95	0.505	0

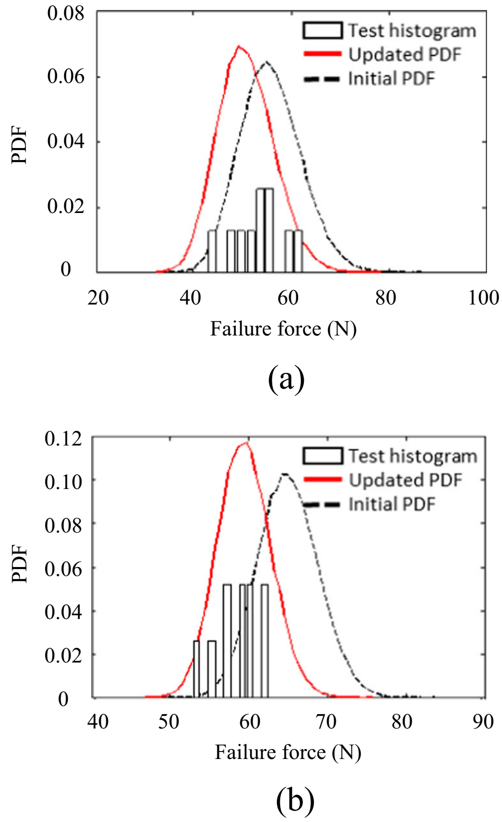


Fig. 17 PDF of calibration results of the refined module **a** with the alignment of Top-X; **b** with the alignment of Bottom-X

5 Conclusions

Several prior studies have proposed systematic approaches for efficiently conducting model calibration and validity checks. However, there has been little discussion to date about systematic methods of model refinement. This study proposed a systematic approach for finding and minimizing the impact of blind and recognized uncertainties in the development of a computational model for engineered products. The proposed approach consists of three main components. First, model invalidity analysis (MIA) is used to identify possible invalidity causes through building of an affinity diagram to determine areas of deficient knowledge that can be supplemented. Then, an invalidity reasoning tree (IRT) is used to identify potential candidates for model refinement in conjunction with the items in the affinity diagram. The IRT determines what specific changes have to be made in an invalid computational model to remove the uncertainties. Finally, invalidity sensitivity analysis (ISA) is used to quantify the effect of improving each potential candidate issue with the goal of removing the uncertainties. The ISA aims to determine the most significant candidates for model refinement.

The benefit of the proposed approach was demonstrated using a real-world problem in the electronics industry: virtual testing of smartphone LCD modules against fracture failure. Possible causes for the invalidity in the computational model were identified, including: incorrect material behavior modeling and invalid boundary condition selection. Through the model refinement process, it was shown that the refined model was appropriate to predict LCD fracture failure over different loading conditions. In the validity check, the validity (i.e., P-value) was significantly improved, moving from 0.1 % to 61.2 %. The impact of blind uncertainty on the computational model could be minimized by uncovering and handling them. We believe that the proposed approach can promote the development of a standard guideline for engineers to build more realistic models when the calibration approach for model verification and validation fails.

Future work is suggested to build a more accurate computational model of engineered products. In this study, the LCD module was broken down into a hierarchy of system, subsystem, and components for model calibration and validation. As the complexity of engineered products becomes greater, this strategy may not be the most effective. Series-decomposition, parallel-decomposition, or a combination of those decomposition strategies can be considered in future work. Another issue is how to uncover and remove blind uncertainty in experiments; this study considered only blind and recognized uncertainties in computational models. Current practice typically relies on personal experience, which delays rapid development of accurate computational models. A successful solution for those issues will enhance accurate prediction of engineered product performance in virtual testing.

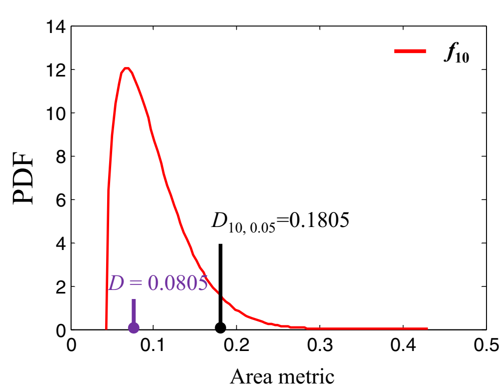


Fig. 18 The validity check shows the refined and calibrated model is valid ($U < D_{10,\,0.05}$)

Acknowledgments This work was partially supported by the Technology Innovation Program (10048305, Launching Plug-in Digital Analysis Framework for Modular system Design) of the Ministry of Trade, Industry & Energy (MI, Korea). This work was partially supported by Mid-career Researcher Program through the National Research Foundation of Korea (NRF) grant funded by the Ministry of Science ICT and Future Planning (MSIP) (2013R1A2A2A01068627).

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