Verification and Validation of ICME Methods and Models for Aerospace Applications

V&V Guidelines
and
Recommended Best Practice
Revision 1

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Preface

It is believed that broad development and implementation of Integrated Computational Materials Engineering (ICME) offers potential for significant benefits to all aspects of aerospace materials and processes engineering – in the form of greatly reduced time, cost and risk of technology development, validation, and sustainment. One major challenge that has been identified is that of verification and validation of ICME models and methods. While other engineering disciplines, such as computational solid mechanics, have addressed V&V in a systematic and rigorous manner, the materials engineering community is regarded less mature in this area.

The USAF organization AFRL-RX sponsored efforts beginning in 2010 to develop a set of verification and validation guidelines and a recommended best practice, suitable for use with ICME applications in aerospace. These efforts included a Technical Interchange Meeting (TIM) on this subject in February 2011, which was attended by more than 40 researchers and managers from government and industry. The TIM was preceded by considerable preparation effort. These efforts and the workshop culminated in documentation regarding relevant V&V practices by other disciplines, development of a proposed philosophy to align ICME V&V with established product and technology development processes, and a set of guidelines for specific V&V applications. The resulting guidelines and recommended best practice included several practitioner aides for implementation, including ICME model and system-level checklists, a Tool Maturity Level (TML) assessment approach, and a recommended process for assessing risk vs. consequences for specific ICME applications.

Since the “V&V Guidelines and Recommended Best Practice” was first published in June 2011, several programs sponsored by AFRL and DARPA-DSO have used them, in whole or in part. In addition, AFRL sponsored a Metals Affordability Initiative (MAI) program (MAI-GE-12) with the specific objective of applying V&V guidelines and uncertainty quantification methods to selected existing MAI programs having significant ICME content. Results of these efforts, and feedback from various practitioners, have been used to develop this revision to the initial V&V Guidelines and Recommended Best Practice for V&V of ICME Methods and Models for Aerospace Applications.

This document summarizes Revision 1 to the recommended approach and best practice for ICME V&V. The revision includes updates to the Systems-Level and Model checklists and guidelines, the ICME tool maturity level (TML) assessment guide, and the Best Practice flow chart and instructions. In addition, some improvements have been made to the hypothetical examples used for illustration. This effort was performed under USAF contract FA8650-06-2-5211, also known as the Metals Affordability Initiative program GE-12.

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Recommended Practice for Verification and Validation of ICME Methods and Models

1. Introduction: It is believed that broad development and implementation of Integrated Computational Materials Engineering (ICME) offers potential for significant benefits to all aspects of aerospace materials and processes engineering – in the form of greatly reduced time, cost and risk of development, validation, and sustainment. In early 2010, AFRL sponsored a "white paper" to assess the current state of ICME for aerospace applications, and to recommend actions to facilitate broader development and implementation [1]. The white paper recommended several topic areas for industrial focus, and a notional 5-year plan for sustaining and improving ICME efforts.

One of the key areas identified for future effort was verification and validation for ICME methods and models – including the need to develop guidelines and standards for this critical activity. The Air Force Research Labs, AFRL-RXLM, sponsored an assessment of V&V activities in 2010 and early 2011, with the objective of developing a recommended approach and practice for ICME V&V. This assessment included review of relevant V&V activities, the development of a proposed general approach and guiding philosophy, development of planning and execution checklists with instructions and examples, and development of a recommended approach for Tool Maturity Level assessment and application.

Initial drafts of these documents and approaches were distributed to selected organizations and individuals for review and comment; and in February 2011 a Technical Interchange Meeting (TIM) on this subject was held in Dayton, OH. This workshop brought together many representatives of government and industry, and provided the opportunity for community review and refinement of the initial documents. The approach, ICME V&V System-Level and Model Checklists, and Tool Maturity Level Assessment Guide were subsequently published in June 2011 [2, 3]. These were also summarized in a paper for Integrating Materials and Manufacturing Innovation (IMMI) in 2012 [4]. The IMMI journal paper includes links to access the original guidelines and associated spreadsheet tools [2, 3].

Since the "V&V Guidelines and Recommended Best Practice" was first published in June 2011, several programs sponsored by AFRL and DARPA-DSO have used them, in whole or in part. In addition, AFRL sponsored a Metals Affordability Initiative (MAI) program (MAI-GE-12) with the specific objective of applying V&V guidelines and uncertainty quantification methods to selected existing MAI programs having significant ICME content. Results of these efforts, and feedback from various practitioners, have been used to develop this revision to the initial V&V Guidelines and Recommended Best Practice for V&V of ICME Methods and Models for Aerospace Applications.

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2. Objectives and Scope:

The objectives of this document were to summarize the recommended approach and associated guidelines for verification and validation of ICME models and methods, specifically for aerospace applications, consistent with Revision 1 updates. The objectives included development and presentation of several tools intended to assist practitioners in planning, assessment, and execution of ICME V&V activities. These include an ICME V&V System-Level Checklist, an ICME Model V&V Checklist, a Tool Maturity Level Assessment Guide, and a recommended approach to address application risks and consequences. The overall objective was to provide guidelines and tools that would be useful and broadly applicable, without being overly prescriptive in nature, and to consolidate current versions of these documents and practitioner aides into a single source. This effort was focused on aerospace applications of structural materials and associated processes.

3. Approach:

The initial approach taken to develop this recommended practice followed three guiding tenets:

1. Utilize current, recognized practices for V&V as the basis
2. Facilitate alignment with established, gated practices for product and technology development.
3. Provide simple, useful guidance and tools to aid practitioners in planning and assessing V&V activities and results for ICME development.

3.1 V&V Background and Philosophy: An assessment was made of historical approaches to verification and validation. Efforts initiated in the 1980’s by the operations research community were refined and extended in later years, notably by The Defense Modeling and Simulation Office, IEEE, the American Nuclear Society, and the International Standards Organization [5]. V&V methodology for the mechanical engineering community remained largely *ad hoc* until the early1990’s. The AIAA then initiated a project entitled “Assessment of Accuracy of CFD Simulations,” in order to establish basic terminology and methodology for assessing the accuracy of CFD simulations. “Guidelines for the Verification and Validation of CFD Simulations” was issued in 1998.[5] Subsequent AIAA interaction with the ASME structural mechanics community led to initiation of a committee effort by ASME to generate what became the “ASME Guide for Verification and Validation in Computational Solid Mechanics.”[6]

It should be noted that development and attaining consensus agreement on this guideline document required extensive effort by a number of participants in ASME over a period of many years. The resultant document provides an excellent set of definitions and guidelines, and appears applicable to a broad range of computational disciplines and applications. It was determined that the ASME V&V Guide 10-2006 document provided an excellent reference and basis for guiding ICME V&V activities. The following pages are intended to briefly summarize background, key definitions, and critical concepts applicable to ICME V&V. It is, however, highly recommended that any practitioner engaged in ICME development, verification, or validation become familiar with the ASME V&V Guide 10-2006 in its entirety.

It is useful to begin with definitions of verification and validation [7]:

- Verification- the process of determining that a computational model accurately represents the underlying mathematical model and its solution –
    - Math issue: "Solving the equations right"
- Validation - the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model –
    - Physics issue: "Solving the right equations for the current problem"

The relationships and process sequences for verification and validation have been illustrated by Schlesinger [8] and were extracted from the AIAA V&V guidelines [6] as shown below in Figure 1.

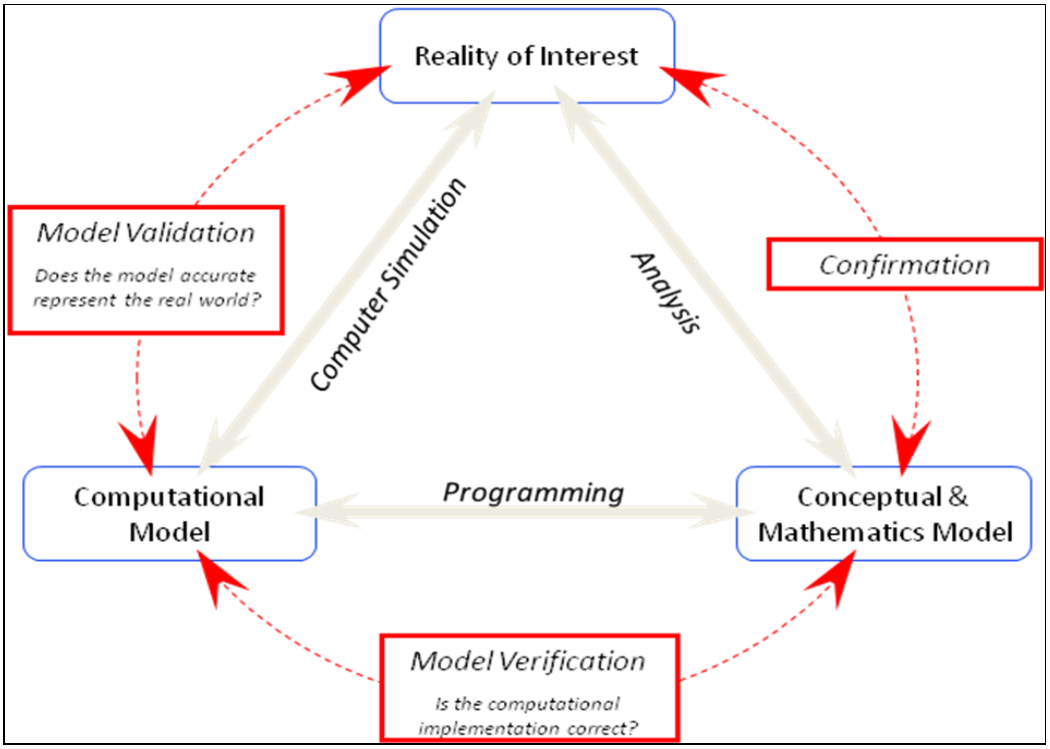


Figure 1: Verification and Validation Process - Level 1 Diagram [6,8]

It is important to note some key guidance from the ASME V&V Guide [6] at this point:

- Verification must precede validation
- The need for validation and the specific computational accuracy requirements depend on intended use, and should be considered as part of the V&V activities
- Validation of any complex system should be pursued hierarchically
- Simulation results and experimental data must be generated independently and have assessment of uncertainty to be meaningful.

These relationships and sequence are illustrated in Figure 2, below.

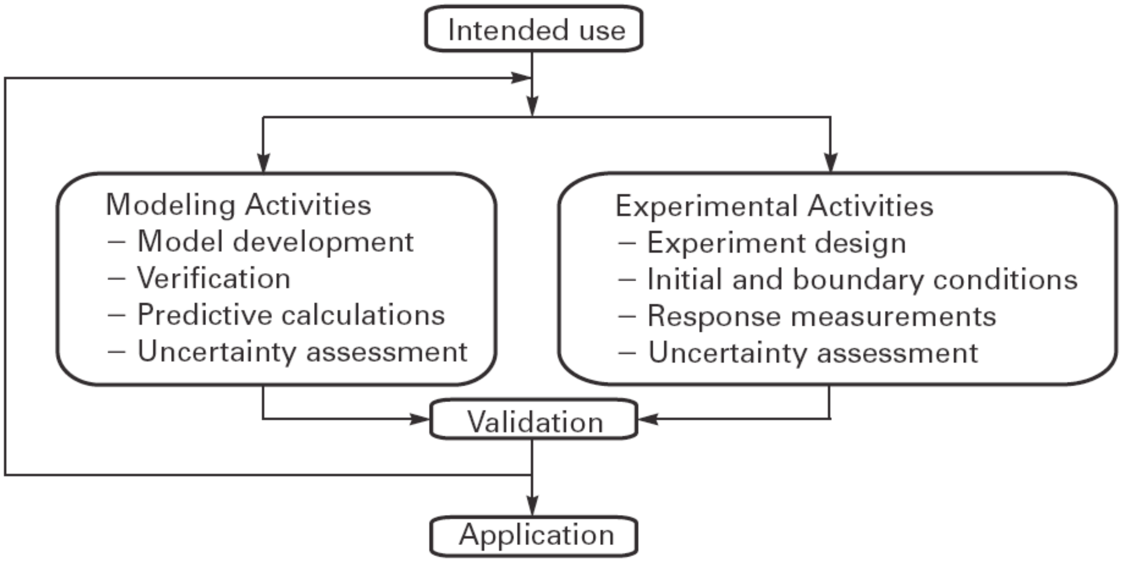


Figure 2: Elements and Sequence for Verification and Validation [6]

Verification can typically be separated into two parts: Code Verification, and Solution Verification. The first step here is clearly aimed at eliminating any mistakes in the source code, finding and removing errors or weakness in the numerical algorithms, and applying software quality assurance methods for best results. The Solution verification step focuses on assuring appropriate input and output data specification, and estimating numerical solution errors such as error due to finite element mesh resolution or time discretization.

Validation is concerned with three activities: model accuracy assessments by comparison to references, application of the model over the range of interest, especially for conditions where no reference data exist, and decisions regarding model accuracy for the intended use. Engineering and science disciplines generally require that any validation reference be based on experimental or measured data. This commonly results in the practice of "model calibration," which necessarily requires caution and judgment for future use and certainly any extension of the declared range of validation for any model.

Perhaps one of the most important concepts for application of V&V methods to ICME is that of “uncertainty quantification,” or UQ. This involves the quantitative assessment of the contribution of model inputs and internal parameters to overall uncertainty of model output, and affects how one assesses the level of agreement of a model relative to both input and output data, as well as the variation in model results. The assessment of uncertainty and propagation through a modeling system are illustrated in Figure 3, below.

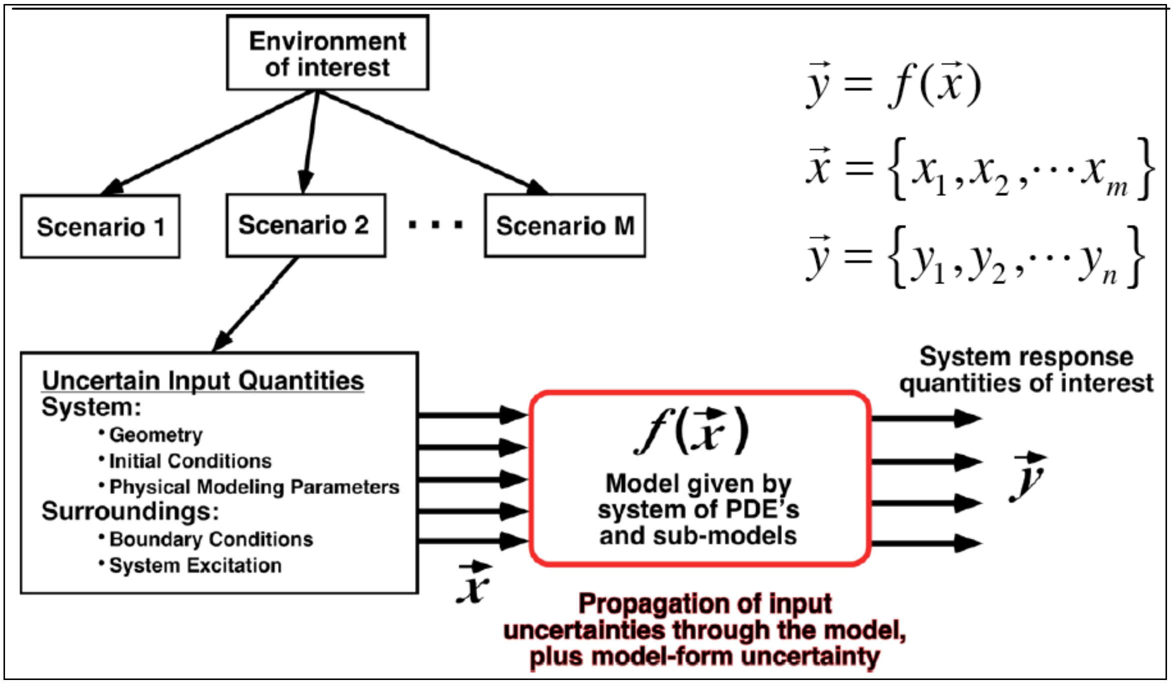


Figure 3: Sources and Propagation of Model Uncertainties [9]

These concepts – for model verification and validation, the relationship of analytical and experimental activities, and the assessment of uncertainty – can be combined and integrated in a Level 2 diagram for an overall Verification and Validation Process Flow Diagram, as shown in Figure 4.

The final concept that is summarized here is the requirement for a “bottoms up,” or hierarchical approach, to V&V. This is regarded especially critical for ICME applications, where many sub-models and/or many sequentially-dependent models may be involved. This necessitates verification and validation for each individual element or contributing sub-model of an overall system. Sole reliance on top-level validation may prohibit isolation of root cause if validation results are poor, or may result in false validation confidence if contributing sub-models can produce cancelling errors. This is especially considered to be a risk if “model calibration” is extensively relied upon. A Model Hierarchy example for the computational solid mechanics community is illustrated in Figure 5.

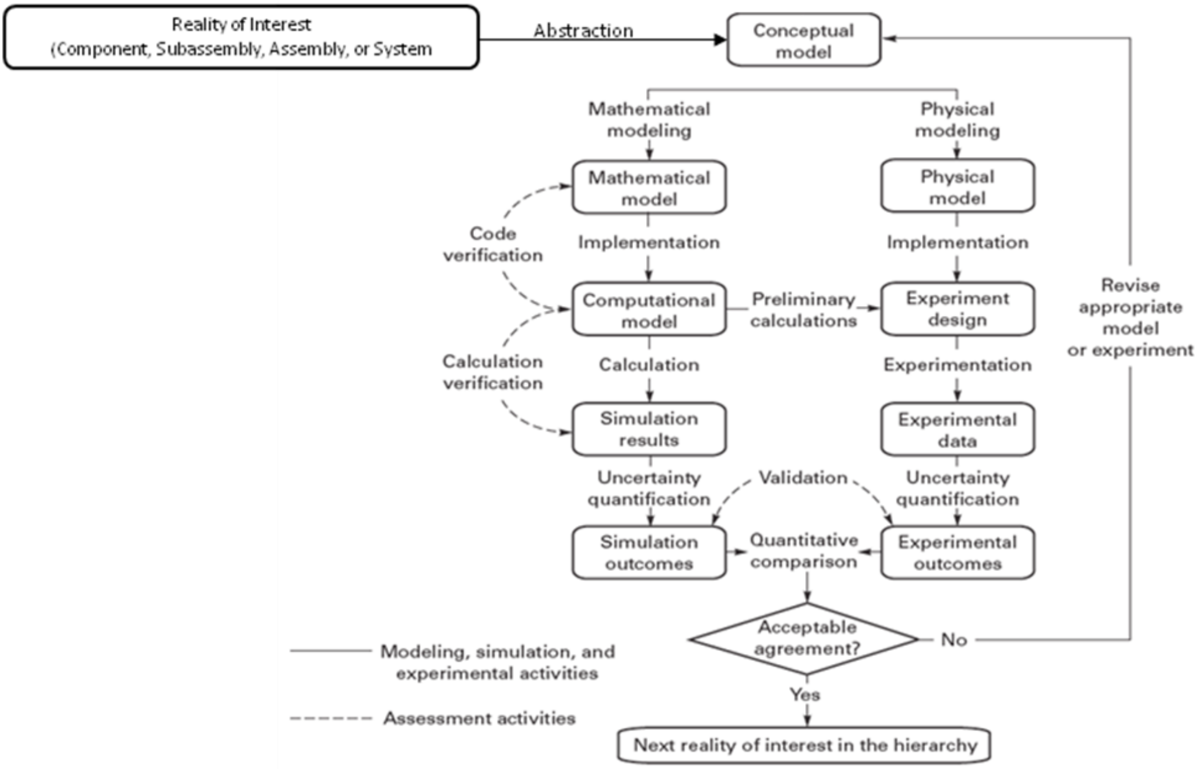


Figure 4: Overall Verification and Validation Process Flow Diagram [6]

There are, of course, many specific considerations for application of this general V&V framework to ICME. However, the fundamental concepts, definitions, guidelines, and cautions are directly relevant to ICME. It is strongly recommended that the ASME V&V Guide 10-2006 be used as the basic reference and set of guidelines for any ICME V&V activity.

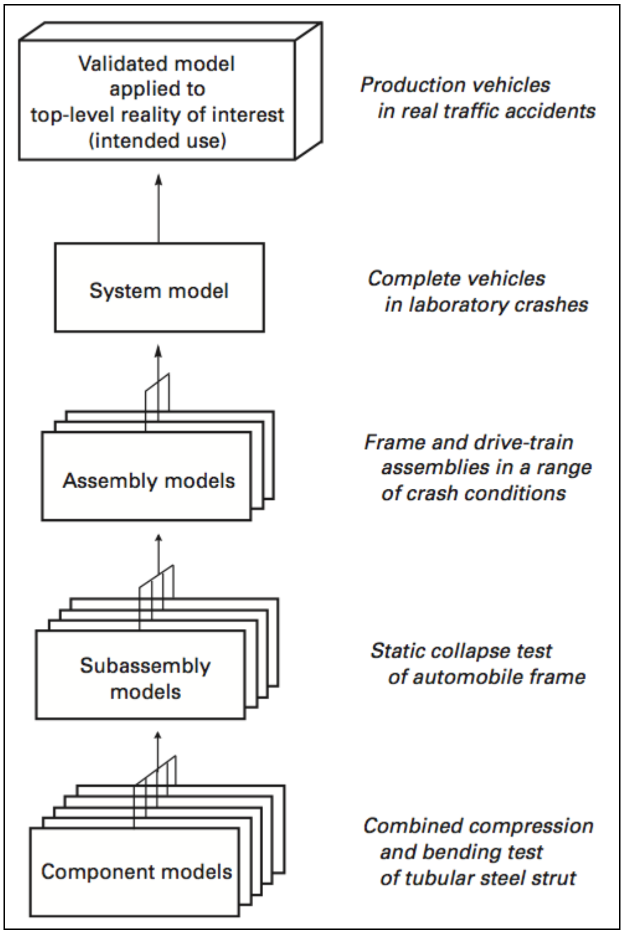


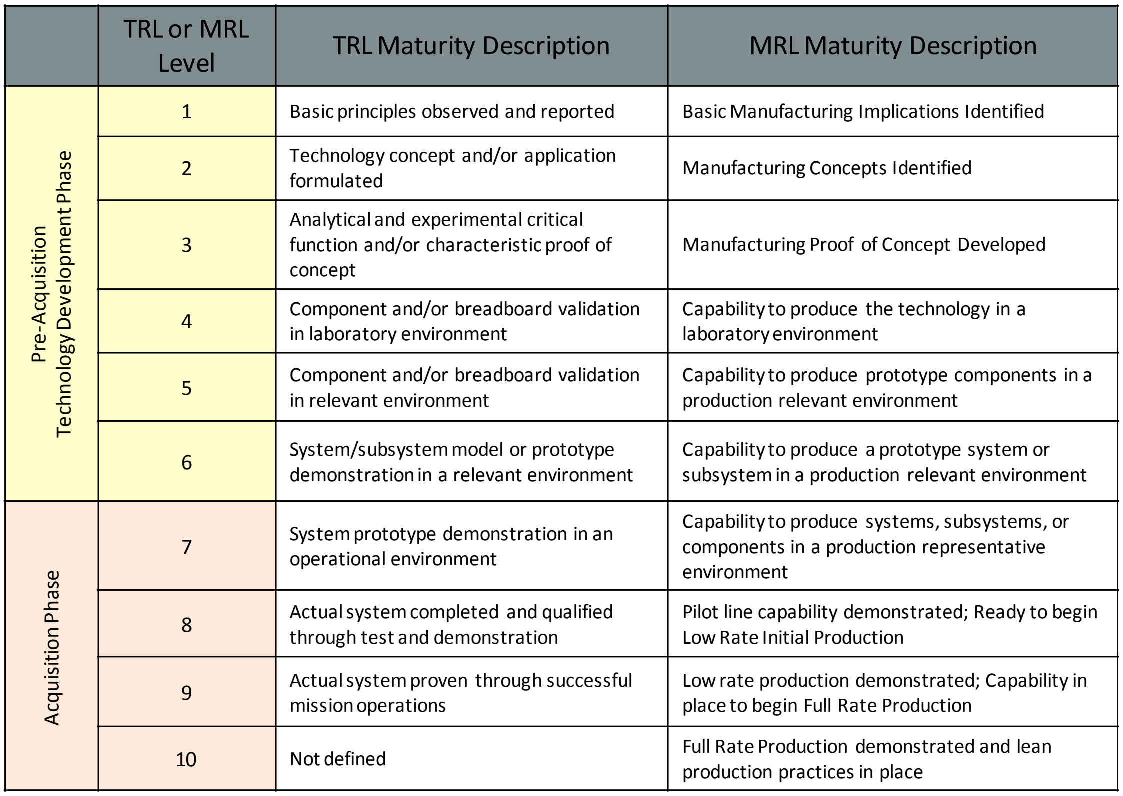
Figure 5: Model Hierarchy Illustration [6]

3.2 Alignment of ICME V&V with Product and Technology Development Processes: Successful, broad implementation of ICME in the future will span an enormous range of applications. ICME encompasses all areas of materials and process engineering, from early development of technology through product support in the field. The application of ICME may involve simple trending or guidance for development, or activities as complex and critical as life prediction in safety-critical systems. Consequences of using ICME for decision-making may be limited to the time and cost required to repeat a set of experiments, especially in the near term. Ideally, however, ICME will become a critical part of important business, product performance, or even safety decisions in future applications. This is certainly consistent with ICME investment goals. Consequently, any V&V guidelines must consider the intended (or permitted) use of such ICME models or methods, including the potential consequences of ICME-based decisions or predictions.

It was intended that the guiding philosophy proposed for ICME V&V align with established product development processes, such as Integrated Product Development (IPD), and technology development processes such as Technology Readiness Level (TRL) and Manufacturing Readiness Level (MRL) processes. These are all "gated processes" – meaning that there are rigorous criteria for assessing completion of a particular gate, and that progressive stages imply more substantial commitment and investment. These processes, or similar ones adopted internally by various companies or agencies, are broadly recognized and widely used. The level of maturity of a particular technology – for a specific application – is now readily communicated by simply stating its current “TRL status.”

The general philosophy was that ICME methods and models would benefit from a Tool Maturity Level (TML) assessment process, which could be used to guide development and application of ICME methods and models. If accepted and broadly used, as is the TRL process, a Tool Maturity Level could readily convey the state of maturity of a particular ICME model or method, and could offer objective guidance on where in the TRL or IPD process its use would be appropriate. TML criteria should be considered in light of the potential decisions or consequences of application. The following section gives a brief description of these gated processes, and summarizes the recommended approach for developing a TML assessment for ICME models and methods.

The Technology Readiness Level process – TRL – was derived from NASA efforts in the 1980’s. Later, corresponding gates and criteria were developed predominantly by the US Air Force (AFRL) for Manufacturing Readiness Level, or MRL. The gate levels and brief descriptions [10, 11] were extracted from the references and are shown side by side for comparison in Figure 6.



	TRL or MRL Level	TRL Maturity Description	MRL Maturity Description
Pre-Acquisition Technology Development Phase	1	Basic principles observed and reported	Basic Manufacturing Implications Identified
	2	Technology concept and/or application formulated	Manufacturing Concepts Identified
	3	Analytical and experimental critical function and/or characteristic proof of concept	Manufacturing Proof of Concept Developed
	4	Component and/or breadboard validation in laboratory environment	Capability to produce the technology in a laboratory environment
	5	Component and/or breadboard validation in relevant environment	Capability to produce prototype components in a production relevant environment
	6	System/subsystem model or prototype demonstration in a relevant environment	Capability to produce a prototype system or subsystem in a production relevant environment
Acquisition Phase	7	System prototype demonstration in an operational environment	Capability to produce systems, subsystems, or components in a production representative environment
	8	Actual system completed and qualified through test and demonstration	Pilot line capability demonstrated; Ready to begin Low Rate Initial Production
	9	Actual system proven through successful mission operations	Low rate production demonstrated; Capability in place to begin Full Rate Production
	10	Not defined	Full Rate Production demonstrated and lean production practices in place

SOURCES: Defense Acquisition Guidebook and DoD/MRL Manufacturing Readiness Level (MRL) Deskbook, ver 2.0, May 2011

Figure 6: TRL and MRL Gate Descriptions [10, 11]

The TRL process is widely used to assess many technologies today – including materials and process technologies. These assessments are used to make decisions on whether to proceed to the next gate – implying further investment – and whether to include a technology in a product development program. Consequently – attaining and demonstrating that critical gate criteria have been met is essential for progression of a technology. The relationship of the TRL process to a typical product development process – IPD for Integrated Product Deployment – is illustrated in Figure 7. Defense Acquisition Milestones A, B, and C, as defined by the US Department of Defense Instruction 5000.02, are shown for reference.

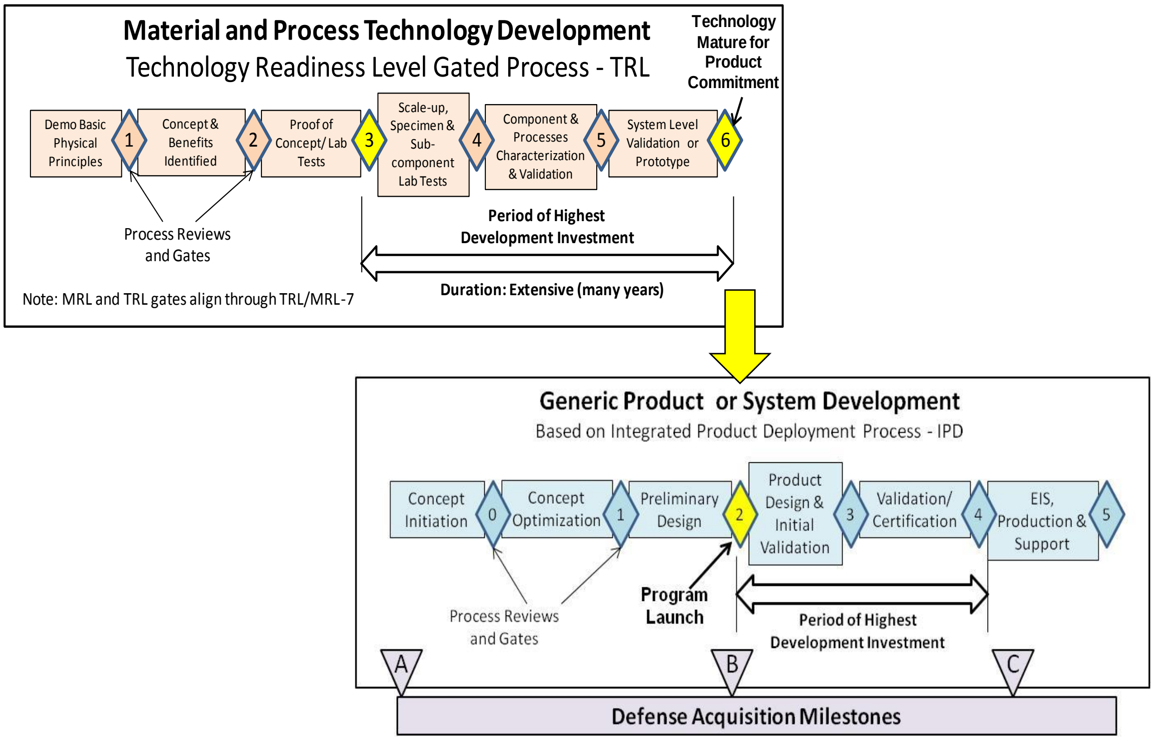


Figure 7: Alignment of the TRL and IPD Product Development Processes

Note that key gates are TRL-3, where significant investment is committed, and TRL-6 (also MRL-6), where the technology is considered mature enough to include in a specific application for a product development program. Typically the key related gate for product development is IPD Gate 2 (and DoD Acquisition System Milestone B) when the product "launch" is committed and detailed design begins. DoD Acquisition Guidelines require that TRL and MRL-6 gates have been achieved for technologies included in a system acquisition before initiating Milestone B. **However, in actual practice, less mature technologies are often included in development programs, with appropriate risk mitigation plans.** Late-stage changes or iterations to a critical technology, especially a materials or processing technology, may cause substantial cost, schedule, system architecture, or system performance impacts. It is obvious that as both TRL and

IPD processes progress, the potential consequences of decisions have increasingly greater impact.

ICME has potential application and benefit for all phases of technology and product development. It is necessary, then, to recognize that verification and validation requirements for ICME should be related to, and aligned with, these established processes for technology and product development.

The concept is useful for ICME V&V process development, and illustrates an approach to align ICME V&V with technology and product development requirements. What is needed here is the development of an ICME-specific Tool Maturity Level process, which would serve as a tool to guide ICME V&V efforts, to communicate ICME tool maturity level in a consistent manner, and to assist decisions on applications and risk of use.

The TML approach can be aligned with both technology and product development processes, as illustrated in Figures 8 and 9. It is presumed that the minimum required ICME tool maturity – and consequently the level and fidelity of verification and validation of a particular tool – would systematically increase as the region of ICME application progressed in the technology or product development process. This is not to say that "high TML" ICME tools are not needed or desired in early stages of technology or product development – but rather that the later stages require

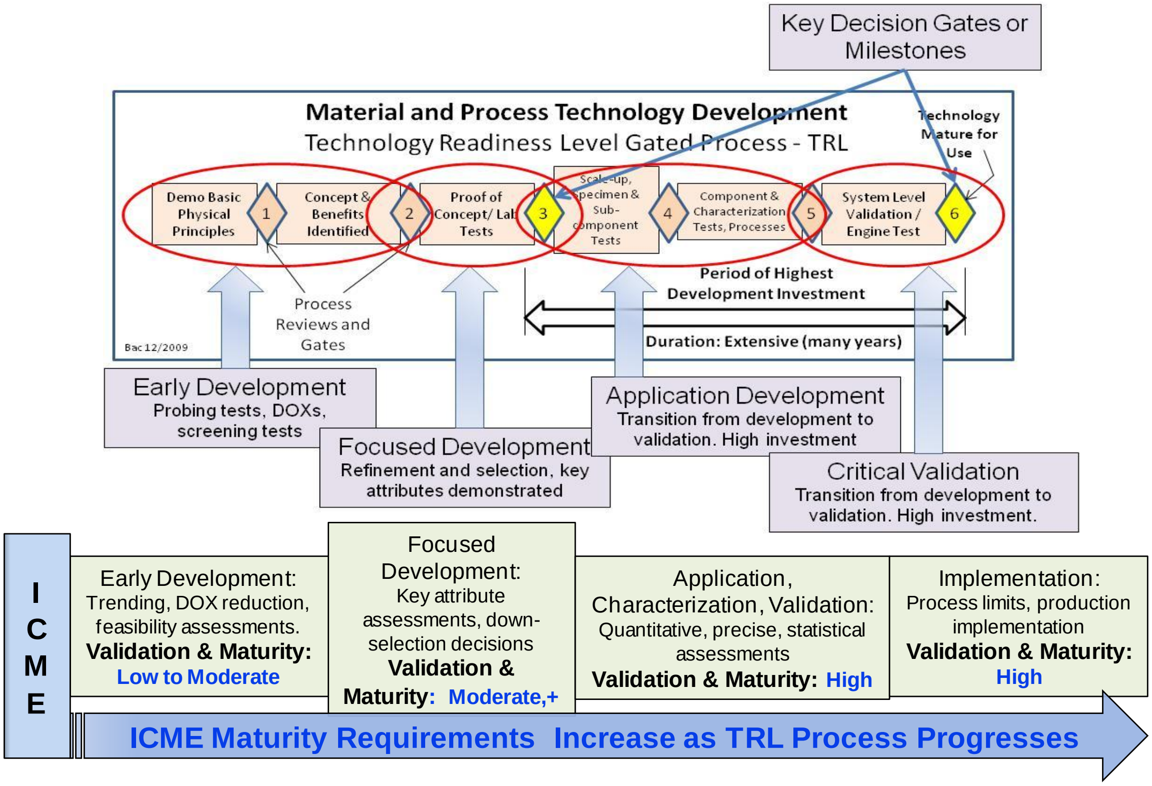


Figure 8: ICME Tool Maturity Level (TML) and the TRL Process

higher TML levels because the potential consequences of application generally become more severe.

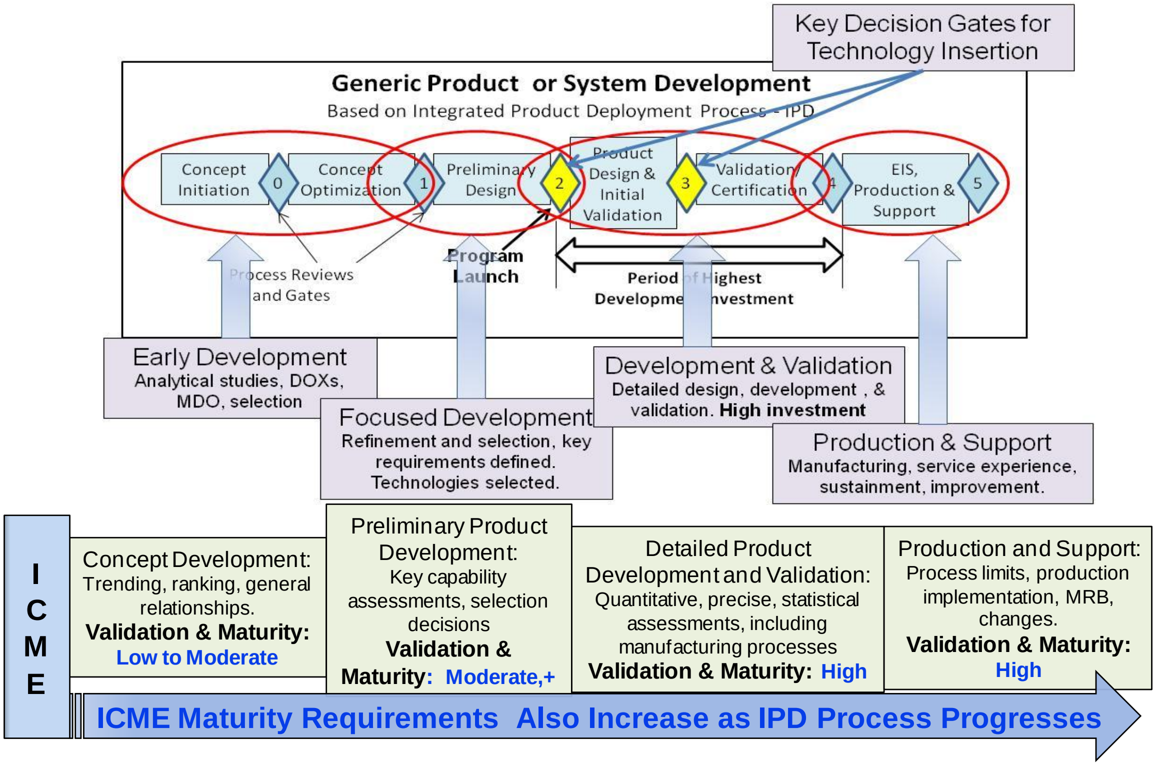
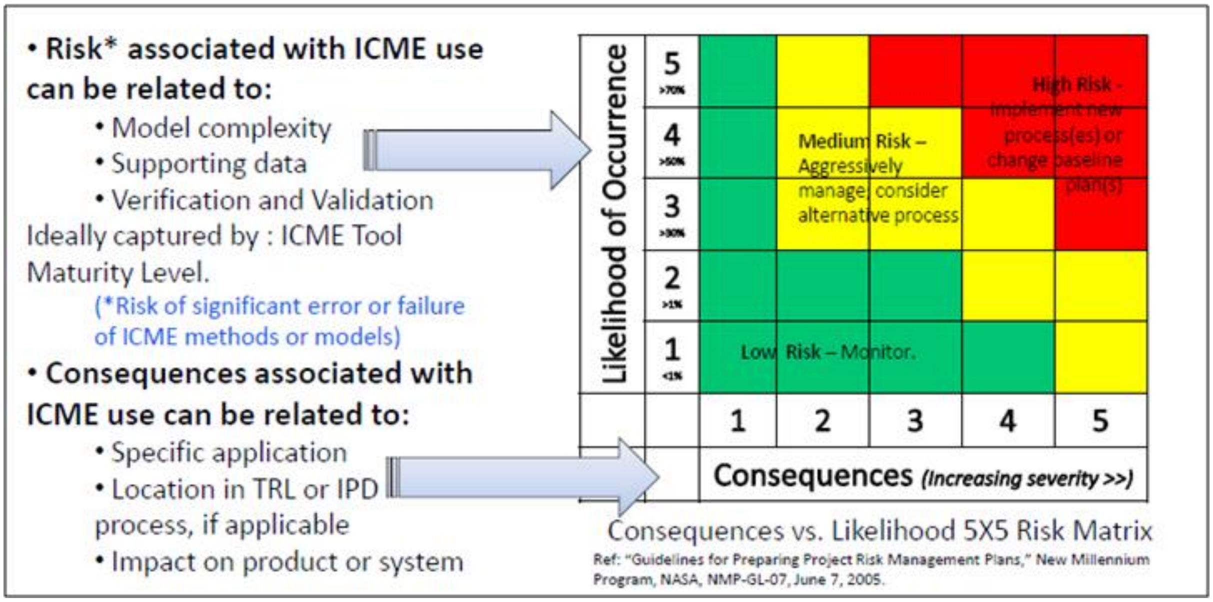


Figure 9: ICME Tool Maturity Level (TML) and the IPD Process

There is no standard, gated process in broad use for assessment and communication of the maturity level of an analytical model or tool – at least not in the same sense as the TRL process. One that was presented by Morris at the 8th International HCF Conference in 2003 [12], offers a useful starting point for ICME. This process defines five levels of maturity level for analytical tools, and was used as the basis for the ICME Tool Maturity Level assessment guide that was developed. It is discussed in detail in section 5.

Since there will likely be many specific ICME applications in the future, developing a prescriptive guideline regarding TML requirements is neither likely nor desirable. It is useful to consider a supplemental means of assessing “risk vs. consequences” of ICME application, and using the outcome to determine whether the V&V status of a specific ICME model is sufficient. An excellent example of a “Risk vs. Consequence” table was developed by NASA [13] and is reproduced below in Figure 10. The associated text boxes and arrows indicate how it relates to ICME model and V&V considerations, and where in the TRL or IPD processes a specific ICME tool might be applied.

Further explanation of this tool is also presented in Section 5 of this document: practitioners are encouraged to use it for ICME tool assessment. The thought process that is stimulated will lead to objective identification and assessment of various application risks and their potential consequences. This process will help identify where mitigation plans are needed, and help objectively assess their impact. Overall, it can be a very useful tool for ICME development and validation planning.



- **Risk* associated with ICME use can be related to:**
    - Model complexity
    - Supporting data
    - Verification and Validation

Ideally captured by : ICME Tool Maturity Level.

(*Risk of significant error or failure of ICME methods or models)

- **Consequences associated with ICME use can be related to:**
    - Specific application
    - Location in TRL or IPD process, if applicable
    - Impact on product or system

Likelihood of Occurrence						
	5 >70%	🟩	🟨	🟥	🟥	🟥
	4 >50%	🟩	🟨	🟨	🟥	🟥
	3 >30%	🟩	🟨	🟨	🟨	🟥
	2 >1%	🟩	🟩	🟩	🟨	🟨
	1 <1%	🟩	🟩	🟩	🟩	🟨
		1	2	3	4	5
		Consequences *(Increasing severity >>)*				

High Risk - implement new process(es) or change baseline plan(s)

Medium Risk – Aggressively manage; consider alternative process

Low Risk – Monitor.

Consequences vs. Likelihood 5X5 Risk Matrix

Ref: "Guidelines for Preparing Project Risk Management Plans," New Millennium Program, NASA, NMP-GL-07, June 7, 2005.

Figure 10: Alternative Risk Analysis Approach to Assess ICME Tool Maturity [13]

The final concept that was embodied in the approach for ICME V&V is that of *progressive validation*. This represents a slight extension of the ASME V&V Guide description of "bottoms up" or hierarchical validation. In addition to the absolute necessity for verification and validation at the building block level for computational models – meaning for individual elements or sub-models – it is likely that the level of validation will be progressive over time for ICME models and tools. This may be driven by practical restrictions regarding validation cases that can be executed, by improving or extending model capability or range of application, or by the development of benchmark validation cases. In any event, the ICME V&V approach must accommodate and facilitate progressive validation. The proposed approach to ensure the efficacy of a *progressive validation* environment for ICME involves the following four steps:

- Establish guidelines for V&V – recommending general standards, but not prescriptive. *(Based on System Level and Model checklists).*
- Establish standards for terminology, data, and model descriptions. *(Based on ASME V&V Guide 10-2006).*
- Establish a common maturity assessment approach *(Based on proposed TML for ICME).*
- Establish databases, or "libraries" – for data, models, and validation cases. *(Databases or at least data standards are considered essential).*

The philosophy and basis for the recommended approach to ICME V&V are relatively easy to describe – but somewhat more difficult to implement in a consistent and sustained manner. It was believed essential that some simple guidelines and tools be developed to facilitate early implementation and refinement of the V&V approach, in order to reach a consensus Best Practice that would be broadly recognized and used. The following sections (Sections 4 and 5) briefly describe these tools: namely the System and Model Level Checklists, and the Tool Maturity Level assessment process including a Risk vs. Consequences assessment.

3.3 Guidelines and Tools for ICME V&V: The preceding text consists of background, relevant historical information, and a guiding philosophy for future ICME V&V activities. These are necessary, of course. But, what is essential for successful launch of a serious, consistent, and sustainable ICME V&V effort are some simple tools for V&V planning and assessment that enable practitioners to get started on ICME V&V immediately. What was developed was a simple guideline, in flow-chart format, and a corresponding set of practitioner aides in Excel™ format. The most important tools for this were considered to be the ICME V&V System-level and Model-level Checklists, and a Tool Maturity Level (TML) assessment guide. It is believed that these tools will enable a consistent approach to ICME V&V, which can be initiated immediately. It is expected that these tools will be refined and improved significantly with time and experience. The simple guideline process concept is shown conceptually in Figure 11, below.

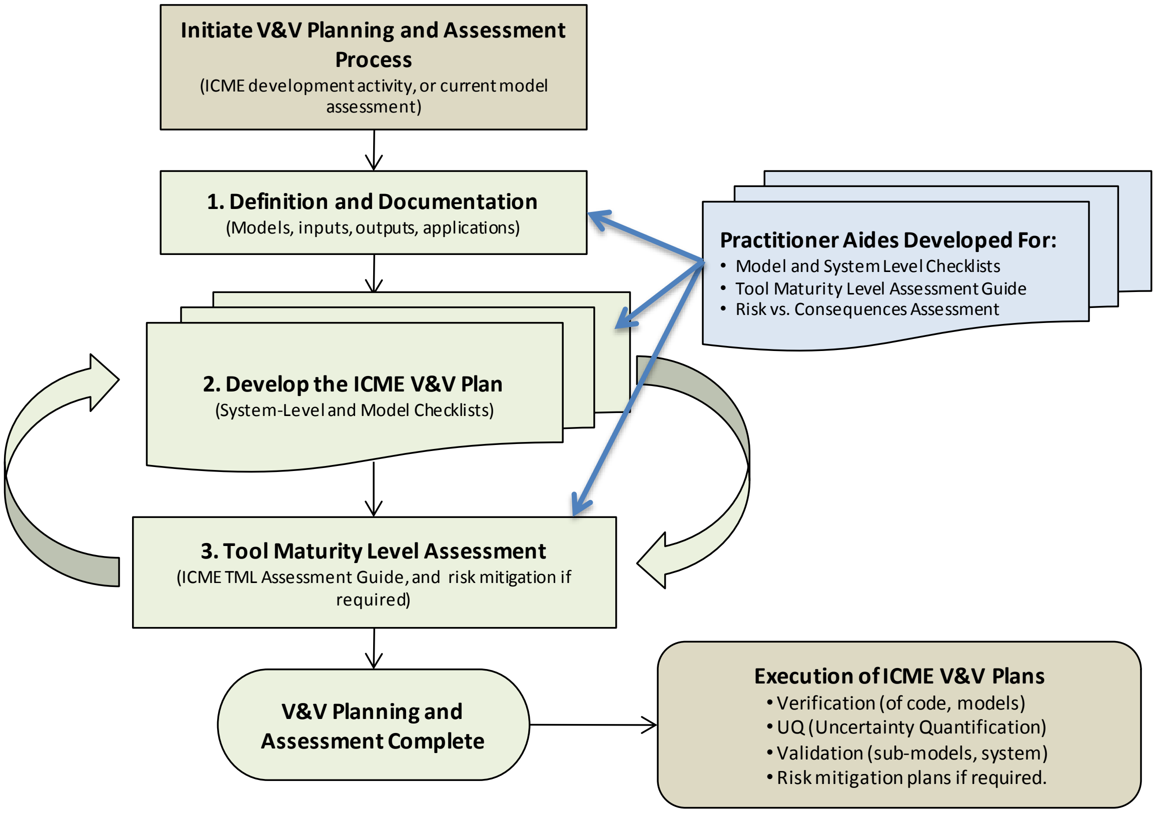


Figure 11: Simplified Flow Chart for ICME V&V Process

Descriptions of the practitioner aides – the checklists, tool maturity level assessment process, and risk – consequences assessment process, are described in detail in the following sections. The more detailed flow chart and description of the Recommended Best Practice are presented in Section 6.

4. ICME Verification and Validation Checklists:

4.1 Introductions and Background

The verification and validation (V&V) checklists are practitioner aides that can help ICME teams to plan and execute V&V activities as well as communicate V&V progress; they support implementation of the V&V guideline described in section [#]. Composing the checklists was motivated by the fact that some MAI ICME program participants are unfamiliar with V&V and associated methods. But even for those ICME teams, which have V&V savvy modelers, the checklists serve to coordinate activities between modelers and less V&V fluent experimentalists, as well as with technical managers and sponsors, who increasingly find confidence in organized, accepted development processes. Subsequent subsections provide a description of (1) V&V checklist precepts; (2) description of checklist items and their organization within the checklists; (3) user notes for V&V checklists; and finally the (4) the V&V checklists.

4.2 V&V Checklist precepts

These precepts provide the flexibility for ICME teams to adapt the V&V Checklists to their particular customer, specific ICME problem, the expertise of some Integrated Product Development Team (IPDT) members, and the ICME program budget and schedule. These precepts include the following:

(1) The ICME V&V checklists are NOT prescriptive. They are offered as a template that an ICME IPDT should/must modify to meet the specific needs of their team's mission and modeling system.

(2) The ICME team should initiate V&V planning during ICME program planning. Too often, the discrepancy between V&V costs and program resource allocation are not recognized early; and ultimately V&V is not carried out fully because allocated funding (if any) was insufficient.

(3) The ICME team should strive to identify early how the ICME program success can help their customers. The IPDT needs to know who their customers are, what their needs are; and how they measure success and determine acceptance, (i.e., accuracy and confidence/uncertainty).

(4) Most IPDT's include engineers from different disciplines with varying levels of expertise, experience, and interests; and some having managerial oversight. For those IPDT members with limited ICME and/or V&V experience, the V&V Checklists provide a consistent framework for understanding the V&V process within the ICME program.

4.3 Organization and content of the V&V Checklists

The V&V checklists were constructed to acknowledge the diversity of ICME program goals and modeling structures and adhere to guidance from the ASME V&V Guide 10-2006 [6].

Checklist Organization

ICME development programs have varying scope, include differing numbers of models, and adopt different approaches for model integration. Some programs may develop a single standalone materials model; some add or improve a small subset of models within an existing commercial code (e.g., DEFORM ™ or ProCAST™); while others develop and integrate a full suite of models within a commercial model integration environment, such as Isight™ or Model-Center™. Yet each of these ICME development scenarios, share a common need to assure that each new model has been verified and validated. Additionally, when ICME development involves an integrated suite of models, the program needs to validate the ICME system performance for any newly developed functionality.

The ASME V&V Guide [6] recommends that V&V activities adopt a hierarchical (tree-like) approach wherein models at the lowest level of the hierarchy are verified and validated first, followed by models at successively higher levels until finally the integrated modeling system is subject to validation. Experience has shown this approach to V&V facilitates identification of errant models when system level validation fails to achieve system validation requirements. It also provides superior uncertainty quantification (UQ) by enabling analysis of error/uncertainty propagation through the integrated model network.

Therefore, there are two ICME V&V Checklists, as shown in Figure 12: one listing activities relevant to the ICME system, and a second checklist form that individually addresses unverified/unvalidated models or sub-models within the ICME system. For example, level 1 models might simulate process, microstructure, and properties, whereas level 2 models might simulate thermodynamics or constitutive properties required by a higher-level model.

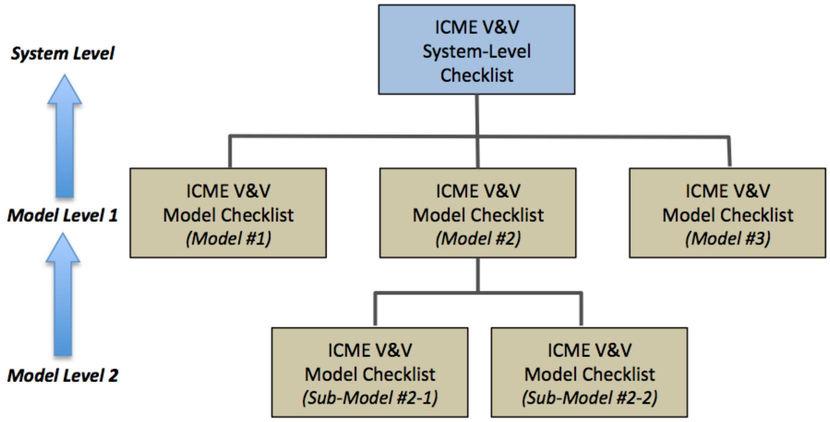


Figure 12: Hierarchical organization of V&V checklists for a hypothetical ICME project

V&V Process Flow

The ICME V&V recommended practice and checklists adhere to the ASME V&V Guide [6] as summarized in ASME's model V&V flow chart, reproduced in Figure 13. Understanding V&V process flow is important because it shows sequencing and interrelationships impossible to capture in a linear listing of checklist items. The process flow begins with the identification of the ICME reality of interest (e.g., precipitation of γ' in a superalloy or residual stress in a heat treated titanium forging). Following formulation of the conceptual model, V&V proceeds along two parallel paths for modeling development and experimental work, respectively. The modeling path includes verification to: (1) confirm that the algorithms of the computational model accurately describe the mathematical model (code verification) and (2) establish that model discretization and solver parameters (e.g., mesh size, and time increments) provide stable and numerically accurate results (calculation verification).

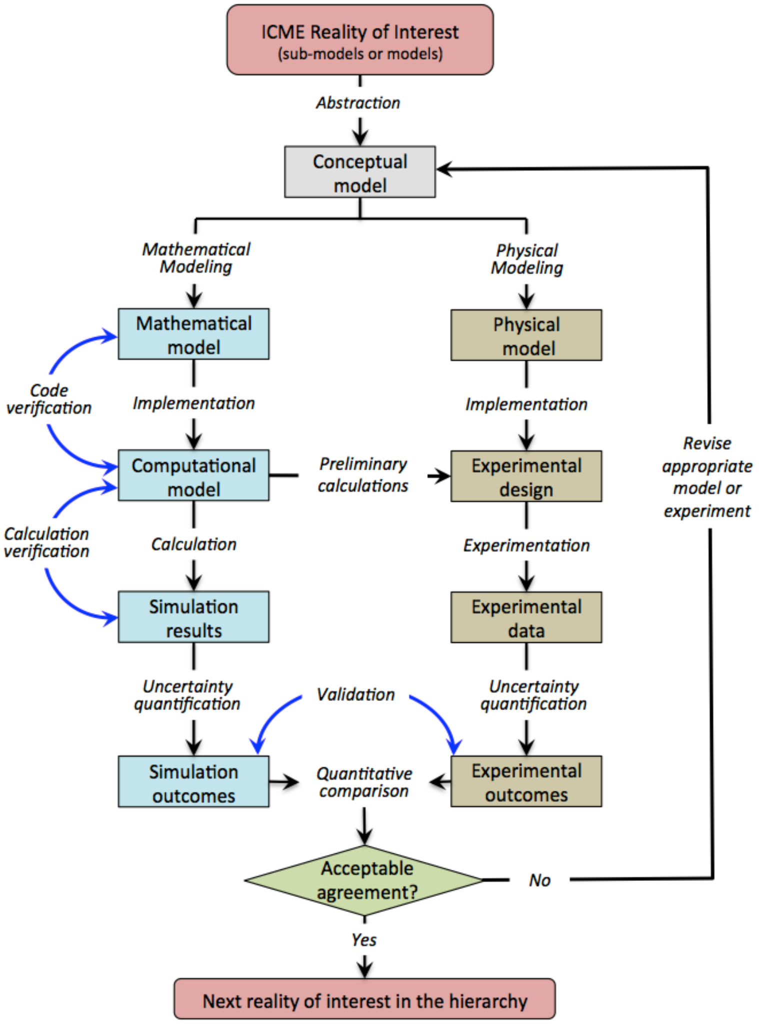


Figure 13: Flow chart describing the model V&V process, ASME V&V Guide [6]

The experimental pathway is easily understood. Following generation, simulation results and experimental data are independently analyzed using UQ and system analysis methods (e.g., DOE's, Monte Carlo analysis) to calculate errors, variation, sensitivities to input and internal parameter uncertainty, and model output uncertainty. The assessment of all simulation and experimental outcomes via UQ validation metrics constitutes model validation. If agreement is unacceptable, it is necessary to revise the model and/or experiment. Note that the model and experimental paths should be conducted independently except for the exchange of preliminary model calculations to aid experimental design and the validation comparison exercise.

ICME system level V&V also follows the ASME V&V process flow, with several modifications as shown in Figure 14, which was adapted from the ASME model V&V flow chart. Owing to the similarities of model and system level flow charts, discussion will focus only on the differences. The system level V&V process begins with the identification of customer needs, which include definition of ICME system output, system accuracy, uncertainty, and tool maturity level (TML) requirements, and quantification of payoff to the customer. The first experimental step involves selecting the component design and materials process that will serve as the vehicle for system level validation. All following experimental steps are identical to the model level V&V process flow. The first modeling system step entails formulating the modeling system from validated constituent ICME models. Following model integration to compose the ICME system, interface verification (rather than code verification) is carried out to insure that model application programming interfaces, model wrappers, and data flow between/among models is properly implemented. If final system level validation is successful, the ICME system is subject to tool maturity level assessment.

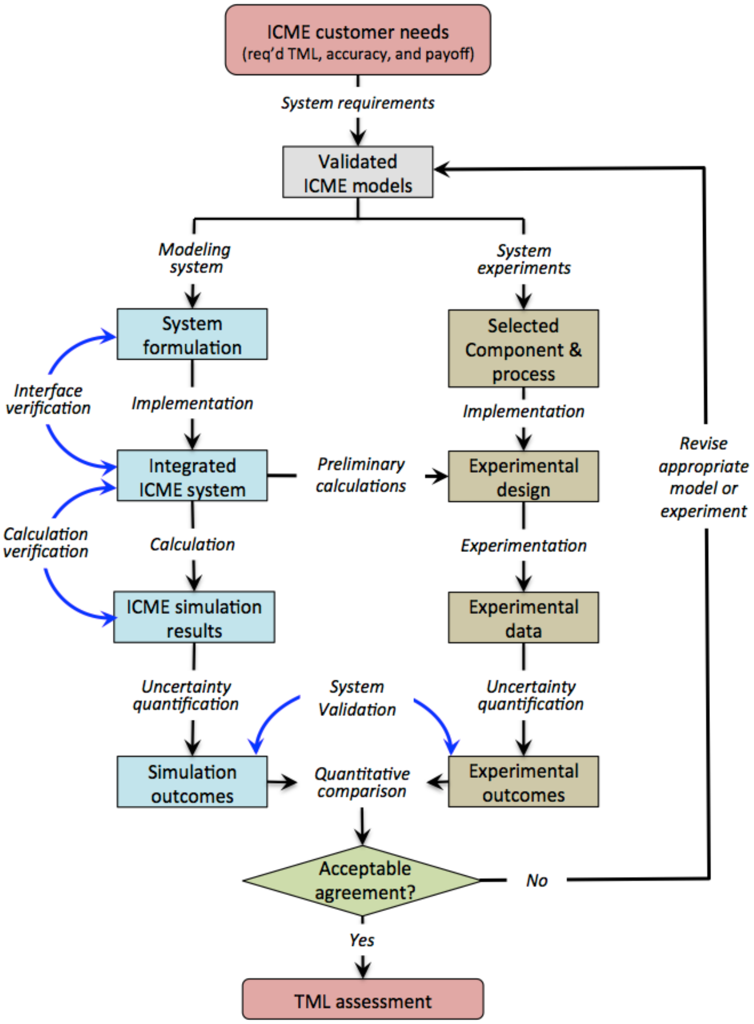


Figure 14: Flow chart describing the ICME system V&V process, after [6]

V&V Checklist Content

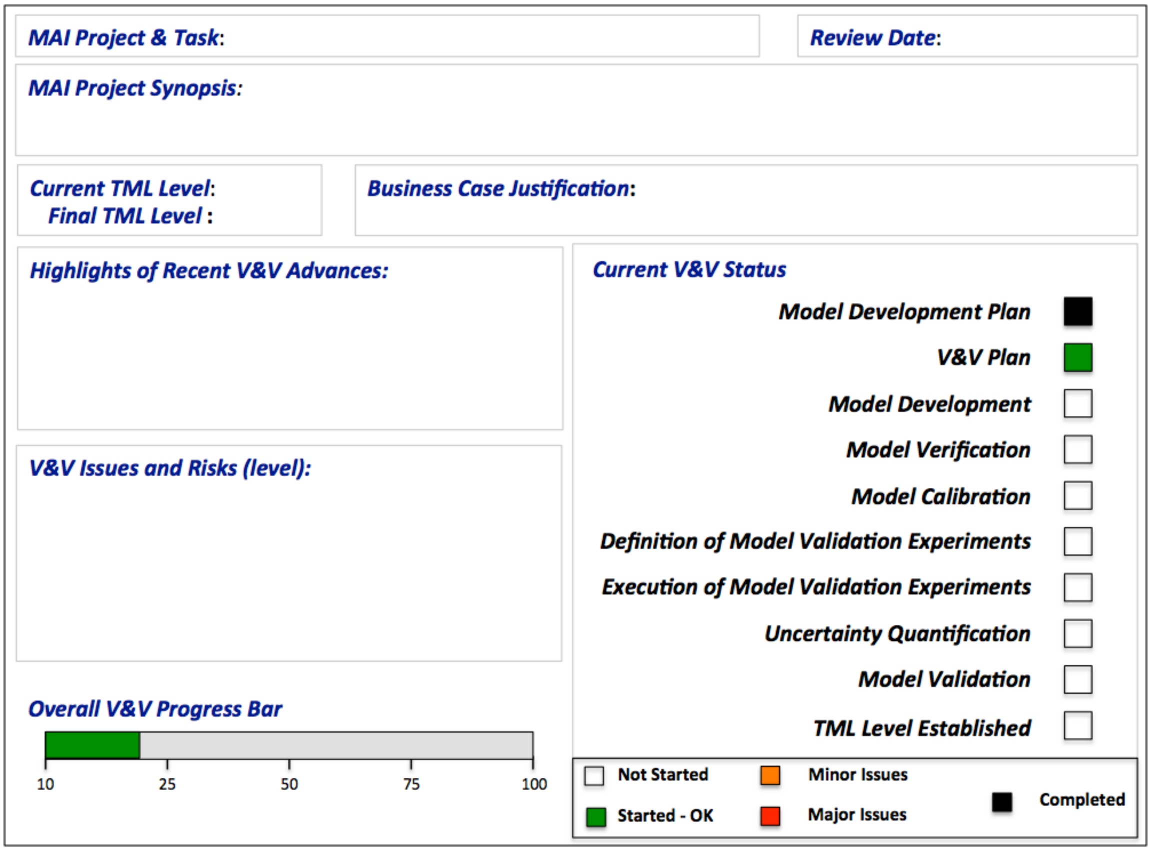
The system level and model V&V checklists were constructed to capture the V&V elements of a typical ICME program in greater detail than possible within the V&V process flow charts, Figures 13 and 14. Also the organized linear listing of V&V activities within the checklists, better serves their intended use: V&V planning, tracking, and intra-team communications. Although ultimately prospective V&V practitioners need to examine and understand the checklists in detail, it is easier to grasp the organizational structure, content, and relationship of the checklists to the V&V process flow charts via the checklist synopses shown in Table 1.

Table 1: Synopses of the V&V Checklists

ICME System V&V Checklist	
Definition of Customer Needs and Business Case	• Identified customer, ICME opportunity, reality of interest, and benefits • Established & refined business case for the ICME system • Defined ICME system accuracy, uncertainty, and TML requirements
ICME Modeling System Formulation	• Formulated the ICME system architecture and constituent modules/models • Selected software platform(s) and integration strategy and tools • Identified and resolved system-wide computation and implement issues
ICME System Uncertainty Quantification	• Established project-wide UQ methods, tools, and application approach • Formulated system level calibration, error/uncertainty propagation analysis strategy
ICME System Level V&V	• Established hierarchical system wide validation strategy • Tested and verified the integrated modeling system • System level model validation and experimental design completed • System level validation exercise and UQ completed
ICME Model Verification and Validation Checklist	
ICME Model Development	• Established detailed modeling approach - Developed mathematical model and initial computational model - Conducted sensitivity studies to assess inputs, internal parameters & BC/ICs - Performed UQ to determine output uncertainty based on inputs uncertainty - Provided support for system level uncertainty propagation analysis
Experimental Support of Model Development and UQ	• Established experimental approach to support model development & UQ • Determined experimental methods and source • Plan and experiments to measure internal parameters, inputs, and outputs • Experiments conducted and UQ applied to determine uncertainty of results • Assess data and uncertainty in support of system level validation
Model Verification	• Established model verification plan • Identified verification benchmark model and/or data • Checked and executed computational model to identify/fix coding problems • Compared model results against benchmark(s) • Identified and repaired computation model deficiencies
Model Validation	• Established model validation strategy and plan • Defined and executed experimental plan for validation - Analyzed results using UQ methods • Defined and executed modeling plan for validation - Analyzed results using UQ methods • Applied UQ methods to determine model accuracy & range of applicability • Completed activities and support for system level validation

4.4 User Notes for the V&V Checklists

The ICME V&V system-level and model-level checklists are presented in Tables 2 and 3. These user notes are intended to provide guidance and suggestions for consideration by the ICME IPDT, particularly those members inexperienced in the use of V&V. Additionally, a scorecard template – for reporting V&V progress to management is shown in Figure 15.



MAI Project & Task:

Review Date:

MAI Project Synopsis:

Current TML Level:
Final TML Level :

Business Case Justification:

Highlights of Recent V&V Advances:

V&V Issues and Risks (level):

Overall V&V Progress Bar

Current V&V Status

Model Development Plan	■
V&V Plan	🟩
Model Development	☐
Model Verification	☐
Model Calibration	☐
Definition of Model Validation Experiments	☐
Execution of Model Validation Experiments	☐
Uncertainty Quantification	☐
Model Validation	☐
TML Level Established	☐

☐ Not Started
🟧 Minor Issues
■ Completed
🟩 Started - OK
🟥 Major Issues

Figure 15: Example of a Dash Board chart to communicate ICME V&V project status

Leaders of the ICME IPDT should formulate an approach for V&V checklist implementation during the early stages of program planning and subsequent execution. Unfortunately there is no single detailed approach that can possibly fit the needs for each and every ICME program; no more than there is a unique approach for technically planning an ICME program, allocating program resources, or executing a risk assessment. The preferred approach for checklist development and execution depends on a number of factors including (among others): (1) the size and complexity of the ICME effort, (2) the size and heterogeneity of the IPDT, (3) the number and maturity level of constituent models in the ICME system, and (4) the depth and uncertainty of existing experimental data and relevant experimental methods. A team checklist process for a simple, single model ICME program will most likely pose many fewer implementation challenges compared with one at the opposite end of the spectrum. It is unfortunate, but often true, that the level of team effort, time, and frustration for implementation of group processes increases non-linearly upwards relative to the number of team members. However, there are several general-purpose tactics/steps that can improve efficiency of generating and maintaining V&V checklists for most ICME programs. These include:

- The IPDT leadership should provide V&V support materials (e.g., MAI V&V and ASME guidelines) to IPDT members before any V&V meetings such as those intended to exercise the V&V checklists. Misunderstanding relative to V&V terminology (e.g., verification versus validation) or the preferred content and structure of V&V activities (e.g., ASME process flow) can create confusion among the IPDT members, consume valuable time, and severely limit meeting productivity. Other useful support materials include: (1) a clear and concise statement of the goals, objectives, and technical requirements of the ICME system; (2) a chart/map of the ICME model structure, along with identification of the qualitative maturity of the constituent models and those models expected to require V&V focus; (3) any available preliminary risk assessment results generated during early stages of proposal preparation; and (4) the results for any Phenomena Identification and Ranking Table (PIRT) analyses conducted. A description of use of PIRT tables and an ICME-related example is presented in section 4.5 of this document.
- For ICME programs that include multiple, uncertain models, the IPDT leaders might consider decomposing V&V checklist discussions and meetings into hierarchical, model specific sub-teams, particularly when modelers and associated experimentalists can be efficiently divided into such sub-teams. For large IPDTs composed of a geographically diverse membership, V&V face-to-face meetings of the entire IPDT can be decomposed into smaller breakout groups that individually address a subset of the decomposed ICME system.
- ICME IPDT leaders can also assign V&V leadership responsibility to a small set of IPDT team members, whose expertise collectively spans the breath of the ICME models and experimental knowledge for the critical sub-elements of the ICME development. Such a group of “domain knowledge” experts can then draft straw-man V&V checklists, for subsequent review, revision, and approval by the collective ICME IPDT.

Serious commitment to upfront planning by IPDT leaders, prior to implementation of the V&V checklists (or any IPDT group process) can reap significant improvements in team productivity and improvements in checklist completeness and acceptance. The sections below provide additional checklist notes and suggestions.

General notes:

The checklists are not prescriptive, in recognition of the diversity of goals, scope, ICME maturity level, and resource availability among ICME development programs. Consequently, each ICME development team has total flexibility to tailor the V&V checklists to meet each ICME program’s individual needs.

> *Checklist Purpose:* The team should determine a strategy of how it intends to use the checklists – whether as a program planning checklist that verifies that appropriate V&V activities have been included in the technical plan and budget

or whether the team decides to use the checklists during the course of the program to track V&V progress. The strategy might also include consideration as to the level of detail that should be included in the checklist, how much customization of checklist details are desirable, and which team member(s) lead the checklist effort. Such early considerations of strategy are of greater programs for large, multi-organization ICME programs.

Checklist Revision: ICME teams own their V&V checklists and are encouraged to modify the checklists to satisfy their particular needs by inserting, modifying, or deleting checklist line items within the Excel checklist file. When a team decides to include significant detail within their checklists, a column can be added to the checklist to signify the "level" of each line-item (much like what is done in a "Work Breakdown Structure"). By filtering this column, detail can be hidden or exposed depending upon the desired level of detail.

Checklist Updating: The checklists contain: (1) a column to denote those line items that the team decides should be addressed during planning and (2) V&V status boxes to specify the state of completion using color codes, located below the system-checklist.

Status Documentation: Some ICME teams have chosen to complement the V&V status boxes using detailed documentation. One ICME team appended an additional column to the checklist spreadsheets to summarize such details; whereas another team built a companion Power-Point presentation to document progress in even greater detail. Additionally, comments can be added to a spreadsheet cell ("Select" –> "New Comment"). Documentation is encouraged because it can greatly augment communication both within the ICME team and with technical management and customers.

V&V checklist implementation builds upon knowledge of V&V fundamentals (per MAI and ASME-CSM V&V guidelines), foundational work to define the goals and UQ expectations for the ICME system, and the identification of the "weak points" and "Achilles heal(s)" of the proposed ICME system that might preclude achievement of ICME system goals/requirements. Methods such as Risk Assessment and the Phenomena Identification and Results Table (PIRT) process are powerful tools that can accelerate identification of V&V targets and approaches that will increase the likelihood that the ICME program will meet customer needs and requirements.

Planning notes:

The V&V checklists, arguably, should have their greatest influence during ICME program proposal preparation and the early stages of program execution, when detailed technical plans are often formulated. It is during these planning exercises that customer requirements, budgets, program goals, objectives, detailed technical plan, and IPDT team member interrelationships are established. Early use of the checklists can improve plan elements by bringing attention to important V&V activities that might otherwise be overlooked.

- *V&V Planning should adopt a top-down approach:* In contrast to V&V execution, V&V planning should begin with the system-level checklist and then proceed downward through the model-level checklist hierarchy. Only through system-level insight of customer needs, required system accuracy and TML level as well as consideration of the entire ICME modeling system, can the IPDT assess which models require V&V focus, identify accuracy and UQ targets for key models, and partition validation experimental resources among key models and the overall system. When a system or model checklist item is identified as important to the planning activity, it should noted by inserting a "P" in the planning column. Note: suggested planning activities are shown in the system level checklist shown in Table 2.

<u>V&V system level checklist:</u>

The system level checklist, as shown in Tables 1 and 2, contains four activities involving: (1) identifying and translating customer needs, (2) formulating the modeling system, (3) establishing the program-wide UQ approach, and (4) defining and coordinating validation of the ICME system. The system level activities have a profound effect on research at the modeling level by setting constituent model requirements, defining inter-model data-flow and interfaces needed for system-level model integration, adopting common V&V methods, and planning and coordinating system level validation. Owing to the pervasive consequences of V&V system level work, the effort should involve participation from across the IPDT to promote communication, achieve consensus, and obtain commonality of purpose and methods within the team.

- *Definition of customer needs and business case:* While ICME program leaders usually identify high-level goals and payoff during proposal preparation, sharpening the definition of customer needs and requirements is essentially early in a program in order to calibrate the technical plan via information about ICME system output, accuracy/uncertainty, and ultimate TML requirements. If such information is obtained too late, ongoing technical effort may be working toward the wrong target. Although the business case is typically generated later in a program, it too can be sidetracked if V&V activities are inadequate to provide the confidence necessary to support critical customer decisions.
- *ICME Modeling System Formulation:* This section of the system checklist addresses the modeling system architecture, the logical (data flow) and computational inter-connections (interfaces) among models, and integration strategy and software. It is critical to also identify whether computation issues (e.g., execution time, computer resources, analyst training) are compatible with pre-existing non-ICME engineering workflow, infrastructure, and budget constraints. These latter "potential" issues could affect the ICME business case and compromise or delay ultimate implementation.
- *ICME System UQ Methods and Tools:* Uncertainty quantification is used during V&V to: (1) determine experimental data error, (2) deduce uncertainty of modeling results caused by natural variation of model inputs and internal modeling parameter uncertainty, (3) support model calibration methods, (4) support validation by defining and calculating validation metrics and evaluating prediction accuracy and uncertainty bounds. UQ tools include a number of software products, ranging from SWRI's NESSUS™ to MatLab™. System

analysis tools (available in some model integration environments) can complement UQ by automating the execution of analytical DOEs, calculating sensitivities, and providing model calibration.

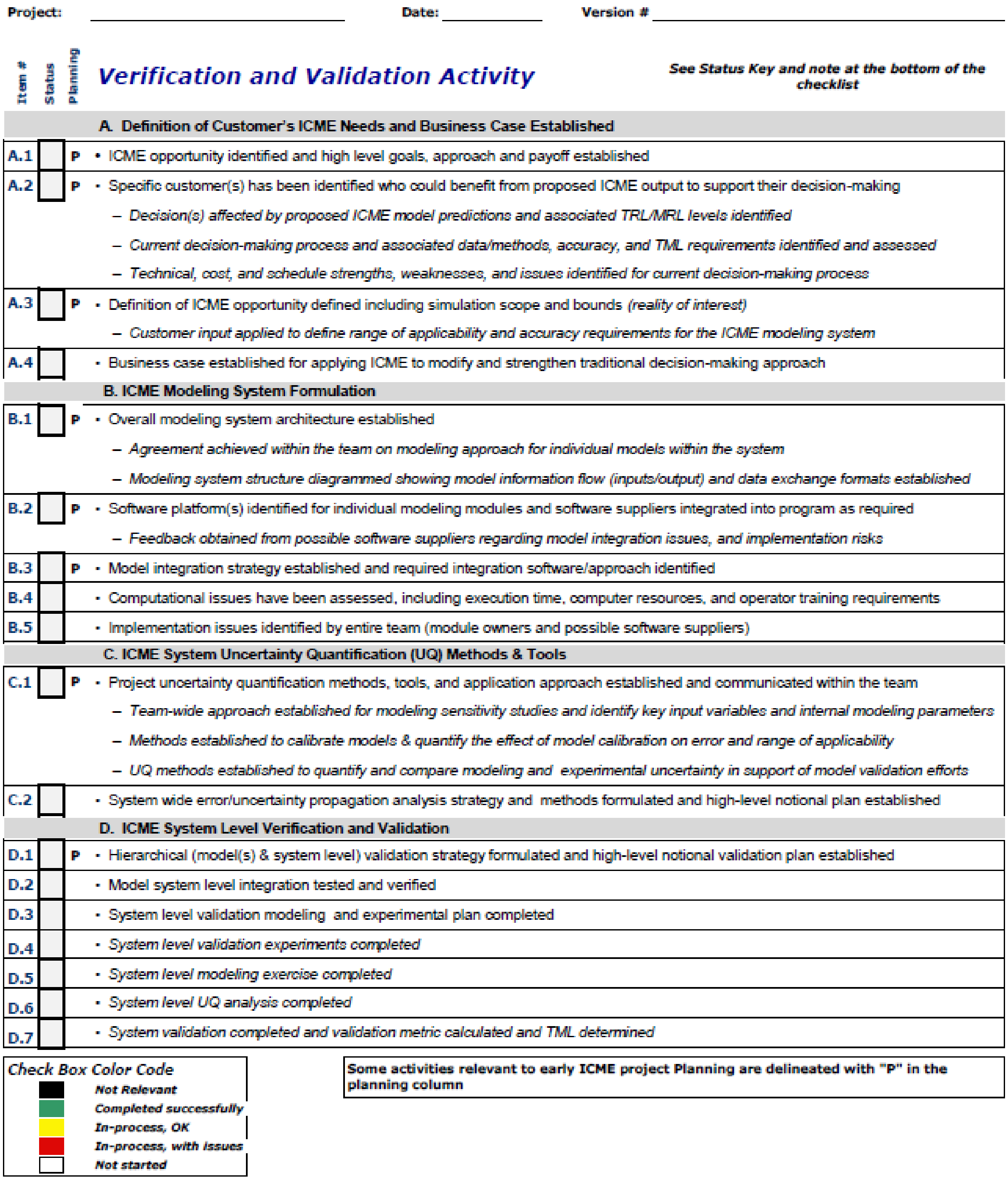
- *ICME System Level Verification and Validation:* System level V&V involves the entire IPDT because it necessarily entails a comparison of system level experimental outcomes against the modeling system outcomes – and the latter involves all models. For this exercise, the IPDT needs to assure that the integrated modeling system has been verified (i.e., the models are communicating properly) and that the validation adheres to the methods and validation metrics established in Section-C of the system level checklist.

V&V model level checklist:

The model checklist was formulated to aid IPDT sub-teams responsible for individual models within the ICME system model hierarchy – specifically those responsible for critical models as identified during system-level assessment. Activities within the model level checklists focus on modeling activities but also include experimental support for determining uncertainty analysis and validation. The level of effort for any given model depends on how sensitively the model influences overall system results, the foundation of the model, and the uncertainty of both the modeling form and internal modeling parameters. The model level checklist follows the ASME V&V process flow except that it explicitly recognized the likely need for model calibration, which is often needed for ICME models, given the often moderate-to-high level of uncertainty of some internal parameter values.

> *ICME model development:* This checklist section follows the left-hand branch of the ASME V&V process flow chart, Figure 13, and includes the path between the conceptual model and creation of the computational model on to subsequent analysis via sensitivity and Monte Carlo analysis to support UQ analysis (discussed previously under the system level discussion). However, note that many industrial ICME model development efforts build upon fundamental university or research laboratory research; and therefore avoid effort to establish the conceptual, mathematical, or even computation models. Also, while the ASME V&V process flowcharts don't include model calibration, it is included in the V&V checklist to acknowledge that often a subset of internal modeling parameters are difficult to measure experimentally and values are therefore uncertain, which can significantly degrade model fidelity.
>
> *Experimental support for ICME model development & UQ:* Experimental support is imperative to generate data-sets with measured inputs and outputs that parallel the inputs used and outputs generated by the model. This activity can be one of the most critical, yet difficult efforts within an ICME V&V program task. The model checklist also includes UQ analysis to determine the uncertainty for measured experimental output for use during validation.

Table 2: ICME V&V System-Level Checklist



Project: ____________ **Date:** ____________ **Version #** ____________

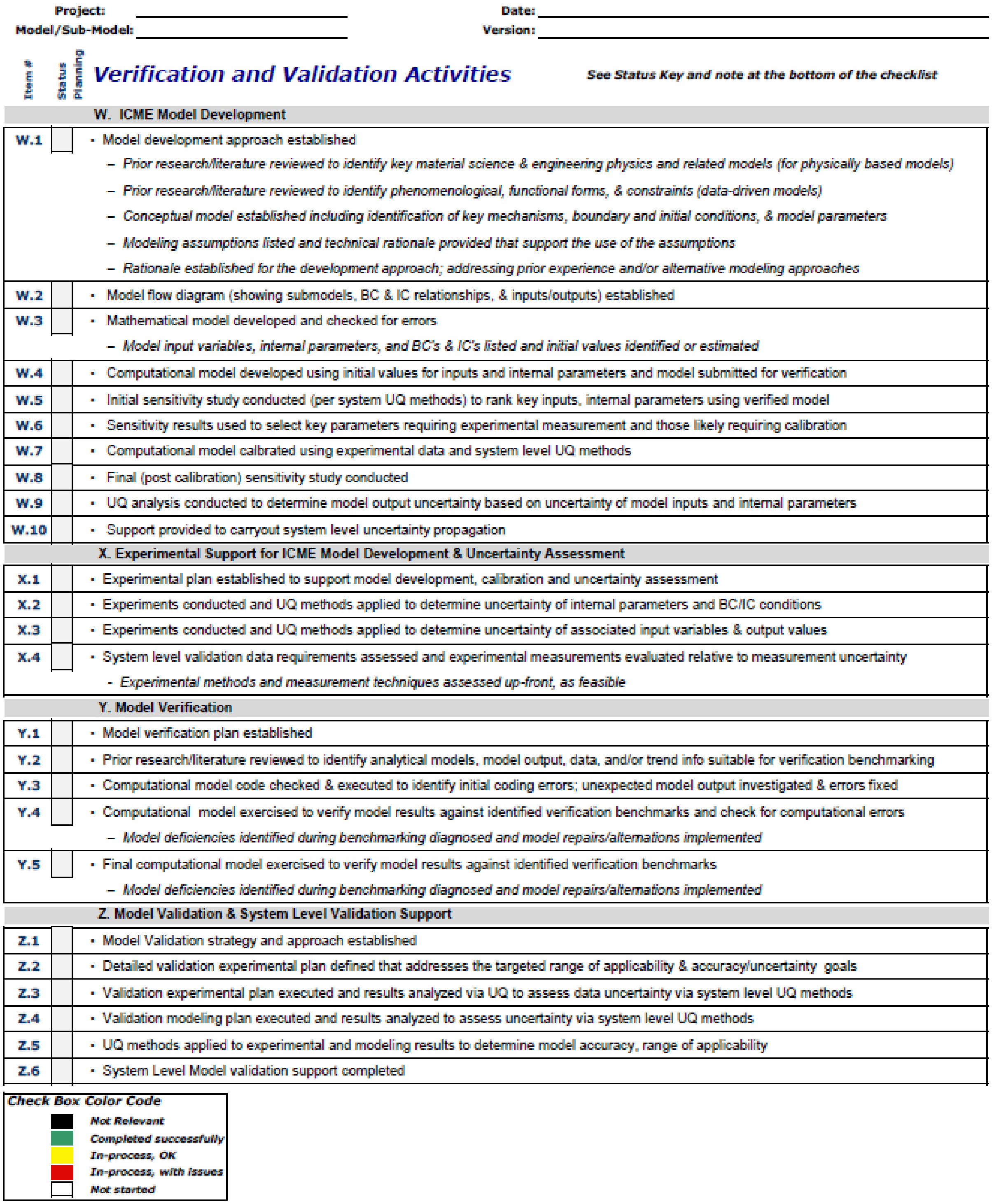
Item #	Status	Planning	*Verification and Validation Activity*
			See Status Key and note at the bottom of the checklist
			A. Definition of Customer's ICME Needs and Business Case Established
A.1	☐	**P**	• ICME opportunity identified and high level goals, approach and payoff established
A.2	☐	**P**	• Specific customer(s) has been identified who could benefit from proposed ICME output to support their decision-making – *Decision(s) affected by proposed ICME model predictions and associated TRL/MRL levels identified* – *Current decision-making process and associated data/methods, accuracy, and TML requirements identified and assessed* – *Technical, cost, and schedule strengths, weaknesses, and issues identified for current decision-making process*
A.3	☐	**P**	• Definition of ICME opportunity defined including simulation scope and bounds *(reality of interest)* – *Customer input applied to define range of applicability and accuracy requirements for the ICME modeling system*
A.4	☐		• Business case established for applying ICME to modify and strengthen traditional decision-making approach
			B. ICME Modeling System Formulation
B.1	☐	**P**	• Overall modeling system architecture established – *Agreement achieved within the team on modeling approach for individual models within the system* – *Modeling system structure diagrammed showing model information flow (inputs/output) and data exchange formats established*
B.2	☐	**P**	• Software platform(s) identified for individual modeling modules and software suppliers integrated into program as required – *Feedback obtained from possible software suppliers regarding model integration issues, and implementation risks*
B.3	☐	**P**	• Model integration strategy established and required integration software/approach identified
B.4	☐		• Computational issues have been assessed, including execution time, computer resources, and operator training requirements
B.5	☐		• Implementation issues identified by entire team (module owners and possible software suppliers)
			C. ICME System Uncertainty Quantification (UQ) Methods & Tools
C.1	☐	**P**	• Project uncertainty quantification methods, tools, and application approach established and communicated within the team – *Team-wide approach established for modeling sensitivity studies and identify key input variables and internal modeling parameters* – *Methods established to calibrate models & quantify the effect of model calibration on error and range of applicability* – *UQ methods established to quantify and compare modeling and experimental uncertainty in support of model validation efforts*
C.2	☐		• System wide error/uncertainty propagation analysis strategy and methods formulated and high-level notional plan established
			D. ICME System Level Verification and Validation
D.1	☐	**P**	• Hierarchical (model(s) & system level) validation strategy formulated and high-level notional validation plan established
D.2	☐		• Model system level integration tested and verified
D.3	☐		• System level validation modeling and experimental plan completed
D.4	☐		• *System level validation experiments completed*
D.5	☐		• *System level modeling exercise completed*
D.6	☐		• *System level UQ analysis completed*
D.7	☐		• *System validation completed and validation metric calculated and TML determined*

Check Box Color Code

■	***Not Relevant***
🟩	***Completed successfully***
🟨	***In-process, OK***
🟥	***In-process, with issues***
☐	***Not started***

Some activities relevant to early ICME project Planning are delineated with "P" in the planning column

Table 3: ICME V&V Model Checklist



Project: ____________ **Date:** ____________
Model/Sub-Model: ____________ **Version:** ____________

Item #	Status Planning	*Verification and Validation Activities* *See Status Key and note at the bottom of the checklist*
		W. ICME Model Development
W.1	☐	• Model development approach established – *Prior research/literature reviewed to identify key material science & engineering physics and related models (for physically based models)* – *Prior research/literature reviewed to identify phenomenological, functional forms, & constraints (data-driven models)* – *Conceptual model established including identification of key mechanisms, boundary and initial conditions, & model parameters* – *Modeling assumptions listed and technical rationale provided that support the use of the assumptions* – *Rationale established for the development approach; addressing prior experience and/or alternative modeling approaches*
W.2	☐	• Model flow diagram (showing submodels, BC & IC relationships, & inputs/outputs) established
W.3	☐	• Mathematical model developed and checked for errors – *Model input variables, internal parameters, and BC's & IC's listed and initial values identified or estimated*
W.4	☐	• Computational model developed using initial values for inputs and internal parameters and model submitted for verification
W.5	☐	• Initial sensitivity study conducted (per system UQ methods) to rank key inputs, internal parameters using verified model
W.6	☐	• Sensitivity results used to select key parameters requiring experimental measurement and those likely requiring calibration
W.7	☐	• Computational model calbrated using experimental data and system level UQ methods
W.8	☐	• Final (post calibration) sensitivity study conducted
W.9	☐	• UQ analysis conducted to determine model output uncertainty based on uncertainty of model inputs and internal parameters
W.10	☐	• Support provided to carryout system level uncertainty propagation
		X. Experimental Support for ICME Model Development & Uncertainty Assessment
X.1	☐	• Experimental plan established to support model development, calibration and uncertainty assessment
X.2	☐	• Experiments conducted and UQ methods applied to determine uncertainty of internal parameters and BC/IC conditions
X.3	☐	• Experiments conducted and UQ methods applied to determine uncertainty of associated input variables & output values
X.4	☐	• System level validation data requirements assessed and experimental measurements evaluated relative to measurement uncertainty - *Experimental methods and measurement techniques assessed up-front, as feasible*
		Y. Model Verification
Y.1	☐	• Model verification plan established
Y.2	☐	• Prior research/literature reviewed to identify analytical models, model output, data, and/or trend info suitable for verification benchmarking
Y.3	☐	• Computational model code checked & executed to identify initial coding errors; unexpected model output investigated & errors fixed
Y.4	☐	• Computational model exercised to verify model results against identified verification benchmarks and check for computational errors – *Model deficiencies identified during benchmarking diagnosed and model repairs/alternations implemented*
Y.5	☐	• Final computational model exercised to verify model results against identified verification benchmarks – *Model deficiencies identified during benchmarking diagnosed and model repairs/alternations implemented*
		Z. Model Validation & System Level Validation Support
Z.1	☐	• Model Validation strategy and approach established
Z.2	☐	• Detailed validation experimental plan defined that addresses the targeted range of applicability & accuracy/uncertainty goals
Z.3	☐	• Validation experimental plan executed and results analyzed via UQ to assess data uncertainty via system level UQ methods
Z.4	☐	• Validation modeling plan executed and results analyzed to assess uncertainty via system level UQ methods
Z.5	☐	• UQ methods applied to experimental and modeling results to determine model accuracy, range of applicability
Z.6	☐	• System Level Model validation support completed

Check Box Color Code

■	*Not Relevant*
🟩	*Completed successfully*
🟨	*In-process, OK*
🟥	*In-process, with issues*
☐	*Not started*

Model verification: Model validation, as specified by the ASME V&V process flow chart (Figure 13) and included in the model checklist, involves code verification (as determined by identifying/fixing coding bugs and comparing results against benchmark results) and calculation verification (as assessed by determining variation of results following changes in numerical spatial and temporal increments as well as FEM element order, if appropriate).
Model validation & system level validation support: Model level validation adheres to the same methods and processes used during system level validation.

Some ICME models are built using commercial software such as DEFORM, ProCAST, or general multi-physics codes. Although these software packages are fairly mature and widely used, V&V nonetheless should be considered by the AIPT team to ensure that internal materials databases, sub-models, and boundary conditions are appropriately selected and that suitable FEM element-type and both spatial and temporal discretization are applied. While code verification is generally neither possible nor required, calculation verification and validation are recommended, particularly when new problems are undertaken or new user-subroutines are involved.

4.5 Use of Phenomena Identification and Ranking Table (PIRT): Contributed by David Riha, Southwest Research Institute: A useful approach for identifying the important physical processes and parameters is to construct a Phenomena Identification and Ranking Table (PIRT). This process has been used and documented for assessment and subsequent tracking of various risks associated with nuclear reactor facilities [14, 15] since the1980’s. It has served as a framework or process for expert elicitation, and for identification, assessment, and prioritization of phenomena or parameters related to important processes and facilities. As such, it is considered a very useful tool to describe and assess ICME computational model elements – including model hierarchy and relative importance or potential impact of various models, sub-models, and parameters.

The PIRT is used to identify key processes and parameters that are important to the system response of interest. It is important to note that the PIRT is a table—a product—and that it is the process of developing the PIRT that is of most value. Ideally, the PIRT is constructed during the conceptual model development and validation experiment planning stages and updated throughout the V&V process for a continual, up-to-date, communication of the physical phenomena, model uncertainties, assumptions, and technical issues relevant to validating the model. The PIRT can serve several roles in the V&V process:

1. Identifies relevant physical process to the responses of interest
2. Identifies key elements and technical issues in both the conceptual and computational models
3. Captures relevant phenomena and simplifying assumptions
4. Describes potential technical issues and barriers

5. Ranks relative importance of these issues
6. Provides information for resource allocation
7. Communicates phenomena, assumptions, and uncertainties
8. Guides the V&V plan and UQ strategy

The PIRT is developed by identifying the important phenomena using engineering expertise, judgment, and subject matter experts and ranking their importance to predicting the system level responses of interest. The table lists the phenomena along with a ranking of its importance (low, medium, high) and the confidence (low, medium, high) in how it is calculated or used. The confidence is sometimes referred to as knowledge level (known, partially known, unknown). An example PIRT for a model that predicts the yield strength for LSHR nickel superalloy is shown in Table 4: Example Phenomena Identification and Ranking Table (PIRT), Table 4 below.

Table 4: Example Phenomena Identification and Ranking Table (PIRT) for Models

No.	Phenomenon	Importance	Confidence	Comments
A.1	Microstructure	High	Medium	Small errors in the tertiary γ' volume fraction and size lead to large errors in yield strength
A.2	Chemistry	High	High	Generally well characterized
B.1	Grain size hardening	High	Medium	Strengthening inversely proportional to grain size, doesn't apply to single crystal systems
C.1	Matrix friction	Medium	Medium	Chemistry/Temp effect. Form is a fit to literature data per material composition
C.2	Precipitate friction	Medium	Medium	Solution strengthening effect
D.2	Interface strengthening	High	Medium	Includes APB effects, coherency strain

The PIRT is a documentation and communication tool and thus its format is flexible to meet the needs of the V&V team. Hierarchical PIRTs are sometimes appropriate for complex models for focused communication of model modules or different experiments. Other columns that may be useful are parameters that are needed for each phenomena or model element, quality/availability of data needed to define model parameters, and uncertainty quantification (UQ) strategies. In some cases, it is worthwhile to create a separate PIRT for the model parameters and identify potential uncertainty ranges for each parameter. This parameter PIRT allows gaining some level of consensus for the importance of the parameters and uncertainty ranges.

A form of the PIRT for experiments can also been useful in V&V efforts to identify the phenomena related to the experiments and facilitate communication between the experimentalists and model developers. This information is useful to identify uncertainties in the experiments, response features for comparison to model predictions, and uncertainties that need to be specifically included in the model for accuracy assessments. An example PIRT for standard tensile experiments to determine the yield stress is shown in Table 5: Example Phenomena Identification and Ranking Table (PIRT) for Experiments, Table 5, below. An optional column is shown to describe how specific uncertainties are characterized or mitigated.

Table 5: Example Phenomena Identification and Ranking Table (PIRT) for Experiments

No.	**Phenomenon**	**Importance**	**Confidence**	**UQ Strategy**
A.1	Force application/ measurement	High	High	Measurement tolerances provided by supplier
A.2	Displacement measurement	High	High	Measurement tolerances provided by supplier
A.3	Temperature application/ measurement	High	Medium	Measurement tolerances provided by supplier
B.1	Specimen geometry	High	High	Measure specimen geometry
C.1	Stress-strain conversion	High	Medium	Use consistent approach

The PIRTs for the model and experiments identify important uncertainties in both the model and experiments. These PIRTS are powerful for planning the model development and experiments for model calibration, validation and gaining consensus about assumptions, importance, and uncertainties. The information can guide resource allocation tradeoffs between the model development and experiments. For example, uncertainties may be economical to include in the model but cost-prohibitive to control in the experiment and vice versa.

5. Tool Maturity Level (TML) and Risk vs. Consequences Assessment:

5.1 Introduction: The Tool Maturity Level (TML) Assessment Guide was intended to facilitate assessment of maturity and capability of ICME models or computational tools relative to intended applications, and to provide a useful method for guiding and assessing ICME V&V activities during model development or refinement, when integrated with the ICME V&V Checklists.

Currently, there is no simple, standard, gated review process in broad use for assessment and communication of the maturity level of an analytical model or tool – at least not in the same sense as the TRL process. Sandia National Laboratories and NASA have published approaches and standards for predictive capability and maturity of computational models and simulations [16, 17]. Both are excellent references and guidelines. The Sandia report describes levels from zero to three in maturity, and contains very specific criteria descriptions for various assessment elements. NASA-STD-7009 describes levels from zero to four (5 levels), and has more general descriptions which would be adaptable for various system level applications. The NASA standard also includes practitioner (personnel) capability and training as one of the major assessment elements. What is proposed for ICME use is based on a simple five-level maturity assessment as presented by Morris [12], at the 8th International HCF Conference in 2003. The five levels of tool maturity – from an initial TML of 1, as least mature, to a fully-mature TML of 5, appear to provide sufficient differentiation without over-complication.

The TML Assessment Guide was primarily intended to facilitate assessment of maturity and capability relative to intended applications. To support this objective, the proposed TML assessment concept was aligned with well-established gated processes for technology and product development, including the TRL, MRL, and IPD processes.

In addition, an approach was selected to provoke assessment of deficiencies or risks that should be addressed in conjunction with specific applications. This approach is based on the NASA risk management tool: "Consequences vs. Likelihood 5X5 Risk Matrix" [13]. This was intended to provide a framework for assessing whether risk mitigation steps are needed for specific applications of ICME methods or models. It is envisioned that this process, used in conjunction with the TML Assessment Guide, would ensure that risk vs. consequences of ICME usage could be objectively assessed for specific applications, and that suitable risk mitigation actions could be identified and integrated with a comprehensive V&V plan.

Overall, the intent was to generate a useful tool and process to meet these objectives - an approach that would be broadly applicable to ICME models and methods, which would provide a consistent guiding framework without being overly prescriptive. Both the TML and Risk Management tools are integrated in the V&V Recommended Best Practice as presented in Section 6 of this report.

5.2 Tool Maturity Level Assessment: The concept for the ICME Tool Maturity Level Assessment is intended to provide a common or standard method for assessing and communicating the maturity of various ICME methods or models. This is believed useful – possibly even necessary - to guide development of V&V plans, as well as for assessment of readiness or maturity of ICME tools for specific applications.

Basis for the TML Assessment Process: The basis for the TML approach was taken from the general analytical TML approach described by Morris [12] as was described above. The five-level structure of the general analytical tool assessment was preserved, and eventually determined to be sufficient for ICME application. The maturity level descriptions were modified specifically for ICME, and are presented in Table 6.

Table 6: Tool Maturity Level Descriptions and Levels for ICME

Tool Level - TML	ICME Tool Maturity Description
1	Analytical process is exploratory in nature. Fidelity of predictions is largely unproven. Provides some physical insight, but cannot reduce development testing.
2	Proven capability for comparative assessment, ranking or trending. Experimental validation is still necessary. Can drive development or assessment plan and test matrix.
3	Material or process can be developed or assessed with significantly reduced testing. Expectation that development iterations will be reduced or eliminated. Accuracy and uncertainty effects must be quantified. Range of applicability well defined.
4	Material or process performance and impact on system or application are understood. Accuracy and uncertainty effects must be verified. Additional data may be required when applied to new materials or processes, or to extend range of application.
5	All material and process performance and system interaction effects are understood within defined range of application. Analytical process can be applied without testing.

The TML descriptions are intended to be general in nature and broadly applicable. They are intended to convey increasing fidelity, supporting data, documentation, and level of V&V, with increasing tool maturity. It is highly desirable to have clearly differentiated criteria for each maturity level. The challenge was to define the criteria in a broadly applicable, useful, and rigorous manner – without being overly-prescriptive. Six general criteria categories were defined during development of the initial concept for a TML assessment process. The assessment elements and gate criteria, while developed specifically for ICME applications, are generally consistent with those in both the Sandia report and the NASA standard previously referenced.

The assessment categories and criteria are described below in Table 7.

These categories can readily be mapped to specific sections and items in the ICME V&V Systems Level and ICME Model V&V Checklists, which were concurrently developed. In addition, the assessment encourages consistency with the ASME V&V Guide 10-2006 for matters of verification and validation, and use of risk vs. consequences assessments to determine whether risk-mitigation plans are warranted for specific applications.

Table 7: Tool Maturity Level Assessment Categories and Considerations

Assessment Category	Description and Criteria Considerations
Model Rationale, Basis and Definition	Definition of the model and its basis, intended application, input variables and outputs, ranges of inputs and outputs, sub-models defined. ICME Systems Level Checklist items.
Complexity and Documentation	Model or method flow diagram, assessment of sequential or interdependent computations, User's Guide. ICME V&V Model Checklist items.
Supporting Data	Identification, adequacy, archiving, and documentation of supporting data.
Model Verification	Computer code and model verification, version control and documentation, consistency with ASME V&V Guide 10-2006.
Range of Applicability and Uncertainty Quantification	Range of applicability and range of all input parameters, UQ plan for model parameter sensitivity and model output uncertainty, limitations defined.
Risk Assessment and Validation	Validation plans and execution for sub-models and system level, benchmark cases, Risk-vs.-Consequence assessment, risk mitigation requirements.

Description of the TML Process levels: Tool Maturity Levels (TML) can be briefly described in the context of the various assessment categories and associated criteria and considerations.

TML-1 represents an analytical model or tool with essentially unproven capability – suitable to provide some physical insight and guidance, but not sufficiently mature or proven to reduce planned experimental or other analytical efforts. TML-1 requires that the model be defined, along with input variables and outputs; that intended applications have been identified; that the model process has been "flow-mapped;" that supporting data has been identified; and that initial plans for verification and uncertainty have been developed. The ICME V&V System Level and Model Checklists provide some specific guidance on model basis and definition.

TML-2 represents a more mature analytical model or tool, where capability for comparative assessments, ranking, or trending has been demonstrated. Accuracy or fidelity of the model may not be sufficient to significantly reduce experimental or other analytical requirements, but the model could potentially drive development or assessment plans and significantly influence experimental or other analytical plans or assessments. TML-2 requires that significant sub-models be identified and assessed, that user instructions be documented, supporting data documented and archived, and computer code and models verified. In addition, the range of intended application must be defined, and sensitivity analyses performed for model input parameters. For TML-2, the Validation Plan must be developed and initiated, and demonstration of model ability to predict trends, or qualitative agreement with known results or expectations demonstrated. The ICME V&V System Level and Model Checklists provide some specific guidance on these items. In addition, at TML-2, it is recommended that a Risk vs. Consequences assessment be made for any application.

TML-3 represents a mature analytical tool or model – one that could significantly reduce or eliminate iterations in a material or process development program, and potentially reduce experimental testing or other analytical requirements. The model could be used directly for assessments or evaluations of derivative materials or processes, or deviations from known practices. Accuracy or fidelity of the model may not be fully validated, but range of application should be well defined and documented. For TML-3, supporting data should represent the entire range of application, a User's Guide fully developed and updated (from TML-2 level), version control for software implemented, and significant sub-model validation completed. The ICME V&V System Level and Model Checklists provide some specific guidance on these items. In addition, at TML-3, a Risk vs. Consequences assessment is highly recommended prior to any significant application.

TML-4 represents a very mature analytical tool or model, where material and process performance and impact within a system or application are well understood. Accuracy and uncertainty of model predictions have been assessed and validated, although additional data may be required to extend range of application or apply to additional materials or processes. Some experimental data or other analytical results may be required to support applications. For TML-4, comprehensive supporting data should exist, be documented and archived; code and model verification should be complete and consistent with ASME V&V Guide 10-2006, UQ analyses performed for overall model performance, and the model validated over the range of interest. Model accuracy, including UQ, should be validated for TML-4. The ICME V&V System Level and Model Checklists provide some specific guidance on these items. In addition, at TML-4, a Risk vs. Consequences assessment should be conducted prior to any significant application, as part of the model application process.

TML-5 represents an analytical tool or model with sufficient maturity that all material and process performance and system interaction effects are well understood and validated within the defined range of application. Demonstrated maturity, verification, and validation confidence is sufficiently high that the analytical process can be applied without testing within the defined range of application. Results are expected to be equivalent to or possibly even better than experimental results over this range. User's guide, all documentation, supporting data, verification and validation activities are mature and complete. Benchmark or standard validation cases have been established and used in validation. The ICME V&V System Level and Model Checklists provide some specific guidance on these items. In addition, at TML-5, a Risk vs. Consequences assessment should be conducted prior to any significant application, or if the range of application is being extended, as part of the model application process.

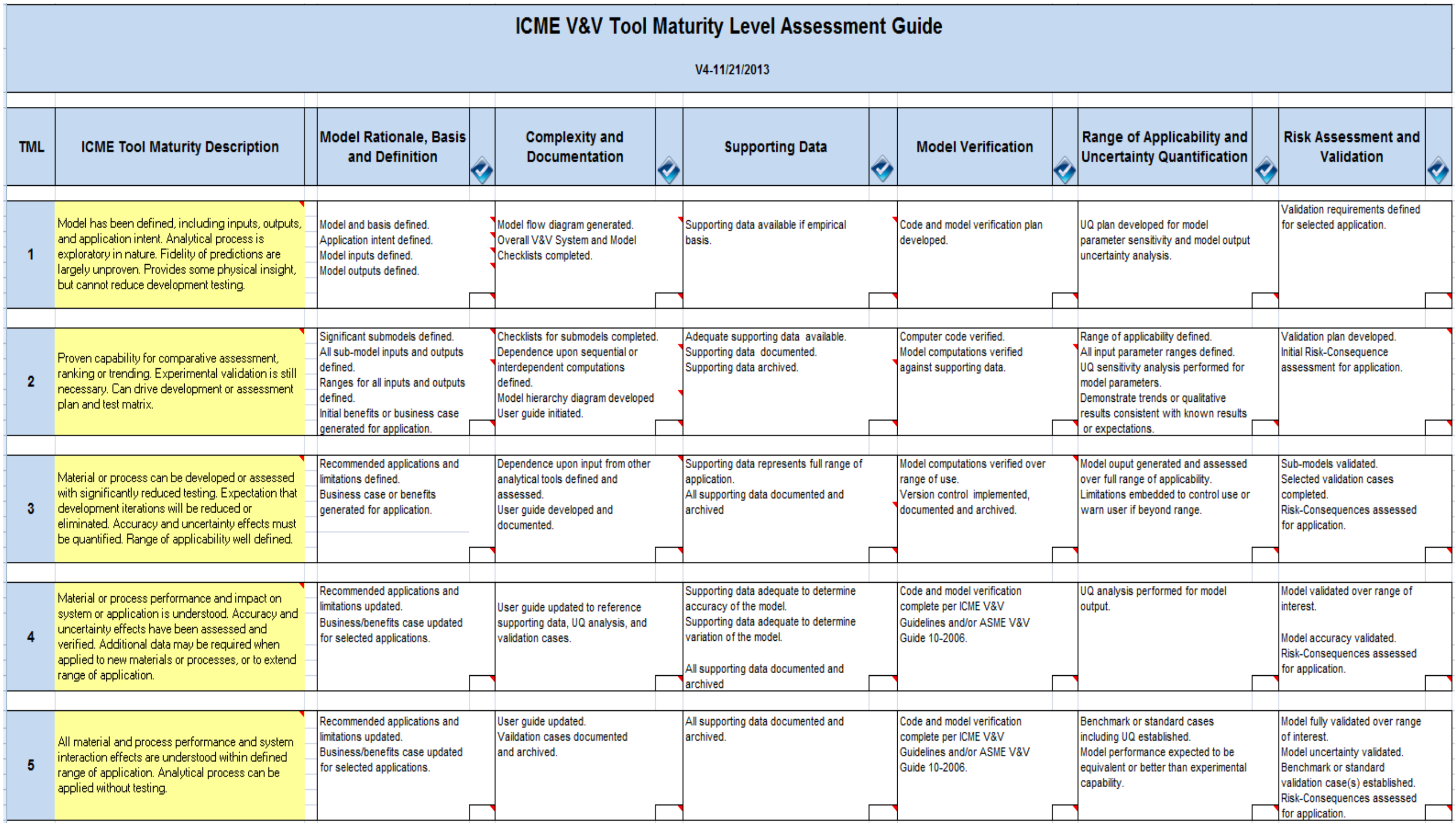
Approach for TML Assessments: A recommended approach was developed to evaluate and apply the various criteria during a TML assessment, in order to determine or assign an overall maturity level. The initial concept considered a binary scoring approach – essentially based on "yes" or "no" responses to a series of questions linked to each TML level and category. This proved problematic to execute in a straightforward way, without making the assessment very prescriptive or cumbersome. The resultant approach which is presented in this document is in the form of a simple table. The assessment is based on general criteria which can be guided by a few important reference documents. The concept is that a TML assessment will address the criteria described in each category at a particular TML level, and use the reference documents to help determine the specific requirements in a manner that is appropriate for the ICME model or tool under review., The reference documents include:

- ICME V&V Systems Level Checklist
- ICME Model V&V Checklist
- ASME V&V Guide 10-2006
- Risk vs. Consequences Assessment Matrix

The Excel™ version of the TML Assessment Guide also includes comments inserted in many of the criteria boxes for additional guidance. As an example, meeting all TML-1 criteria would, at a minimum, require completion of selected items on the Models and Systems Level Checklists. At higher TML levels, additional line items in the two checklists are referenced, consistency with the ASME V&V Guide is recommended for verification and validation criteria, and "risk vs. consequences" assessments are either recommended or required.

The need for flexibility and interpretation of how to meet these criteria is recognized; the intent was to provide sufficient guidance to be useful and encourage consistency. The table was developed in Excel spreadsheet format, so that notes associated with various entries could be inserted and recalled as needed. An image of the table is presented in Table 8.

Table 8: ICME Tool Maturity Level (TML) Assessment Guide



ICME V&V Tool Maturity Level Assessment Guide

V4-11/21/2013

TML	ICME Tool Maturity Description	Model Rationale, Basis and Definition	Complexity and Documentation	Supporting Data	Model Verification	Range of Applicability and Uncertainty Quantification	Risk Assessment and Validation
1	Model has been defined, including inputs, outputs, and application intent. Analytical process is exploratory in nature. Fidelity of predictions are largely unproven. Provides some physical insight, but cannot reduce development testing.	Model and basis defined. Application intent defined. Model inputs defined. Model outputs defined.	Model flow diagram generated. Overall V&V System and Model Checklists completed.	Supporting data available if empirical basis.	Code and model verification plan developed.	UQ plan developed for model parameter sensitivity and model output uncertainty analysis.	Validation requirements defined for selected application.
2	Proven capability for comparative assessment, ranking or trending. Experimental validation is still necessary. Can drive development or assessment plan and test matrix.	Significant submodels defined. All sub-model inputs and outputs defined. Ranges for all inputs and outputs defined. Initial benefits or business case generated for application.	Checklists for submodels completed. Dependence upon sequential or interdependent computations defined. Model hierarchy diagram developed User guide initiated.	Adequate supporting data available. Supporting data documented. Supporting data archived.	Computer code verified. Model computations verified against supporting data.	Range of applicability defined. All input parameter ranges defined. UQ sensitivity analysis performed for model parameters. Demonstrate trends or qualitative results consistent with known results or expectations.	Validation plan developed. Initial Risk-Consequence assessment for application.
3	Material or process can be developed or assessed with significantly reduced testing. Expectation that development iterations will be reduced or eliminated. Accuracy and uncertainty effects must be quantified. Range of applicability well defined.	Recommended applications and limitations defined. Business case or benefits generated for application.	Dependence upon input from other analytical tools defined and assessed. User guide developed and documented.	Supporting data represents full range of application. All supporting data documented and archived	Model computations verified over range of use. Version control implemented, documented and archived.	Model ouput generated and assessed over full range of applicability. Limitations embedded to control use or warn user if beyond range.	Sub-models validated. Selected validation cases completed. Risk-Consequences assessed for application.
4	Material or process performance and impact on system or application is understood. Accuracy and uncertainty effects have been assessed and verified. Additional data may be required when applied to new materials or processes, or to extend range of application.	Recommended applications and limitations updated. Business/benefits case updated for selected applications.	User guide updated to reference supporting data, UQ analysis, and validation cases.	Supporting data adequate to determine accuracy of the model. Supporting data adequate to determine variation of the model. All supporting data documented and archived	Code and model verification complete per ICME V&V Guidelines and/or ASME V&V Guide 10-2006.	UQ analysis performed for model output.	Model validated over range of interest. Model accuracy validated. Risk-Consequences assessed for application.
5	All material and process performance and system interaction effects are understood within defined range of application. Analytical process can be applied without testing.	Recommended applications and limitations updated. Business/benefits case updated for selected applications.	User guide updated. Validation cases documented and archived.	All supporting data documented and archived.	Code and model verification complete per ICME V&V Guidelines and/or ASME V&V Guide 10-2006.	Benchmark or standard cases including UQ established. Model performance expected to be equivalent or better than experimental capability.	Model fully validated over range of interest. Model uncertainty validated. Benchmark or standard validation case(s) established. Risk-Consequences assessed for application.

It should be noted that the Excel™ version of the table includes comments in many of the cells to clarify intent and stimulate consideration of items regarded relevant at selected TML levels.

The long-term vision for the TML Assessment is that it become a "gated process," where expectations are that all prior TML criteria are met before a particular analytical model or tool can progress to the next level, yet where flexibility is maintained to permit tailoring to the many, diverse applications which ICME will surely entail in the future.

5.3 Risk vs. Consequences Assessment: The previous discussion regarding TML must always be considered in the context of specific applications. There may be many application-specific considerations which could affect content of the associated V&V plan. Certainly one consideration must be "what risks are involved if an ICME-based analysis or decision is made?" The related question, of course, is "what are the potential consequences associated with that risk?" ***These questions are usually posed in the context of a program, especially programs for technology or product development, rather than as an aide to development and assessment of analytical tools.*** Note that this is not intended to be an assessment of a specific ICME model – but rather the project or program risks that should be considered in association with ICME application. They are considered appropriate here for ICME V&V planning, however, because the intent of ICME in general is to replace historical, empirically based processes with more analytical, physics or science-based processes. Benefits of ICME may be realized through reduced development time and cost, reduced experimental test and validation requirements, fewer iterations or unplanned events in technology development or implementation, new "development space" being predicted from analyses, etc. In most or all of these cases, integration of ICME and ICME-based decisions with current technology or product development processes will be required. The more dependent a technology or product development program is upon ICME, the more important the state of verification and validation will become. And, the more significant the decisions or impact of ICME applications become, the more important an assessment of any associated risks and their related consequences will be.

Earlier in this document, the philosophy and approach for ICME V&V was described. This included the desire to align V&V of ICME models and methods to established, gated processes such as TRL and MRL for technology development, and IPD for product development. The approach was to link the level of V&V required, as indicated by TML, to the intended application. It is recognized, however, that this linkage could be somewhat subjective. Consequently, an approach is proposed to assist evaluation of risks and consequences of ICME applications, with intent to help develop V&V plans and to identify any risk-mitigation actions that might be prudent.

The proposed approach is based upon the NASA "Consequences vs. Likelihood 5X5 Risk Matrix" [13], modified slightly for ICME use. The philosophy and alignment with gated processes was presented earlier in this document. Slight modifications to the likelihood percentage cutoffs were made, and notes related to consequences were developed specifically for ICME. These are embedded in the Excel versions for easy recall and reference. An image of the "5X5 Risk Matrix with ICME-relevant notations was presented previously in Figure 10.

It is intended primarily for use during the planning phase for programs or ICME model development efforts, when V&V plans are being developed, and also when program plans that involve ICME-based decisions are being generated. The process consists of three steps:

1. Identification of specific risks. This may be in the form of a short list.
2. Estimation of the likelihood of occurrence and the potential *program or ICME application* consequences. These are plotted on the 5X5 Risk matrix.
3. Development of risk mitigation actions *where appropriate*, to reduce likelihood of occurrence or potential consequences. Risk mitigation actions might be defined in the form of alternative processes, backup plans, additional testing or measurement data, etc.

Effective risk mitigation plans should reduce likelihood of occurrence and/or consequences to a level deemed acceptable for the application. These would typically be considered "green," or possibly "yellow," in the assessment matrix.

TML Assessment and "Risk vs. Consequences" Example: As with the ICME V&V example described in the previous section, example applications of the Tool Maturity Level assessment guide, and associated risk vs. consequences assessments, are needed to help practitioners accelerate and strengthen the application of V&V within ICME development programs. The best and most relevant examples will ultimately be drawn from successful ICME projects involving an integrated system of models targeted for specific applications. A hypothetical example is provided below.

Consider a comprehensive ICME effort aimed at predicting bulk residual stresses in an aerospace component, which will include process-induced residual stresses from forging and heat treatment, and the redistribution of these stresses after final machining. The goal of this ICME program is to reduce the machining cost by predicting and managing any distortion within the desired final part envelop and to integrate the analytically predicted bulk residual stress effects into final component service-life predictions. Model development includes new modules as well as the extension of existing tools by incorporating new data related to the specific material and application. V&V plans have been developed in accordance with the Checklists with the intent to achieve TML-3 at completion.

TML-3 [4] represents a mature analytical tool or model – one that could significantly reduce or eliminate iterations in a material or process development program, and potentially reduce experimental testing or other analytical requirements. At TML-3, the model can be used directly for assessments or evaluations of derivative materials or processes, or deviations from known practices. While the accuracy or fidelity of the model may not be fully validated, the range of application should be well defined and documented. In addition, supporting data should represent the entire range of application, a User's Guide should be fully developed and updated (from TML-2 level), version control for software implemented, and significant sub-model validation completed. Finally, at TML-3, a Risk vs. Consequences assessment is highly recommended prior to any significant application.

In this hypothetical example, it is uncertain whether TML-3 will be totally achieved, and what impact that might have on realizing all the program and project goals. Further, it is uncertain whether TRL-3 is an adequate maturity level to achieve the most ambitious project goal: use of the predicted residual stress fields in the component life predictions for fatigue and damage tolerance. Consequently, the developers and project team generated a high-level flow diagram from their System and Model level checklist information, to help assess the critical elements for V&V, as illustrated in Figure 8.

The project and development team identified five specific items that appear to be significant risk areas that warrant additional consideration in the V&V plan for this application. These are indicated with numbered symbols in Figure 16.

Process Step	**Starting Billet Stock**	**Forging and Heat Treatment**	**Machining and Finishing**	**Assembly**	**Service**
ICME Focus Areas	Description of starting composition and microstructure	Microstructure-property evolution and **residual stress field**	**Residual stress field** evolution and part distortion	**Final residual stress field** in part after assembly	Integration of residual stress field with service stress for life prediction
Critical Elements (for the ICME effort)		• Temperatures (1) • Time transients • Microstructure evolution (3)	Part geometry and removal sequence (4)	(4) Assembly tolerances	High fidelity and confidence in residual stress field predictions (5)
Critical Validation Elements		• Temperatures and transients • Heat transfer coefficients (2) • Measured RS field	• Dimensional changes • RS field in finished part (2)	• Dimensional tolerances for assembly fit	• Life prediction validation

Figure 16: Simple Flow Map for Hypothetical Example – ICME Prediction of Residual Stresses in Heat Treated and Machined Forgings

The team then constructed a working table to list the specific risks, estimated the likelihood of occurrence and the severity or potential impact to the project. This is illustrated in Figure 17, below.

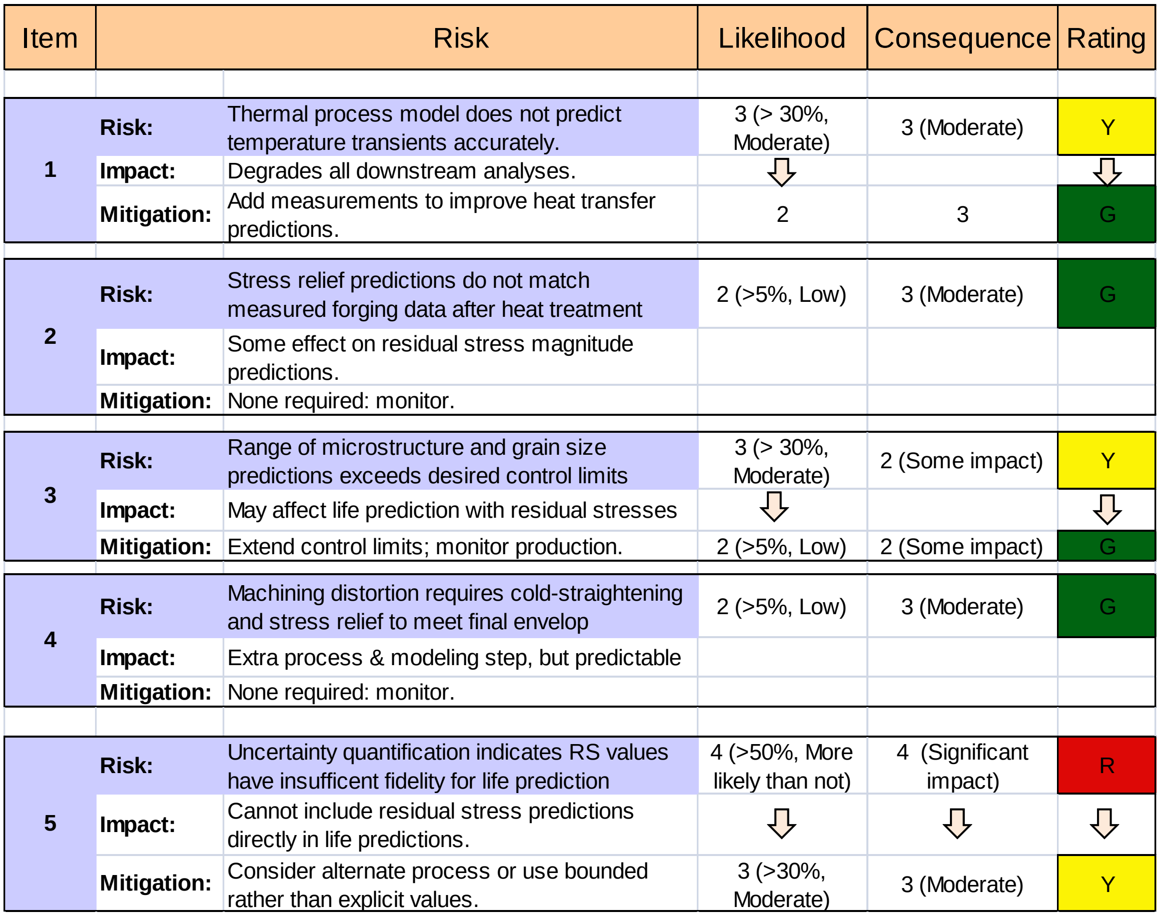
The developers and project team determined risk mitigation actions, where appropriate, and estimated the effect on reducing program risk and potential consequences:

1. *Thermal process modeling must accurately predict temperatures and temperature transients during processing in order to predict resulting residual stress fields.* The project team performed a parametric analysis where such predictions were evaluated for typical aerospace rotating components. This analysis found that determination of accurate heat transfer coefficients, especially for use during high

transient thermal processes, was critical. Consequently, additional measurements of part temperature during processing and use of complementary methods to estimate heat transfer coefficients were deemed necessary.

2. *Measured residual stresses must reasonably validate predicted values for the intended purpose.* Virtual uncertainty quantification (UQ) experiments were performed with combined error sources using nominal magnitudes in order to estimate the current stress prediction error for the residual stress measurement technique. In performing the simulations, emphasis was placed on simulating "worst-case" scenario error sources in order to understand the lower bounds of accuracy associated with the method. Based on the results of the virtual experiments the team planned additional, more sophisticated stress-relaxation mechanical tests to ensure adequate constitutive data to support the modeling efforts. The team also decided to use multiple methods for residual stress measurement validation.
3. *Variation in final microstructures must be within desired control limits for the intended application* – to ensure that material properties and behavior meet design intent. The project team recognized this as a potential risk, but has experience with microstructure evolution modeling for this material and determined that the risk can be mitigated or eliminated with early production monitoring and controls.
4. *Distortion during finish machining may result from redistribution of process-induced residual stresses.* This may relate to placement of the final part within the forging envelope, and any variations in that placement. For the rotating parts considered in this project, the team regarded this risk as low but required simulation of final part placement in the forging envelop, and assessment of machining sequence effects on distortion.
5. *Fatigue and damage tolerance life predictions require high fidelity stress values for required accuracy.* The project team was concerned that the accuracy of residual stress predictions may be suitable for use in defining forging shapes, reducing input weights, and predicting or controlling part distortion during machining, but not sufficiently accurate to use directly in life predictions. Further, potential errors in residual stress measurement accuracy may preclude or limit validation. The project team regarded this as a risk that was likely to occur based on similar studies [19], and that would have significant impact if it did occur. The team adjusted this specific project goal and decided to use the residual stresses for static assessments such as potential impact on rotor burst limits, rather than directly in Low Cycle Fatigue (LCF) and fracture mechanics life predictions. The team agreed to reassess at a future date, pending improved elements of the ICME modeling efforts, measurement techniques, or demonstrated ability to achieve TML-4 for this process.

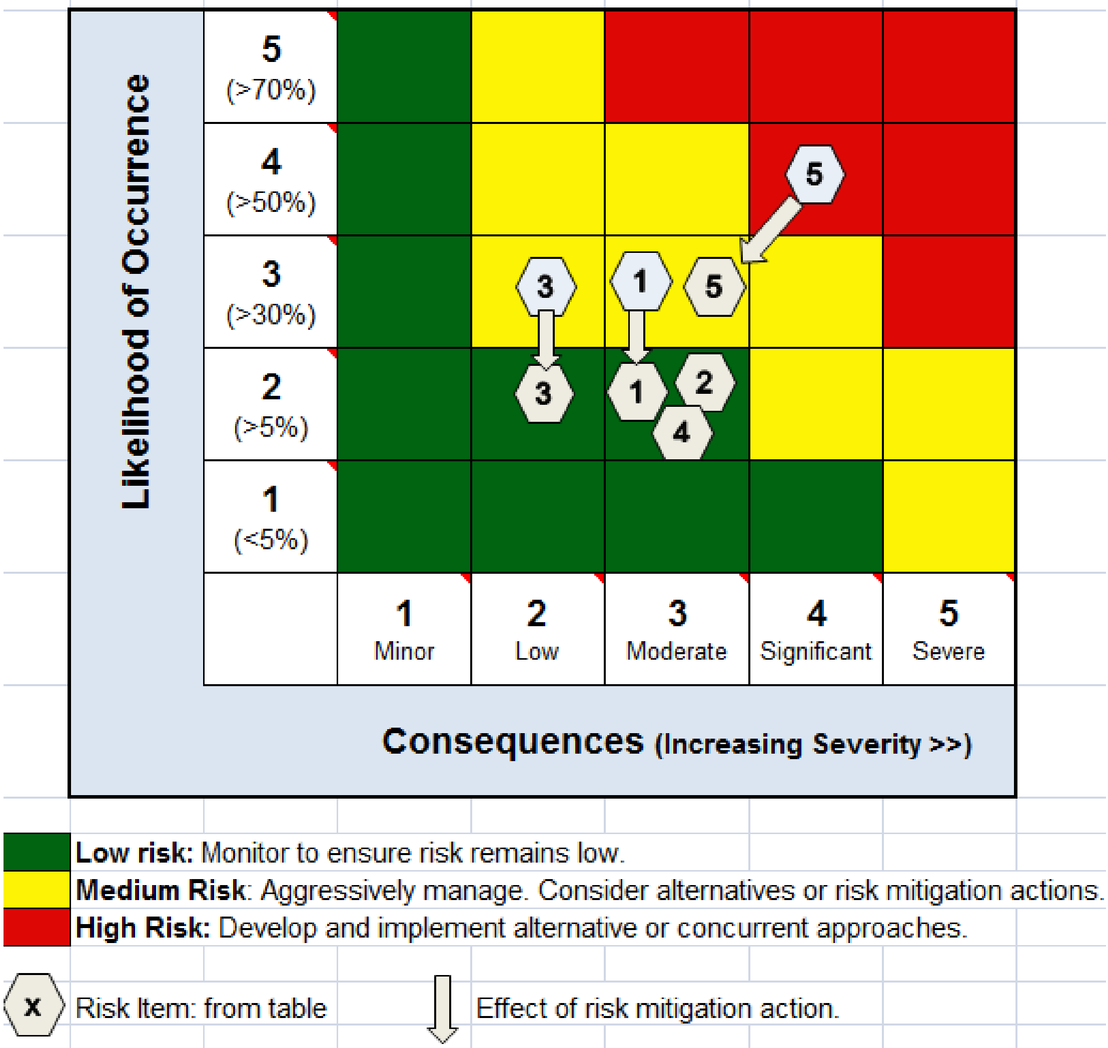
The resulting list of risks, estimated likelihood of occurrence, estimated consequences, and a simple “red-yellow–green” assessment of importance are summarized in Figure 9.



Item	Risk		Likelihood	Consequence	Rating
1	**Risk:**	Thermal process model does not predict temperature transients accurately.	3 (> 30%, Moderate)	3 (Moderate)	Y
	Impact:	Degrades all downstream analyses.	⇩		⇩
	Mitigation:	Add measurements to improve heat transfer predictions.	2	3	G
2	**Risk:**	Stress relief predictions do not match measured forging data after heat treatment	2 (>5%, Low)	3 (Moderate)	G
	Impact:	Some effect on residual stress magnitude predictions.			
	Mitigation:	None required: monitor.			
3	**Risk:**	Range of microstructure and grain size predictions exceeds desired control limits	3 (> 30%, Moderate)	2 (Some impact)	Y
	Impact:	May affect life prediction with residual stresses	⇩		⇩
	Mitigation:	Extend control limits; monitor production.	2 (>5%, Low)	2 (Some impact)	G
4	**Risk:**	Machining distortion requires cold-straightening and stress relief to meet final envelop	2 (>5%, Low)	3 (Moderate)	G
	Impact:	Extra process & modeling step, but predictable			
	Mitigation:	None required: monitor.			
5	**Risk:**	Uncertainty quantification indicates RS values have insufficent fidelity for life prediction	4 (>50%, More likely than not)	4 (Significant impact)	R
	Impact:	Cannot include residual stress predictions directly in life predictions.	⇩	⇩	⇩
	Mitigation:	Consider alternate process or use bounded rather than explicit values.	3 (>30%, Moderate)	3 (Moderate)	Y

Figure 17: Example of Risk Identification, Impact and Mitigation Estimates for Hypothetical Forging Residual Stress Example

Expected effects of the planned mitigation items are also shown in Figure 17, with changes indicated by the small arrows. The five risk items are plotted on the 5X5 Risk vs. Consequences Matrix in Figure 18, at the assessed levels for likelihood and consequence. This figure illustrates the effect of the planned mitigation actions, and improvements to the V&V plan for this ICME project. The assessment indicated that Items 1 and 3 could be improved from "yellow" to "green" with mitigation actions, and that Items 2 and 4 posed some risk but did not require any risk mitigation actions. Item 5 obviously posed a high risk which could be reduced with mitigation actions but would still warrant attention of the project and development team.



🟩 **Low risk:** Monitor to ensure risk remains low.
🟨 **Medium Risk**: Aggressively manage. Consider alternatives or risk mitigation actions.
🟥 **High Risk:** Develop and implement alternative or concurrent approaches.

Risk Item: from table
Effect of risk mitigation action.

Figure 18: Example Use of Risk Matrix and Effect of Mitigation Actions

This is just a hypothetical example, of course, but it shows how a project risk management tool can be used in conjunction with the ICME System Level and Model V&V Checklists, and the TML Assessment guide to assist ICME V&V planning, especially for developmental ICME models or methods, or when development program decisions will be ICME based.

5.4 Summary Comments Regarding TML Assessment Guide and Risk vs. Consequences: The TML Assessment guide was developed as a tool to aide practitioners in assessment and communication of the maturity of ICME models and methods, especially as they relate to intended applications. The Risk vs. Consequences approach was adapted from well established risk matrix approaches for program risk assessment and mitigation planning. Both tools were developed to be compatible with well-established processes such as TRL, MRL, and IPD for technology and product development, where many future ICME applications will be focused. When used in conjunction n with the System-Level and Model Checklists that were also developed under this project, it is believed that consistent, rigorous, and comprehensive V&V will result. If these tools become broadly accepted and used, they will form the basis for communication of the maturity of ICME models and methods, hopefully in a manner similar to current TRL assessments.

6. Recommended Best Practice: Process Flow Chart and Description:

6.1 Introduction: This document is intended to succinctly present a recommended best practice for assessment and planning of Verification and Validation for ICME methods and models (V&V). It was developed specifically for aerospace structural materials. It was intended to include a simple listing of recommended steps in the best practice, an illustration of the recommended best practice in flow-chart format, and the various support tools and references that have been developed to assist practitioners. These support tools are in the form of Excel spreadsheet tables, and include an ICME V&V System-Level Checklist, an ICME V&V Model Checklist, a Tool Maturity Level (TML) Assessment Guide, and a Risk Matrix tool for assessment and mitigation of application risks.

6.2 Recommended Practice for ICME V&V Planning and Assessment: Rigorous, systematic verification and validation is regarded critical to successful development and broad implementation of ICME. Development of a comprehensive V&V plan and model assessment is highly recommended whenever a new or derivative model is under development, and whenever a new program or project application is planned. The recommended practice for V&V planning and assessment can be simply stated in the following steps:

- Define and document the model and the intended application.
- Develop a comprehensive V&V plan for the modeling system and constituent models.
- Assess the tool maturity level that is required and that will be attained at completion of model development and V&V efforts.
- Iterate the V&V plan and develop any risk mitigation plans that may be required for the application.
- Execute the development and V&V plans and assess the outcome.

The recommended process was conceptually illustrated in its simplest form by the flow chart in Figure 11. Note that the V&V Plan and Tool Maturity Level Assessment are related and are intended to be interactive. Criteria in the TML Assessment Guide relate to V&V Checklist items, and an objective assessment of the expected state of tool maturity is of course dependent upon the plans and execution of the ICME V&V Checklist items.

The recommended practice is illustrated in more detail in Figure 19. The intent is to show all of the key process steps, and indicate where the various support tools should be applied.

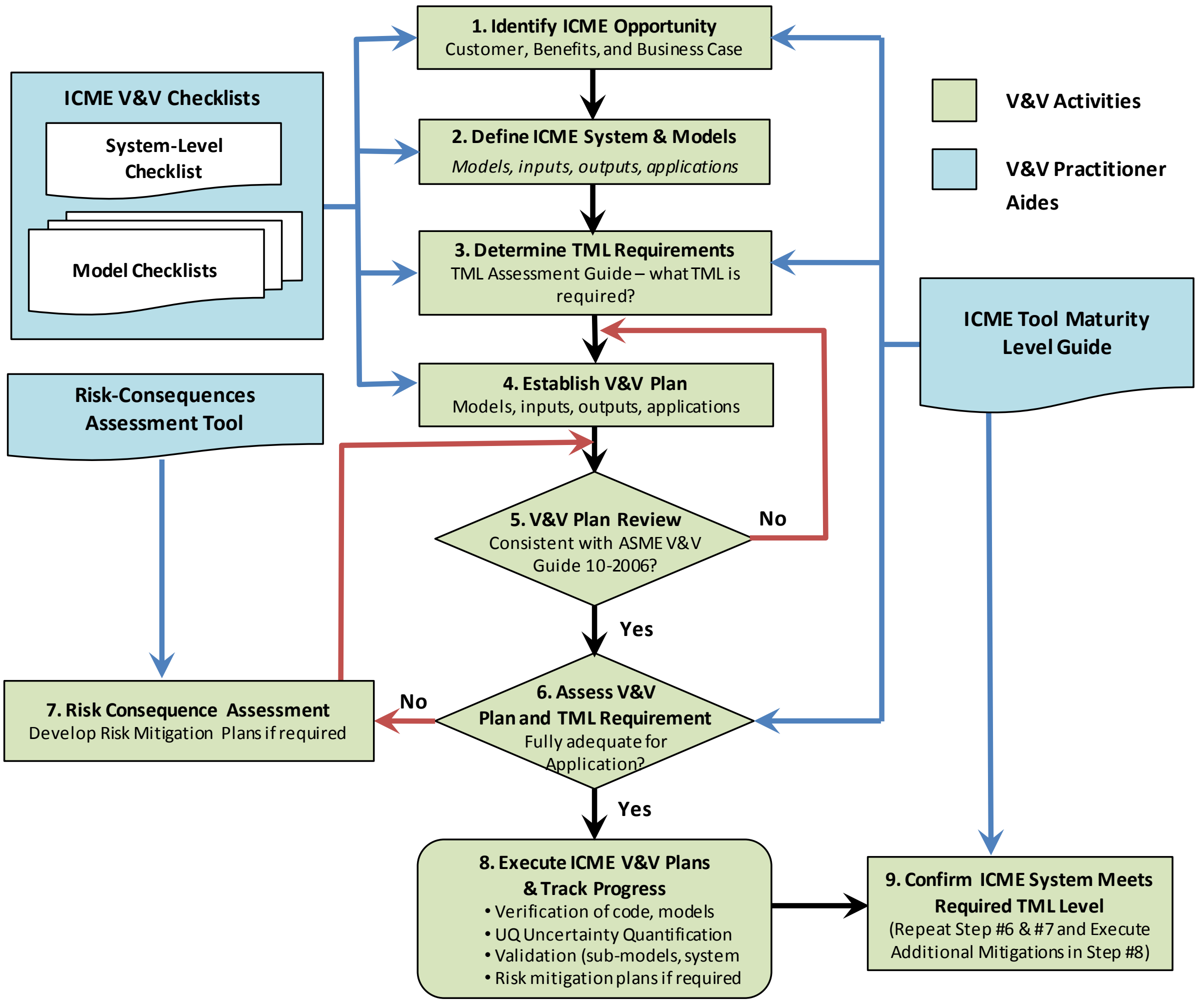


Figure 19: Flow Chart of Recommended ICME V&V Planning and Assessment Process

The recommended process can be described by the following steps:

1. **Identify ICME Opportunity:** when a new or derivative ICME method or model is proposed or under development, or when an existing model is planned for use in a new application. This step represents a formal commitment to enter into V&V assessment and planning activity. It includes discussion with the end use customer, determination of the requirements for the specific application, and understanding of the benefits or business case. The System Level Checklist (section A) should be considered in this step.

2. **Define the ICME System and Models:** intended to formally document the model or method, including the model inputs, outputs, the intended application, and any required or supporting analyses or data that may be required. It is when the model developer(s) or researcher(s) must consider

customer or project requirements and determine at a high level how the proposed or current ICME approach relates. The objectives of the ICME model or method development and V&V activity should be specified in this step. The System and Model Level Checklists (sections B and W) should be considered in this step.

3. **Determine Tool Maturity Level (TML) Requirements:** The TML requirements for the intended application should be assessed in this step. This requires that the TRL, MRL, IPD, or other appropriate technology or product development requirements be assessed for the intended application, and a determination made as to what Tool Maturity Level is appropriate or required for the ICME method or model. This assessment is key to guiding the level and fidelity of the activities that are required for successful V&V. Trending or ranking applications may require limited V&V demonstration; use of ICME models to significantly guide or reduce experimental or other analytical efforts may require more detailed V&V activities, and use of ICME for key decisions or analyses with limited supporting data may require extensive V&V activity including benchmark case demonstrations. The TML Assessment Guide as well as the System Level Checklist should be used in this step.

4. **Establish the V&V Plan:** V&V requirements, detailed planning, and tracking methods for the execution of the V&V plan should be addressed in this step. Both the ICME V&V System and Model Checklists should be used in this step. In addition, it is recommended that practitioners use PIRT (Phenomena Importance Ranking Technique) or similar method for describing and understanding the hierarchy and relative importance of various parameters and models to the overall ICME system under development. Individual checklists should be developed for each model or significant sub-model used in the process.

5. **V&V Plan review:** should include an assessment and review of the overall plan for completeness and adequacy. It is highly recommended that the plan be reviewed for consistency with the guidelines presented in the ASME V&V Guide 10-2006. Any recognized deficiencies in the plan should be addressed or documented in this step**.** If the review indicates deficiencies or unacceptable risk, the V&V plan developed in Step 4 should be reviewed and revised.

6. **Assess V&V Plan and TML Requirement:** should include an assessment of the plan and TML requirements **specifically for the intended application**. Any recognized deficiencies in the plan or specific risks for the application should be addressed or documented in this step**. It is intended that this step represent a "gate review," where passing the review constitutes program or project concurrence with the V&V assessments and plan for the ICME model and application.** If the review indicates deficiencies or specific application risks, a Risk vs. Consequences Assessment should be made and any necessary mitigation plans generated.

7. **Risk-Consequences Assessment:** This step is recommended to determine if some form of risk mitigation is appropriate for use of the ICME methods or models for the intended specific application. It is highly recommended that this process be utilized whenever significant program or project decisions will be based on the ICME methods or models under development or review. The recommended project risk management approach is based on the NASA "Likelihood vs. Consequences 5X5 Risk Matrix" [13]. The matrix modified for ICME V&V application is recommended.

8. **Execute ICME V&V Plans and Track Progress** This step represents the execution of the V&V plan, including verification of codes and models, uncertainty quantification, validation of sub-models and models, and execution and assessment of any risk mitigation activities. Results should be used to update status of items in the Checklists and Tool Maturity Level (TML) Assessment Guide.

9. **Confirm ICME System Meets Required TML:** This step is intended to determine whether the desired model maturity was achieved. As such, it should be regarded as an assessment of exit criteria and perhaps also constitute either a gate review or preparation for a gate review, where the model developers in conjunction with program or project representatives determine whether the ICME system is approved for use in the intended application, or if additional risk mitigation is warranted.

Completion of the preceding process ensures that the execution phase for ICME V&V can be initiated with confidence, including all verification, uncertainty quantification, and validation efforts. It is certainly expected that periodic review and reassessment would be conducted, and any appropriate changes implemented.

6.3 Closing Comments: It was the intention of the authors to provide a useful, rational, and structured process to facilitate and standardize ICME V&V activities. Associated support tools were developed, documented, and integrated to aid in practitioner implementation. The intent was to develop a process that would be broadly applicable and flexible, but not overly prescriptive. In the end, successful use is dependent upon the practitioners who employ the process and those who require its use.

7. Summary:

ICME has the recognized potential to greatly benefit the materials science and engineering communities, and to greatly enhance integration with other engineering disciplines. The potential benefits of ICME to reduce time, cost, and risk of materials and process technology development, and to enhance future "design" of materials and processes, are enormous. Verification and validation of models and methods pose significant challenges to broad development, implementation, and acceptance of ICME. This is believed especially relevant where significant decisions will be ICME-based. These decisions may affect technology or product development, legacy system sustainment actions, supply base decisions, or quality assessments. As was concluded in a 2013 study organized by the Minerals, Metals & Materials Society (TMS), methods and standards for effective verification and validation of ICME methods and models is a cross-cutting issue – one that affects aerospace, automotive, and maritime industries. [18]

AFRL/RX initially sponsored activity to assess the current state of V&V for ICME, compare it with the approach to V&V taken by other engineering disciplines such as computational solid mechanics, and to develop an approach and tools for use by the ICME community. Subsequent feedback from various programs and practitioners was solicited for the purpose of updating and improving the initial versions.

The resulting approach and tools are aligned with current well-established technology and product development processes such as TRL, MRL, and IPD. The guidelines are consistent with, and frequently reference, the well-established ASME V&V Guide 10-2006, developed by the computational solid mechanics community over many years of effort. Finally, the practitioner tools that were developed and improved in Revision include an ICME V&V System-Level Checklist, a Model V&V Checklist, a TML Assessment Guide, and a risk matrix tool for project risk assessment and mitigation.

Much effort went into making these tools broadly applicable, useful, simple, and flexible - and then integrating them to ensure compatibility. Instructions for their use, and examples of their application were developed. Finally, a simple Recommended Best Practice, presented in Section 6 of this report, was developed and illustrated to aide practitioners in selection and use of these tools.

The authors recognize that this will be an evolving effort. It is hoped that the tools and approach will be continuously improved and updated, with increasing application experience. Most of all, we hope they prove useful.

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Acknowledgements

The authors would like to acknowledge Dr. Rollie Dutton of AFRL/RXM for his continued support and insight in development of this document and its predecessors. Dr. Dutton, and AFRL/RX, recognized the need for more rigorous ICME V&V, and the importance of it to future development, implementation, and acceptance of ICME. The continued support for this effort, including the original concept development and this most recent revision, and the timely integration of it with other AFRL, MAI, and industry efforts, has been key to success.

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Appendix A

ICME Verification & Validation Example

A.1 Introduction

The Verification and Validation (V&V) process description, as presented in this V&V Guideline, has been abstract by necessity, because it was meant to serve the full spectrum of ICME programs that include diverse materials technologies, ICME maturity levels, program scopes, and application requirements. This section of the guideline intends to go beyond abstraction, by giving a real example; and by design, a simple one that avoids complexity and helps delineate key issues more clearly. The example will also show how V&V tradeoffs are unavoidable to combat limitations imposed by technical, budgetary and schedule constraints. The selected ICME example involves the prediction of the strengthening precipitate size distribution and its effect on yield strength (hardness) for Aluminum 6000 series alloys, within a larger ICME modeling system. The subsections that follow will follow the workflow of this real, yet simple, ICME V&V example.

A.2 V&V Plan

The reality of interest for the "example" ICME system involved the prediction of mechanical strength (e.g., □□□□□□□□□e□□□□) of an extruded and heat-treated thin-wall Aluminum 6082 alloy panel. The customer's technical lead intended to build an ICME system to help plan and guide development of extrusion and heat treatment processes for such structures using the ICME system shown in Figure A-1.

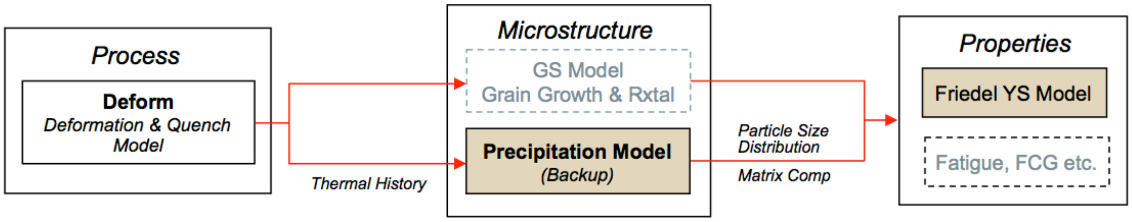

Figure A-1: Flow chart showing the V&V case study ICME flow; Boxes, colored brown, show the focus of V&V effort for the V&V example

At the outset of this ICME program, the team initiated adaptation of a state-of-the-art precipitation model, which had been successfully applied to nickel-based superalloys. However, when this development encountered unexpected delays, a short and very modest effort was undertaken to apply a simplified precipitation model and a yield strength model, which were based on the published work of Myhr [A-1, A-2].

The customer had only moderate expectations for performance of the backup precipitation model; it needed to replicate trends previously reported by Myhr (i.e., a targeted maturity level of TML-2). Despite the low TML level, the backup model required V&V to: (1) assure that the Myhr mathematical models were properly implemented within the programs computational model, (2) verify that spatial and time increments were properly selected, and (3) confirm that the models were applicable to the aluminum A6082 alloy, which lay at the extreme bound of the range of applicability for the models.

Like other ICME development efforts, V&V for this program was constrained by both schedule and budget. V&V for backup models in this program needed to be brief and economical owing to the provisional nature of the models and the lack representative extruded A6082 for yield strength measurements. The V&V plan followed the ASME V&V process flow, Figures 13 and 14, but focused solely on model verification and system level validation. It was argued that Myhr [A-1, A-2] had validated the precipitation model by using TEM precipitate size analysis and validated of the yield strength model for the alloys, used in their research, via hardness testing. System level verification was deemed unnecessary because both models were integrated via a single MatLab™ script. System level validation, within this program, involved the comparison of predicted and measured A 6082 hardness values for a series of heat treatment trials. Yield strength measurements could not be included in the study because there was insufficient thin wall extruded A6082 material to machine tensile test specimens.

A.3 Model Formulation

The backup precipitation model followed the formulation described by Myhr [A-1, A-2]. This model is physically based upon classical nucleation and growth theories; albeit it utilizes several simplifications to circumvent lack of knowledge about several unknown parameters and to streamline computation. The major elements of the precipitation model are described below:

- Thermodynamics: The model assumes that precipitation of the strengthening β” phase is governed by a reduced-order relationship describing the solubility of Mg and Si in Al and uses the Gibbs-Thompson relationship to account for the influence on particle size on solubility. A simplified relationship is used to account for the fraction of silicon consumed by alpha phase formation.
- Nucleation Rate: A classical heterogeneous nucleation rate equation is used to determine the number of nuclei added to the particle size distribution at each time step of the computation. This rate equation includes a fitted parameter, j_0, to describe the nucleation rate constant and the free energy, ΔG^*_{het}, is described using a fitting parameter, A_0, determined via experiment. The approach is lacking because it takes no account for precipitate incubation or the variation in potency among heterogeneous nucleation sites.
- Growth Rate: The model uses a very simple growth equation wherein the particle interface velocity is a linear function of the difference between the matrix interface composition, C_i, and the average matrix composition, C_{bar}. This formulation ignores both the non-linear compositional profile in the matrix away from the particle interface and the potential for impingement effects (i.e., overlap in compositional profiles between adjacent particles).

The yield strength model includes strengthening relationships based on Friedel’s formulation to derive alloy yield strength and hardness values based on the size distribution of the strengthening precipitates.

The equations representing these phenomena and ancillary mathematical relationships representing these phenomena are solved numerically as an initial-value problem using internal modeling parameters provided by the Myhr research. The backup precipitation model was implemented within MatLab following the Myhr solution scheme, outlined in Figure A-2.

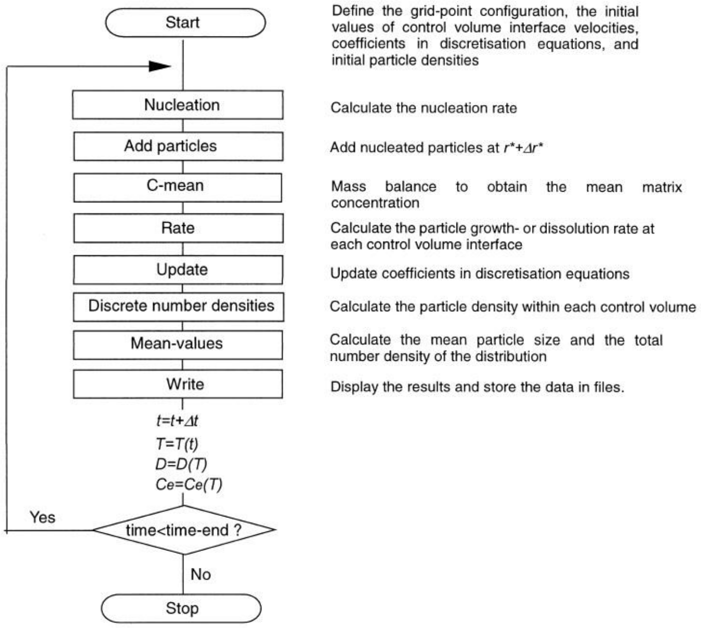

Figure A-2: Flow diagram showing the main elements of the particle size simulation loop, from Myhr [A-1].

A.4 Verification of the MatLab™ Computational Model

Verification for the A6082 precipitation model included three steps that involved checking the MatLab™ code to identify and resolve errors; comparing simulation results against a benchmark computation; and examining model output for anomalies. The original Myhr papers described the computational implementation thoroughly (except for radius and time increments), thereby reducing debugging to little more than correcting several simple code syntax and typographical errors.

The benchmark verification entailed comparing output for the MatLab™ implementation against results reported in Myhr [A-1]. The comparison included checking predictions of nucleation rate, particle number density, mean particle radius, and the particle size distribution at discrete times during isothermal aging. For each output characteristic, output from the MatLab™ implementation matched the published Myhr results very well. A comparison of predicted precipitate particle size distributions is shown in Figure A-3. The two sets of modeling results nearly overlay each other except near the peak of the distribution; this discrepancy was attributed to likely small differences in the time and/or radius (particle size) increments used for numerical integration.

The benchmark verification demonstrated that the model was properly implemented within MatLab™. However, subsequent application of the model for A6082, using a modified thermodynamic relationship provided by Myhr [A-2], revealed an unexpected anomalous secondary spike in the predicted particle size distribution. This peak, shown in Figure A-4, was transient, forming and disappearing within a relatively brief time window. The presence of the anomalous peak required additional verification that involved determining whether it reflected a numerical instability, a discontinuity in the revised thermodynamic formulation, or a spurious nucleation event.

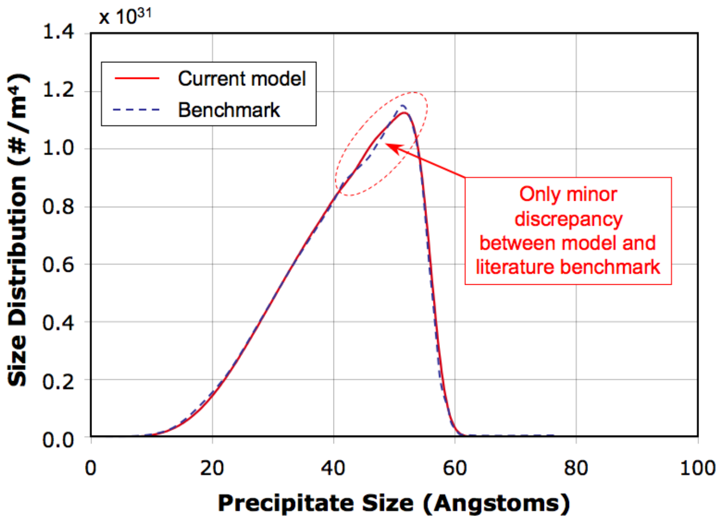

Figure A-3: Comparison of particle size distributions calculated by Myhr [A-1] (benchmark) and the current MatLab™ implementation following 10 hours age at 180 ºC .

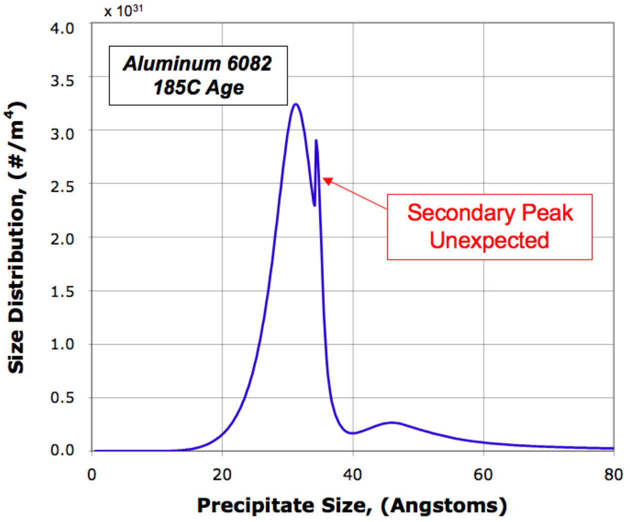

Figure A-4: A6082 precipitate size distribution exhibited a transient anomalous peak following a 2 hour aging heat treatment at 180 ºC.

Study of the anomaly, involving changing the integration time and spatial increments along with use of the earlier thermodynamic relationship, failed to eliminate the anomalous peak. However, careful examination of mass flows among cells in the vicinity of the peak and inspection of the local cell mass balance, indicated that the anomalous peak was a natural consequence of the nucleation formulation. Specifically, the Myhr model assumes that all nuclei forming during a time step have a fixed radius, which leads to an exaggerated increase in number density for that precipitate size. This conclusion was confirmed by "turning off" nucleation during the critical time window, which eliminated the secondary peak. Despite this finding, the team decided against attempting to fix the nucleation formulation (e.g., by dispersing the nuclei radius) because no data was available to guide or validate such an adjustment; and furthermore, the spurious peak had no significant effect on yield strength predictions, as verified via analysis using the ancillary strength model (with the spurious peak turned "off" and "on.

A.5 Validation of the A6082 Precipitation Model

The Myhr research team [A-1, A-2] had rigorously validated the foundational model for a range of aluminum-magnesium-silicon alloys and select thermal cycles. This work included activities such as electron microscopy to measure precipitate sizes and number densities, and hardness testing to infer yield strength. System validation and uncertainty assessment of the A6082 MatLab implementation was significantly more modest and included both experimental and modeling activities. In overview, system validation consisted of comparing simulation of precipitation and subsequent hardening against experimentally determined aging curves that describe A6082 hardness as a function of aging time. Specific elements of the study included:

- Measurement of temperature variation during heat treatment and hardness measurement error;
- Heat treatment trials involving the aging of coupons for differing lengths of time;
- Replicated hardness measurements for each coupon coupled with subsequent calculation of hardness uncertainty;
- Simulation of precipitate size distributions and associated hardness values for A6082 coupons heat treated per the experimental plan; and
- Synthesis of a lower bound of system simulation error via the Monte Carlo method using the results of a sensitivity analysis and uncertainty estimates for model inputs and parameters. The results were judged to represent a lower bound because undoubtedly not all sources of uncertainty were included in the analysis.

The results of the validation exercise and embedded uncertainty assessment are shown in Figure A-5. The graph shows that results of the A6082 precipitation model in combination with the yield strength model show similar hardening trends; qualitatively the agreement appears good. The data averages at each ageing time appear close to the model results, at least for those times greater than 30 minutes; and the uncertainty of the data (2 σ error bars) and of the model (shaded area from Monte Carlo analysis) are comparable.

Application of one validation metric, which is determined by calculating the area between the cumulative distribution functions (CDF) for experimental and simulation results, more clearly delineates the level of validation. An example of this validation metric, as calculated for ageing times of 30 minutes and 10 hours is shown in Figure 5-6. The poor validity at 30 minutes is made quite clear, given that the validation metric is greater than 6 times larger (poorer) than for the 10 hour case. Yet, the poor model performance at short ageing times is understandable, because the nucleation model ignored incubation effects and experimental errors associated with specimen heat-up and transfer times (furnace to the quench media) have a greater impact during shorter aging treatments.

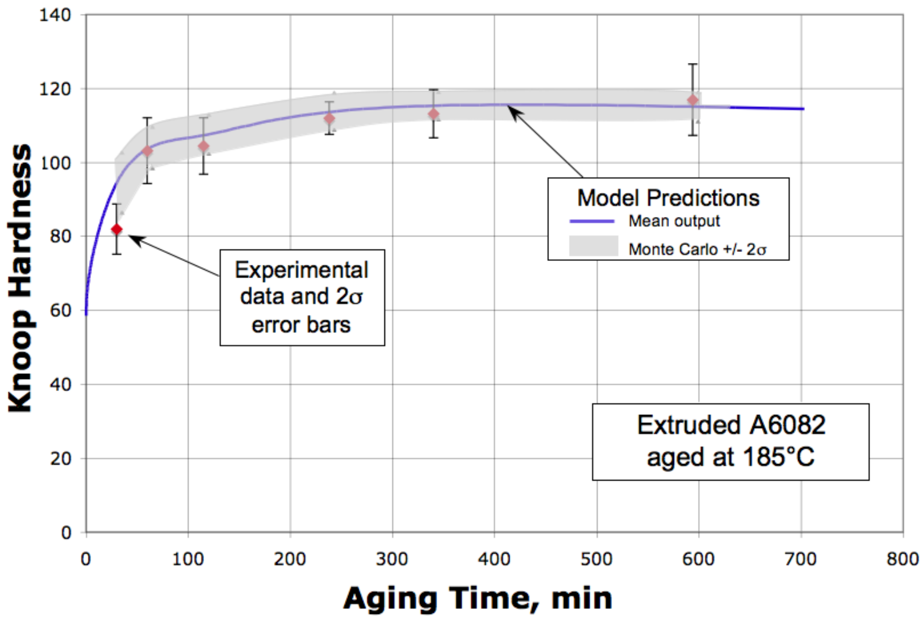

Figure A-5: Comparison of experimental and system validation results for the MatLab implementation of the Myhr precipitation model.

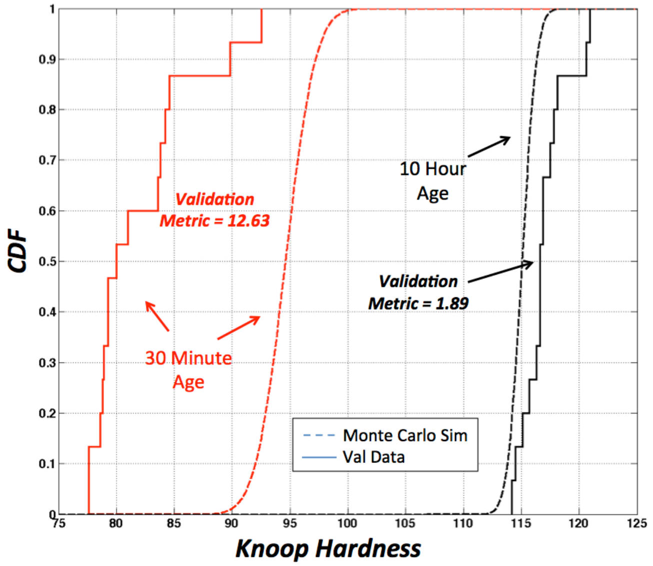

Figure A-6: Chart showing the difference between the data-derived empirical CDF curve and the system simulation-based CDF curve for A6082 specimens aged for 30 minutes (red) and 10 hours (black). The validation metric for each aging time denotes the area between the empirical and simulation based CDF curves.

A.6 Final TML assessment and conclusions

It is useful to review the V&V results of this case study, to determine whether the combination of the precipitation and yield strength backup models met the up-front requirement of TML-2. This assessment will be carried out by gaging the program's V&V information and findings against the TML-2 criteria within the ICME V&V Tool Maturity Level Assessment Guide, column-by-column as shown below:

Model rationale, basis, and definition: Both the precipitation model and yield strength model were defined and justified in peer-review, published research by Myhr [A-1 and A-2], which predated the program. The range of inputs and outputs were established in the present work.

Complexity and documentation: The dependencies between all models within the system defined and both the precipitation and yield strength models were integrated within the system code.

Supporting data: Data supporting internal modeling parameters, microstructural characterization information, hardness testing results, and aging furnace temperature records were obtained and documented by Myhr [A-1 and A-2] and within the present program. Values of the nucleation rate, pre-exponential constant j_o, were determined via calibration within Myhr's research effort.

Model verification: The MatLab computational code used in the present program was subject to "code verification" and errors were fixed. Subsequently, a three step "calculation verification" was conducted to: (1) verify that radius and time increments were sufficiently small to provide stable precipitate size distributions, (2) demonstrate that the MatLab implementation replicated Myhr's (benchmark) results, and (3) resolve an anomalous short-lived peak in the β'' particle size distribution.

Range of applicability and UQ: The program expanded the range of applicability to include the Aluminum A6082 alloy. UQ analysis included determination of uncertainty of the ageing heat treatment temperature, uncertainty of hardness measurements, determination of sensitivities for key internal modeling parameters, model inputs, and model outputs. Model output uncertainty was estimated by using Monte Carlo analysis.

Risk assessment and validation: Risk-Consequence analysis was conducted during initial assessment of the Myhr [A-1 and A-2] precipitation model, and several model simplifications were identified as possible problems; indeed the absence of nuclei incubation is likely to degraded model accuracy for short ageing times. The model system was validated using hardness test results from ageing trials that were compared to the dispersion of simulation results predicted via Monte Carlo analysis.

The case study V&V outcomes of the case study precipitation and yield strength models meet all TML-2 criteria and therefore are deemed satisfactory as provisional models within the ICME system.

A.7 References for Appendix A

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