DISSERTATION

ON THE INTEGRATION OF MATERIALS CHARACTERIZATION INTO THE PRODUCT DEVELOPMENT LIFECYCLE

Submitted by

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ABSTRACT

ON THE INTEGRATION OF MATERIALS CHARACTERIZATION IN THE PRODUCT DEVELOPMENT LIFECYCLE

The document is broken down into four sections whereby a more complete integration of materials characterization into the product development lifecycle, when compared to traditional approaches, is researched and considered. The driving purpose behind this research is to demonstrate that an application of systems engineering principles to the characterization sciences mechanism within materials engineering and development will produce a more efficient and comprehensive understanding of complex material systems. This will allow for the mitigation of risk, enhancement of relevant data, and planning of characterization procedures proactively.

The first section proposes a methodology for Characterization Systems Engineering (CSE) as an aid in the development life cycle of complex, material systems by combining activities traditionally associated with materials characterization, quality engineering, and systems engineering into an effective hybrid approach. The proposed benefits of CSE include shortened product development phases, faster and more complete problem solving throughout the full system life cycle, and a more adequate mechanism for integrating and accommodating novel materials into already complex systems. CSE also provides a platform for the organization and prioritization of comprehensive testing and targeted test planning strategies. Opportunities to further develop and apply the methodology are discussed.

The second section focuses on the need for and design of a characterizability system attribute to assist in the development of systems that involve material components. While materials characterization efforts are typically treated as an afterthought during project planning, the argument is made here that leveraging the data generated via complete characterization efforts can enhance manufacturability, seed research efforts and intellectual property for next-generation projects, and generate more realistic and representative models. A characterizability metric is evaluated against a test scenario, within the domain of electromagnetic interference shielding, to demonstrate the utility and distinction of this system attribute. Follow-on research steps to improve the depth of the attribute application are proposed.

In the third section, a test and evaluation planning protocol is developed with the specific intention of increasing the effectiveness of materials characterization within the system development lifecycle. Materials characterization is frequently not accounted for in the test planning phases of system developments, and a more proactive approach to streamlined verification and validation activities can be applied. By applying test engineering methods to materials characterization, systems engineers can produce more complete datasets and more adequately execute testing cycles. A process workflow is introduced to manage the complexity inherent to material systems development and their associated characterization sciences objectives. An example using queuing theory is used to demonstrate the potential efficacy of the technique. Topics for further test and evaluation planning for materials engineering applications are discussed.

In the fourth section, a workflow is proposed to more appropriately address the risk generated by materials characterization activities within the development of complex material systems when compared to conventional engineering approaches. Quality engineering, risk mitigation efforts, and emergency response protocols are discussed with the intention of reshaping post-development phase activities to address in-service material failures. While root cause investigations are a critical component to stewardship of the full system lifecycle during a product's development, deployment and operation, a more tailored and proactive response to system defects and failures is required to meet the increasingly stringent technical performance requirements associated with modern, material-intensive systems. The analysis includes a Bayesian approach to risk assessment of materials characterization efforts through which uncertainty regarding scheduling and cost can be quantified.

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1.1 Introduction:

Material systems are increasing in complexity. Meanwhile, the activities associated with research, development, engineering, and manufacturing are being squeezed into increasingly restrictive timeframes. Tools exist to manage concurrent manufacturing efforts, but frequently the inherent complexity of novel material systems is overlooked. For example, as time progresses, technical requirements become more specific and extreme, and new material compositions and processing techniques are developed to meet project specifications, as seen in the evolution of superalloys over time depicted in Belan, 2012. With more complicated compositions and processing, characterization efforts, likewise, become more complex. The aim of this document is to propose a new, systems-driven approach to characterization, specifically tailored to complex materials development, that will allow for the mitigation of risk, enhancement of relevant data, and planning of characterization procedures proactively.

A material can be defined as a substance displaying definable properties. Characterizing a material can be defined as the process by which a material can be understood or interpreted. Therefore, for the purposes of this document, materials characterization can be defined as the act of determining the properties, structures, or distinguishing features of a material with the intention of broadening the knowledge base surrounding that material space or enhancing the utility of the material. Note that this definition includes a pragmatic addendum to separate a more engineering-framed definition from the more abstract uses of the nomenclature.

Furthermore, and again for our purposes, material systems can be defined as an integrated assemblage of substances where the composition and associated properties define a value proposition for the innovator and product manufacturer. The expectations for the performance of these materials are higher than they have ever been. They are expected to be able to accommodate stringent requirements and be integrated wholistically within products designed, developed, and produced for specialized needs and with novel components. It is becoming increasingly difficult to understand and define the properties of materials and problem-solve within the materials science space due to the high complexity of these new systems. Furthermore, tracking and applying the understanding found in fundamental research throughout the development and manufacturing phases of the product, while these phases are happening concurrently, is becoming a more difficult task than traditional methods of materials innovation can accommodate.

An opportunity exists to apply systems engineering methodologies to materials innovation and characterization such that complex materials systems can be quickly, efficiently, and successfully designed and developed to facilitate the materials innovation process. This method is named Characterization Systems Engineering (CSE). The goal of this document is to create an approach that facilitates materials science innovation by applying systems engineering principles to materials characterization throughout the system lifecycle. Frequently, the fundamental understanding generated in the research phase of a product development is not communicated downstream, and likewise downstream processes are not considered in the initial needs analysis and product design. This isolates rather than integrates different phases of the developmental process. CSE aims to provide a more efficient toolkit for developing novel material technology and translating understanding and requirements throughout the process. In doing this, CSE integrates the various materials development methodologies into a more unified and complete process.

Traditionally, material systems are developed according to a more traditional format. The bulk of the development time is spent on basic research to work out the major problems with a series of materials. Materials are then evaluated and selected according to a trade-off analysis. Applied research and development activities begin after selection, followed by cost reduction efforts, and completed with a transition to production (Gell, 1995). The conventional method is designed to iron out most of the wrinkles in the design prior to adjusting to specifications required for subsequent phases of the development cycle. Frequently, impatient organizations select a material and begin their product lifecycle in the development stage attempting to fix a myriad of problems that require a combination of fundamental and applied research efforts. This results in a substantial amount of resources being dedicated to rework and redesign efforts. Furthermore, modern concurrent engineering practices demonstrate a limited degree of compatibility with the more linear conventional materials development methods.

Manufacturing and processing methods are becoming increasingly complex and in need of research and development efforts in their own right. Traditional manufacturing ramping periods are no longer sufficient to discern problems, trace root causes, and implement controlled solutions for long-term consistency (Saleh et al., 2020). Emergent behaviors within material systems caused by the complex chemical and physical interactions that dictate the material properties no longer allow for conventional production start-up. While digital twins are frequently used to predict process-structure-property relationships and accelerate the development cycle, these models must be trained by good quality data. They can struggle to predict the effect of process changes and the inherent variability associated with the start-up of a production line (Xu et al., 2014). While these techniques hold tremendous value, being able to properly characterize a material, in its entirety, provides data on the developing situation, and modeling efforts that have historically been asked to provide a prediction with a small or non-existent set of data typical of new products can be trained with this good quality, comprehensive characterization data.

On the topic of modeling, material informatics has demonstrated a high degree of value for generating compositions and targeting experimentation to produce specific process-structure-property relationships. Innovation within the materials space that used to be propelled forward by trial-and-error experimentation has been distilled into a more efficient high-throughput discovery cycle leveraging the latest modeling, simulation, and artificial intelligence-assisted techniques (Rajan, 2015). While the power wielded by material informatics is impressive, it is unfortunately a victim of its own efficiency. Compositions can be computationally calculated, and samples can be generated in the laboratory, but the characterization mechanism critical to understand those samples and further inform the model and the next steps of the experimentation serves as a bottleneck and significantly limits the pace of development.

While more conventional models for materials development are sufficient for simple systems, an intensive definition and integration focused methodology is required for the complex, material systems that are rapidly becoming the common request from the market. The methodology process development will consider common challenges to materials engineering, cultivate proposed solutions for those challenges, and test the framework against case studies systematically (Hernandez and Pollman, 2022).

In a complementary design to the systems engineering method, the CSE method will be iterative and allow for the subdivision of complexity into manageable, discrete portions. The SE method consists of four steps which include requirements analysis, functional definition, physical definition, and design validation (Kossiakoff et al., 2020). Through the evaluation of this sequence, complex systems, processes, and interactions can be defined and developed to best serve the project goals over the full system lifecycle.

To design a method for CSE, the needs for the framework will need to be considered:

- The methods needed to address material compositions.
- The methods needed to address interfaces and integration, both within the material system as well as a likely integration within a larger system.
- The methods needed to incorporate materials processing as a component of the system development.
- The methods needed to cover engineering efforts over the full system life cycle.
- The methods needed to provide an improved return-on-investment when compared with traditional engineering approaches by minimizing the bottleneck effect typical of characterization efforts.

1.2 Materials and Methods:

A CSE method will be developed based upon a combination of material design techniques and systems engineering principles to better understand the root of the problem as well as design an appropriate and complete toolkit for characterization of the development of complex systems. A series of case studies will then be evaluated against the CSE method to validate the method and determine how the factors of the method influence the development of complex systems. For each factor of the method, the presence (+), absence (-), or substantial presence and absence (/) of elements will be noted on a table along with an associated outcome of the project, defined as either positive (+) or negative (-). The resulting table will summarize the presence and efficacy of the tenants of CSE against real world case studies. To develop a method that adequately addresses the needs associated with characterization, the attributes, integration processes, and constraints of developing and understanding complex, material systems require diagnosis and attention.

1.2.1 Attributes of Characterization

A systems approach to materials development has been reviewed by Arróyave and McDowell, 2019. In their investigation, process-structure-property (PSP) relationships were highlighted as the core relationship within materials design that serve as the aim for elucidation and manipulation for research teams. With the need for an accelerated design cycle, better targeting and control of PSP relationships drives project progress and requirement satisfaction (Arróyave and McDowell, 2019). By applying systems engineering to materials development, a more efficient and iterative engineering cycle can be deployed to manage these complex material systems.

The aim of this document is the characterization of materials to develop a complete understanding throughout the system lifecycle, therefore a characterization-focused redefinition of the PSP relationship can be crafted. The three major attributes of complex, material system characterization are (1) compositions, (2) interfaces, (3) processes. From these characterized attributes, PSP relationships can be derived and understood. Iterative evaluation of these three attributes follows the systems approach for lifecycle design, deployment, and operation (INCOSE, 2015). As systems are developed, engineers must be cognizant of the compositions in play, the interfaces amongst those compositions, and the processes involved to create and use these materials.

Research and in-depth understanding of interfaces amongst materials and integration of multiple materials to achieve specific properties is rapidly becoming the norm for system developments as varied as microfluidic arrays (Nge et al. 2013), thermal management systems (Li et al. 2023), and battery and renewable energy systems (Xi et al., 2021), with further investigation and characterization of the interactions between these materials being specifically called out as critical for the advancement of the technologies. With the advent of specialized sub-disciplines, such as additive grain boundary engineering, specifically catered towards interface management, increasingly efficient and targeted approaches are being developed and utilized to manipulate PSP relationships under stringent requirement conditions (Seita and Gao, 2022). Interface engineering has even emerged as a technical discipline in its own right, and is employed in circumstances where technological advances lie primarily at the interfaces of materials (Graetzel et al., 2012). Identification and rapid characterization of complex interfaces drives a high throughput experimentation cycle that defines key associations among the material attributes. Developing a clear understanding of material interactions and coupling that exploration with the innovation-fertile landscape of diverse material community interactions serves as an auxiliary mechanism for materials design and discovery inherent to the interface engineering research space.

It is worth noting that environmental interfaces for material systems have historically been a major design consideration and a primary requirement for property specifications. Substantial resources in any project for complex material systems will involve not only the routine use of environmental scenarios and modeling, but also edge case extreme environmental considerations. As more demanding requirements are generated for materials, more rigorous and complete requirements management will be needed to manage their complexity.

1.2.2. Systems Integration

The method will have to incorporate a mechanism to ensure integration. Langford makes the argument for seven principles of engineering systems integration. Of the seven, the principles of limitation and forethought are the most applicable to material systems. The principle of limitation dictates that system architecture, in conjunction with the concept of operations (CONOPS), are inherently resource constrained. It is the responsibility of the system designers to accept these constraints and address the stakeholder needs through requirements design as the functionality of the system is subdivided into realistically achievable portions. The principle of forethought dictates that integration must be considered proactively, as early in the planning stages as possible, and defined as a requirement (Langford, 2012).

The system integration will consist of a bottom-up integration process, whereby the smallest discrete units of the material system are characterized, defined, and tested as the system is integrated. An important perspective must be maintained by the systems engineers involved with the product development that incorporates a top-down understanding of eventual functionality and proactive approach to mitigate possible problems associated with critical technological linkages. (Kossiakoff et al., 2020). Testing data must be accumulated through the integration process and used for training models and simulations. Digital twins of the material system can guide post-development upgrades, future process refinements, and new product lines. There is an opportunity for digital twins of these development cycles to substantially reduce the time and resources associated with experimentation while successfully directing targeted problem solving.

The test architecture governing test and evaluation of systems uses test planning, test measurements, and test equipment requirements as inputs, as shown in Figure 1.1 (Kossiakoff et al., 2020). While, these inputs are sufficient in an abstract sense, a high specificity and required level of expertise is required for the comprehensive characterization of materials. This is especially true in the research and development portions of the system development where highly specialized tools and skillsets may be required with high costs or long lead times (e.g., atom probe tomography). This contrasts with more routine and expected analyses, whereby experience and equipment has typically been developed in-house across several phases associated with the system life cycle (e.g., optical microscopy). Further investigation and elaboration of test and evaluation protocols for characterization systems will be discussed in further research. The challenges associated with complete testing within prescribed timeframes and budgets for the inherently labor, time, and cost intensive process that is materials characterization is a complex problem in its own right.

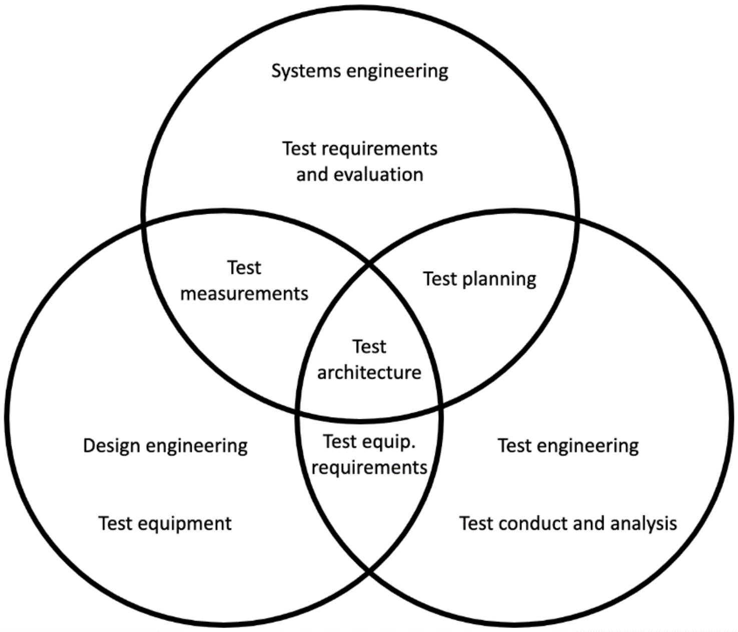


Figure 1.1: Test and Evaluation engineering responsibilities (adapted from Kossiakoff et al., 2020)

1.2.3 Theory of Constraints

The theory of constraints (TOC), developed by Goldratt, is based on the concept that all systems have constraints that restrict productivity and efficiency. The five steps to address the constraint consist of identifying the constraint, exploiting the constraint, subordinating everything else to the constraint, elevating the constraint, and reevaluating the system. This theory led to the development of critical chain scheduling

(CCS) and has been shown to be an effective process for reducing wasted time and resources in complex systems development (Pinto, 2019).

Material systems involve an inherent amount of uncertainty with respect to scheduling, making buffer time calculations difficult. With the time attributed to delays and project setbacks being highly variable, depending on the equipment and expertise available, and nature of the project scheduling will likewise be variable. CSE is aimed to minimize these variations, and using critical chain scheduling techniques to manage scheduling uncertainty aids in the work consistency required for complex projects. By heralding the use of CCS as refined by Kulejewski et al., 2021, this necessary consistency can be achieved. As opposed to conventional CCS, the Kulejewski-refined method includes the use of inflow buffers to secure the starting time of feeding chains. This protects the start date of supporting chains of the projects and more adequately allows for the management of characterization backlogs and delays.

Within the context of this document, characterization and the process by which materials are understood and developed is a constraint within the system. To properly address the constraint, we can evaluate the “problem” of materials characterization through the lens of the theory of constraint. In a preliminary sense, the constraint (characterization) has been identified, exploited, and subordinated by focusing attention on this bottleneck through the use of the CSE attributes and integration scheme. The elevation of the constraint can become the focus of the process endeavor. The fifth step (reevaluating the system) can be included within the iterative approach of the method. As engineers cycle through the SE method and CSE method during the concept development, engineering development, and post-development portions of the project, reevaluation of the system occurs in perpetuity throughout the full system life cycle. The elevation of the constraint can be considered as the third phase of the CSE method. It serves to eliminate the constraint problem and improve the project position in the long term.

On the point of communication, it has been demonstrated that organization of processes to increase efficiency cannot be implemented without reinforced communication efforts, both horizontally and vertically, throughout the organization (Zhang, 2022). To properly implement any CSE methodology, an efficient and open communication network throughout the organization will be necessary to provide context for the project members and carry a historical record of the project progress into future endeavors. When considering improvements, upgrades, and next-gen product lines, it is especially important to emphasize documentation and information management systems rather than word-of-mouth advice and guru-based guidance.

A schematic detailing the cyclic nature of the characterization attributes leading into the integration scheme, which is followed by the elevation of the constraint, is given in Figure 1.2. The CSE method is meant to coincide with the utilization of the SE method in an iterative manner throughout the system lifecycle.

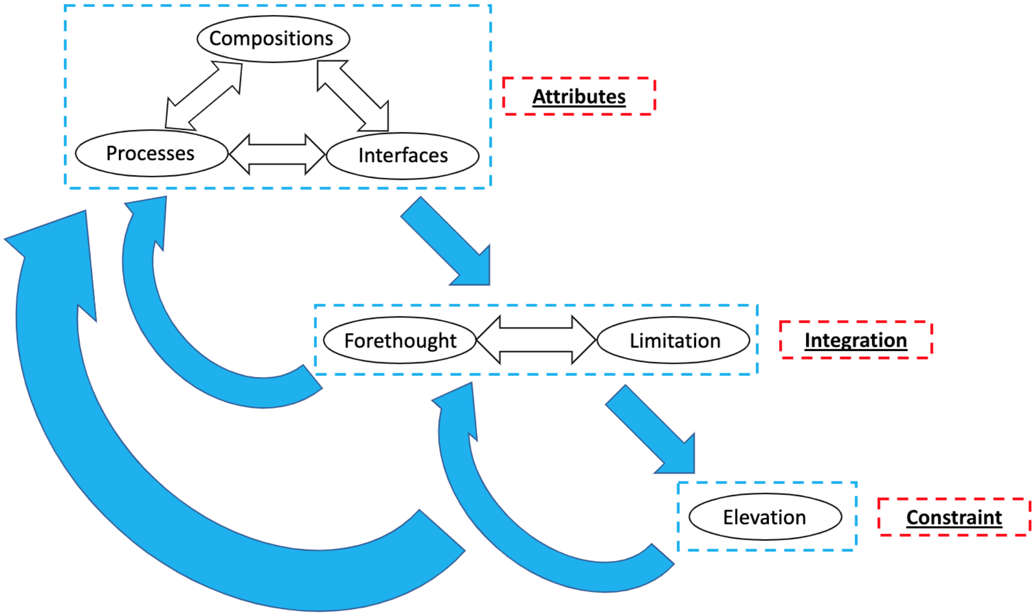


Figure 1.2: CSE method diagram

1.3. Results:

The information resulting from the evaluation of the case studies by means of the CSE method is detailed in Table 1.1. The case studies are summarized in this section to provide context for the analysis and subsequent discussion in later sections of the document. A series of questions will be used to determine which aspects of the CSE method are evident within each case study.

The questions guiding the evaluation are:

For the factors of CSE -

- Is the factor of CSE being sufficiently considered and understood such that the project time, budget, and performance requirements are met?

For the project outcome -

- Is the outcome of the project a success or a failure?

The working hypothesis is that the CSE method will provide value when aspects of the method are used (i.e. positive outcomes) and will result in setbacks or project failure when not used (i.e., negative outcomes). Because the majority of the case studies are failure analyses, an effort will be made to diagnose the major contributing factors of the failure for categorization within the evaluation matrix. Also, corrective actions and emergency response efforts associated with failure will be evaluated according to the CSE methodology.

Table 1.1: CSE evaluated case studies (Compositions is abbreviated as "Comp.")

Case	Comp.	Interfaces	Processes	Forethought	Limitation	Elevation	Outcome
1	-	-	-	-	-	-	-
2	-	-	/	+	+	+	+
3	-	-	-	-	-	-	-
4	-	-	/	-	-	-	-
5	-	-	-	-	-	-	-
6	/	-	-	-	-	-	-
7	-	-	-	-	-	-	-
8	-	-	-	-	+	+	-
9	-	-	-	-	+	+	-
10	-	-	-	-	-	-	-
11	+	+	+	+	-	+	+

1.3.1. Case Study #1

The cooling tower associated with the power plant being built in Willow Island, West Virginia, was under construction (Gagg, 2014). A jump form system of concrete building was used in the construction, whereby scaffolding is bolted into the side of the structure as the higher areas of the structure are poured. During the subsequent investigation into the incident, it was determined that the concrete, which had been exposed to lower-than-expected temperatures overnight, had not been given an appropriate time to cure given the loads being applied during the construction (Lew et al., 1979).

1.3.2. Case Study #2

The Fontana dam was constructed to generate hydroelectric power from the Little Tennessee River. A gravity dam style design was selected for the project. In a gravity dam, the dammed water is held back only by the weight of the dam and the resistance of the dam components to sliding against their foundation. The design, furthermore, required vertical contraction joints to allow for variable stresses due to the southward orientation of the downstream face of the dam and extended periods of heating from the sun. Upon observations that the dam was cracking, an investigation of the concrete indicated that an alkali-aggregate reaction was occurring generating the cracks, which were further worsened by the heat due to long sun exposure. In addition, it was discovered that cooling pipes ran through the dam during its construction, lowering the temperature of the dam interior compared to its exterior during the curing process (Gagg, 2014).

1.3.3. Case Study #3

The Malpasset dam in France was constructed over 30 months with several construction stoppages. The periods of inactivity allowed portions of the concrete to harden substantially before new sections of concrete were added. The inconsistent concrete construction resulted in unplanned variability in the material properties of the dam, and the structure failed. Furthermore, the rock against which the dam was constructed was insufficient to support the structure, and inadequate initial surveying failed to identify an unknown fault. Hot, dry summers and wet winters further exacerbated the geological failure mode (Gagg, 2014).

1.3.4. Case Study #4

A highway overpass in Montreal, Canada collapsed after 36 years of service. Portions of concrete were observed falling from the structure prior to the collapse (Gagg, 2014). An investigation into the failure determined that improper design of the rebar reinforcement, inadequate installation of the rebar, and the use of low-quality concrete during the construction of the overpass were the causes of the incident. Possible contributing factors included a design vulnerability to shear stress, lack of waterproofing, and insufficient repair work in prior years (Commision, 2007).

1.3.5. Case Study #5

The roof of terminal 2E of the Charles de Gaulle International Airport partially collapsed less than a year after opening (Gagg, 2014). The investigation into the cause of the incident pointed to poorly positioned steel supports, lack of mechanical redundancy, concrete beams with insufficient resistance to stress, and poorly positioned metal supports within the concrete structure.

1.3.6. Case Study #6

The Ynys-y-Gwas bridge was a segmental post-tensioned concrete bridge in South Wales (Gagg, 2014). Post-tensioning of supports within concrete is a process by which slabs are composed ahead of time and only need to be installed and tensioned during construction. Post-tensioned slabs contain reinforcing tendons within sheaths in the concrete, and tension is applied to the supports after the installation. The bridge collapsed due to inadequate protection of the tendons around the joints, which resulted in corrosion of the tendons. The corrosion was likely accelerated due to the presence of road salt on the bridge during the winter months (Woodward, 1989).

1.3.7. Case Study #7

A series of wharves were inspected for degradation in Portugal (Gagg, 2014). The wharves were composed of pre-cast, pre-stressed concrete beams and pre-stressed, cast-in-place concrete slabs. The portions of the wharves were exposed to different effects from the surrounding marine environment, which included the splash zone impacting the upper parts of the beams, the tidal zone impacting the lower parts of the beams, and the near complete submergence of the pile foundations impacting the bottom of the structure. The tendons and ducts were severely corroded with evidence of stress corrosion cracking in several areas. Poor installation practices led to ungrouted ducts which increased the rate of degradation due to corrosion, and a lack of adequate drainage led to increased salt deposits that further worsened the situation (Costa and Appleton, 2002).

1.3.8. Case Study #8

The Channel tunnel ("Chunnel") is a tunnel that connects the northern coast of France and the southern coast of England (Gagg, 2014). The interior of the tunnel is lined with pre-cast, high strength, reinforced concrete rings. In sections of the tunnel where concrete reinforcement was not sufficient, cast iron supports were used. An incident occurred where a train carrying polystyrene caught fire causing substantial sections of concrete within the heated area to begin spalling off the walls and ceilings and impacting emergency responders on the scene.

1.3.9. Case Study #9

The Mont Blanc tunnel runs between Chamonix, France and Courmayeur, Italy. The roadway was built of reinforced concrete, but the tunnel lining was not reinforced. An incident occurred where a truck caught fire within the tunnel, and the subsequent spalling of concrete caused significant damage to the structure. Insufficient emergency precautions resulted in a substantial loss of life (Gagg, 2014).

1.3.10. Case Study #10

The Heathrow Express rail tunnel being engineered using the New Austrian Tunneling Method (NATM) at Heathrow airport collapsed during construction. The collapse generated a crater in the ground between two runways of the airport that disrupted aircraft operations for a prolonged period of time. A study launched into the challenges associated with NATM projects showed that the most common root causes of failures resulted from engineers encountering unexpected ground conditions during construction, especially during the application of the sprayed concrete to the tunnel lining.

1.3.11. Case Study #11

Several examples of Roman-built piers and harbor structures have remained intact for more than 2,000 years. The longevity and durability of the concrete material is substantially advantaged compared to modern analogues. Through a mineralogical investigation, a formula has been rediscovered for ancient roman concrete that has generated interest from materials researchers into concrete experimentation using plate-like minerals for enhanced structural resistance properties (Witze, 2017). These newer families of concrete, while not necessary for conventional applications, can be applied to more extreme environments or situations where more complex interfaces must be considered.

1.4. Discussion:

There is a correlation between the unsuccessful application of CSE and failed projects. In this study, a series of failure analyses were investigated, which presented thorough reports and investigative documents but lacked a certain breath in terms of the variety of the application. The evaluated case studies involved concrete structures and compositions for structural application. While complex, additional investigation into other materials, coatings, thin films, and processing procedures would be of value to further test the method and ensure compatibility with other engineering disciplines. While most of the evaluated case studies resulted in failure, case study #2, regarding the Fontana dam, was of particular interest due to its partially positive outcome: the dam is still being used. An initial oversight in the failure to adequately characterize the composition of the concrete was eventually identified through a comprehensive investigation, and corrective actions were taken.

It is worth noting that the absence of the factors of CSE in these systems' development and operation frequently resulted in significant downtime for the system or a catastrophic destruction of the system. While concrete may be thought of as a fairly well understood material family, even during the timeframes of some of the older case studies, complexities with the system application and lack of attention to system integration resulted in project setbacks. As new materials, processes, and applications are designed, it is important for development teams to dedicate sufficient resources to manage the complexities involved with material systems.

Application opportunities for CSE include any system with novel materials or materials that interact complexly. The aim is to reduce inefficiency due to the constraint of characterization, understand the materials being used proactively, and apply that knowledge to eliminate setbacks and rework at later stages of the project. CSE is particularly well suited to projects that exist within the technical intersections of advancing technologies. For example, the targeting of tumor microenvironments for cancer treatment with coated drug-encapsulated nanoparticles (Ma et al., 2023).

1.5. Conclusion:

In conclusion, the methodology of Characterization Systems Engineering (CSE) was investigated. The method was tested against a series of case studies to evaluate the utility and value of the tool, and a relationship was observed between the absence of the factors of CSE and failed projects. In several cases, factors of CSE being present in a project led to a less catastrophic failure or a positive outcome.

CSE provides a more adequate management approach for material systems within a concurrent engineering format. Allowing for the knowledge base for the material to be built and communicated throughout the organization as the system is developed and deployed reduces rework and redesign, as well as limits the risk of catastrophic failure. CSE also provides for complete and robust datasets, which can serve as inputs for materials informatics tools, further enhancing the upgradability of current systems and providing insight into new intellectual property space for materials discovery.

As with many systems methodologies and frameworks, a certain amount of tailoring is required depending on the specific system under development, however the current method demonstrates a degree of robustness by subdividing material systems into their fundamental components. These components can then be properly defined, integrated, and tested, mitigating the risks associated with materials system in a more universal fashion than conventional design and scheduling.

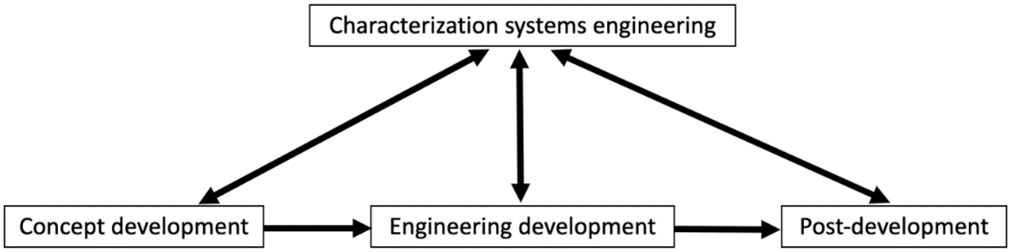


Figure 1.3: Phases of the System Life cycle (adapted from Kossiakoff et al., 2020)

In further applications, the CSE method could be applied more specifically to the system life cycle phases to enhance individual aspects of the process (Figure 1.3). Requirements definition and management could be further classified using CSE terminology to more comprehensively interpret customer needs, translate those needs into engineering specifications, and track those specifications through the system life cycle. CSE could be applied to the final stages of the life cycle by guiding the termination, disposal, and recycling of components and materials as reclamation and reusability are increasingly becoming important values for system stakeholders.

Chapter 2: Designing for characterizability in the synthesis of materials systems

2.1. Introduction:

While materials characterization is understood to be a valuable part of the materials design and development process, the planning and utilization of characterization techniques is frequently left unincorporated into the concept development phase and project scheduling efforts. This leads to delayed project timelines and a misallocation of resources related to the understanding of novel materials and their interfaces. An opportunity exists to leverage the empirical information gathered by materials characterization efforts, enhancing models and simulations while better constraining and predicting downstream problems and opportunities. By applying systems engineering methodology to materials characterization, systems engineers can mitigate risk, enhance data retrieval and utilization, and plan characterization procedures proactively. Generating a metric that defines characterizability directly can serve to weigh trade-off options in system-wide decision-making efforts.

With a proactive approach to characterization, project schedules can be maintained and characterization can be thought of as an innovation process whereby process-structure-property (PSP) relationships can be better investigated driving both downstream troubleshooting, through the gathering of fundamental knowledge, as well as generating novel directions for intellectual property space exploration. By planning for in-depth materials analysis as part of the design phase, project teams can maximize the value of the time and activities associated with the synthesis of material systems.

It is widely accepted that materials characterization is an expansive and diverse field of study. Especially with the more widespread use of in situ and in operando measurements, the time and expertise associated with material development increases to match the increasingly complex questions that must be answered during product evaluation and production. As the complexity of models and simulations increases concomitant with the increasing digitization of engineering, the datasets used to teach these models must become more multi-faceted and of a higher quality, such that these models are accurately taught and can point scientists and engineers in the right direction for efficient project completion.

Therefore, the important notions related to leveraging the capabilities of materials characterization include:

- Informing downstream processes by establishing strong fundamental materials knowledge early in the product development lifecycle
- Informing upstream processes and redesign efforts by continuing materials characterization efforts through the post-development phase (e.g. production, operation, in-service failure, disposal) to incorporate the fill product lifecycle
- Informing future product innovation and intellectual property space exploration by establishing a good understanding of the process-structure-property relationships of current products

A good perspective on the potential of materials characterization as an innovation tool has been considered in Ash, 2016. In this commentary, innovation through characterization is visualized using a triangle where empirical study is the base and intellectual property is the top. As an engineer attempts an IP-based materials investigation, the throughput of the materials characterization is low, while the complexity and cost become high. Empirical investigations can have high throughput, low cost, and low complexity, but lack intellectual stimulation and usually produce less advanced technical capabilities. Part of the issue here is that materials characterization has been traditionally viewed as a laboratory service, whereby the design/formulation and the analysis of the material have been separate organisms. More completely integrating materials characterization into the materials system development lifecycle provides an opportunity to draw more value from the process with minimal cost added.

Leveraging the capability of characterization to enhance the development of systems, while appearing to be an intuitive next step in accelerated materials discovery, is frequently hindered by decision making processes that minimize the value of materials characterization while emphasizing the expenditure of time and cost associated with characterization. Increasing emphasis is typically placed upon high throughput techniques and delivery of data to the project team with the minimum necessary information to inform the decision at hand. This encourages abandoning complete material datasets that quite frequently can mitigate or eliminate problems later in the development lifecycle and accelerate next-generation product development.

There exists an opportunity to implement characterization in the design phase by treating characterization as a non-functional system property (e.g. maintainability, reliability, etc.). For the purpose of this document, non-functional system properties, system attributes, and “-ilities” will be considered synonymously.

System attributes are criteria that are used to define the system’s operational behavior and evaluate the system’s performance. They ensure that the system operates according to the customer needs and serve as an architectural guide for the system development team.

The current use of material characterization does not include characterization scientists in the design and planning processes, largely robbing the project team of the opportunity to consider the value of the characterization effort itself. By incorporating “characterizability” into the design process, the value of characterization can be weighed against the value of other system attributes, in tools such as trade-off analyses, and tied directly to project goals and requirements during schedule planning efforts.

While the use of systems engineering principles can certainly aid in designing a system for robustness by considering system attributes in the earliest phases of the system life cycle, materials characterization is frequently regarded as a laboratory service somehow outside of the design and innovation process. Design engineers typically lack fundamental understanding of the science behind the characterization technique, experience in the laboratory operations of the characterization process, and/or knowledge of the lead times and scheduling challenges of different techniques from a project management standpoint.

While systems engineering can address some issues related to the product lifecycle, a specific approach must be developed to assist engineers in the design of systems for characterizability, since characterization efforts are typically blamed for incomplete datasets and delayed project schedules. Considering characterization early in the design process can eliminate uncertainty related to these specialized engineering efforts, especially when novel materials are being evaluated for integration into the system in question.

While previous work on this topic does not deal with characterizability specifically, similar design and evaluation of system attributes (maintainability, reliability, etc.) have been explored in established research. By examining these techniques, characterizability can be better designed for and considered pragmatically.

Luo et al., 2015 use maintainability design attributes to evaluate systems in the design phase. The methodology breaks the maintenance attributes down to be focused on simplicity, modularity, standardization, diagnosability, and identification to better constrain and define the contributing factors of a maintainable system, while further defining accessibility, assembly/disassembly, ergonomics, and maintenance safety as maintenance processes critical to addressing the time and effort required to maintain systems. By separating processes and operations into two categories and further defining those categories with specific and quantitatively discrete sub-attributes, the maintenance task development and deployment was evaluated against a case study for efficacy.

Ingwersen et al., 2015 use a Resource Description Framework (RDF) to enhance the Life Cycle Assessment (LCA) process by making data associated with technical architectures more interoperable, integrable, and transparent. By addressing the data associated with the LCA process rather than the process itself, the research allows systems architects to better use and track data relationships as design complexity increases. While part of the work addresses the construction of an architecture ontology to label data with more appropriate and actionable nomenclature, the researchers also consider system flexibility and automated integration of increasingly complex datasets.

Wan et al., 2018 consider the relevance of a nature-inspired approach to materials innovation for energy storage applications. By using a ground-mountain-vegetation design metaphor, the researchers were able to produce a novel high-power density heterostructure with a long cycling life. The team was able to innovate within the material space using newly generated categories for the material system constituents.

Beesemeyer et al., 2012 propose system property categories to increase a system's robustness and/or changeability. They propose that the value of the system increases substantially when these factors are considered in the design phase, therefore catering to this design priority warrants specialized tools for the early phases of the project. The researchers design categories including the trigger for system change, the type of agent executing the change, and the life cycle phase for execution, such that these system-change characteristics more adequately provide context for the relationship between system attributes and design decisions.

The conventional approaches to product design would not be adequate to address the issues that most commonly occur during the development of complex material systems due to the added uncertainty surrounding the involvement of materials characterization processes. In a similar fashion, principles of systems engineering, as they currently stand would also not serve to control the variability associated with the unknown unknowns of the characterization effort. While a systems approach focused on the full system life cycle is beneficial, problems arising from incomplete or improperly used materials characterization efforts rob the product team of the fundamental knowledge associated with the material process-structure-property relationships. This information is valuable for training models and simulations, driving materials innovation in future projects, and proactively mitigating downstream issues associated with unforeseen material interactions and failures.

This is especially relevant in the modern world of concurrent manufacturing. Comprehensive materials characterization can eliminate problems amongst complex material interfaces, reduce uncertainty related to novel material emergent behavior, and proactively minimize variability associated with ramping up manufacturing processes. Materials characterization can even predict and proactively mitigate in-service operational failures that can prove costly both financially (e.g. product recalls) and in terms of customer relationships (e.g. lost trust / lost customers).

As part of this process, engineering teams must relearn how to design material systems by tailoring their efforts to leverage materials characterization. By collecting comprehensive datasets, more complete digital twins of these systems can be produced to make experimentation more efficient in future projects. While the temptation exists to minimize time and resources not specifically accomplishing project goals, a new, more strategic mentality must be formed to leverage the data generated by materials characterization efforts.

Materials characterization is, inherently, a multi-scale and multi-resolution endeavor. A variety of equipment and techniques may be required given the questions being asked by the design team. Instead of the basic requirements being addressed, the systems engineers involved with the project should not only ask “Does this material meet our requirements?" but also ask "How is this material meeting our requirements?". The question that asks "How?" provides more comprehensive and intensive information on the true material interactions and accelerates problem solving moving forward.

Given the history of work conducted in related fields, an appropriate process by which to design the attribute of characterizability would be to designate relevant sub-attributes and test the design process against the conventional design methodology to determine practical efficacy. By testing one method versus the other, a more quantitative comparison can be generated.

2.2. Materials and Methods:

Characterizability can be defined as the ease and completeness with which the relationship between the properties, processes, and structures of materials can be discerned. Certain materials have extensive industrial and institutional histories in the innovation, manufacturing, and operational spaces (e.g. steel components for railways), while others are fairly young in that they are newly designed, manufactured, or applied to a new industry, where most knowledge surrounding their characterization comes from small, laboratory scale experimentation. Designing for characterizability, in these circumstances involving less mature materials, can increase process efficiency with respect to understanding the material within its newfound application and scale of production.

Ricci et al., 2014 propose the System-of-systems architecting with ilities (SAI) method which provides guidance for systems engineers to design for ilities from the concept development phase onward. This allows the product development team to proactively manage and prioritize system attributes that will be of value during the system's operational lifetime and not only consider the immediate functional requirements of the system. This provides a more robust system in the long-term that can adapt to a changing environment and variable operational conditions.

Lee and Collins in 2017 subsequently proposed an extension of the SAI method into the sub-system levels demonstrating that communicating non-functional properties to component owners early in the system development process can be essential to meeting customer needs. Bringing component and service engineers into the system attribute design and trade-off analyses frequently lends technically specific guidance to the non-functional system attribute implementation and translates the priorities of the project throughout the product development team and across the product development lifecycle. By involving the whole team, specialized technical perspectives and experiences of which the systems engineer may not have a deep understanding can be leveraged to ensure that the customer needs are met.

The formulation of the characterizability attribute and associated sub-attributes will be carried out in a similar manner, considering the full life cycle and full technical diversity of the task to be completed.

Addressing characterizability will consist of several sub-attributes. These sub-attributes will allow the project team to better define the system and constrain the scope of the project. The sub-attributes will consist of:

1. Material Novelty
2. Technique accessibility
3. Data integrability

Using these three sub-attributes to clarify characterizability provides a more rigorous and traceable design metric through to the most basic levels of the product.

2.2.1. Material Novelty

A key component to this characterizability system attribute is the management of innovation and intellectual property (IP) space. It has been established that the material process-structure-property relationships are valuable to understanding materials currently under development while also providing strong fundamental knowledge of material families for further research and intellectual property exploration in the future.

Material novelty as a characterizability sub-attribute requires the evaluation of future requirements as aspects of the current project. For example, a strategic goal for a company designing thermionic generators might involve exploring novel materials with high electrical conductivity and low thermal conductivity. The project team may be working largely with commercial off-the-self (COTS) equivalent materials that were not intended to contribute to this long-term, strategic goal, but through adequate curiosity and characterization due-diligence, certain process-structure-property relationships can be discovered that not only mitigate development issues likely to arise in downstream processes, but also contribute to the working body of knowledge regarding the company's strategic materials objectives.

As was stated previously, an objective of this conceptual workflow development is to provide guidance on treating characterization as an information generating mechanism. Characterization data will need to be labeled, stored, and relatable, such that data can be accessed when problem-solving during the system lifecycle and innovating during future projects.

A material with high material novelty will require complex, expensive, and time-consuming characterization efforts but pays forward advanced knowledge of a potentially valuable intellectual property space or can more adequately address downstream development, production, and operational issues. An emergency effort in response to a manufacturing upset or an in-service product failure will already have a platform of fundamental knowledge of the material to serve as a jumping off point for speedy conflict resolution. Note that materials with low novelty are simple to characterize and use within a new system but promise lower innovation potential.

2.2.2. Technique Accessibility

The process by which characterization methodologies, tools, and equipment are selected and planned for can be defined as technique accessibility.

It is quite common for project engineers to have a limited understanding of the materials that they are designing or selecting. Characterization specialists are collaborated with to best understand the properties of the materials being chosen. During the evaluation of different materials, especially novel materials, more in-depth and complex characterization efforts need to be performed to understand the strengths and limitations of the materials under evaluation.

It is important in this context to comment on the complexity and variety of techniques available for materials characterization. These range from highly available, mature technologies (e.g. optical light microscopy, or hardness testing) to newly accessible, specialized pieces of equipment (e.g. atom probe tomography, or micro x-ray computed tomography). Lead times for using this type of equipment, likewise, vary from immediate availability, with immediate feedback, to long leads times requiring an application or reservation, with extensive requirements for data analysis to understand the conducted characterization effort.

Figure 2.1, below, summarizes the problem. With complex materials, equipment and techniques are more specialized, and longer lead times are incurred for both equipment and data. However, this intensive effort leveraging new characterization capabilities allows engineers to more completely understand materials at the frontiers of what is attainable by modern technology. The dashed blue arrow corresponds to simultaneous increasing process complexity and innovation value.

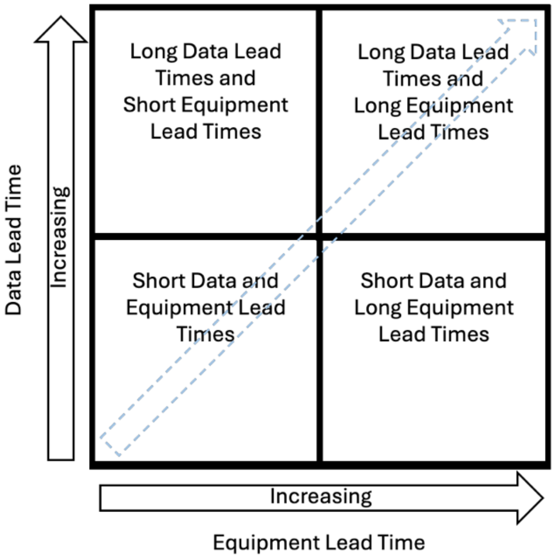


Figure 2.1: Diagram describing characterization lead time.

It is worth noting that, as new techniques become available that characterize materials in new ways and become popular within the academic and industrial communities, lead times associated with these new techniques extend due to high demand. Much like in the field of economics, cost (i.e. time) increases substantially when a source of value (i.e. data) is in high demand with limited supply. This phenomenon leads to a scheduling issue and, by extension, a risk issue. The certainty with which a characterization effort can be conducted and concluded depends on the complexity and availability of the technique. Planning ahead for appropriate lead times in accordance with new tools, techniques, and characterization goals can allow for project schedules to remain valid, even when substantial resources are being dedicated to complex characterization efforts.

Therefore, technique accessibility becomes an important issue with respect to project opportunity and risk. Much information can be gathered to ensure requirements qualification and inform future activities. Expense, however, in terms of time and resources, can quickly extend past that which was scheduled/budgeted if the project lead is unprepared.

2.2.3. Data integrability

The manner in which data can be integrated into the product lifecycle is paramount to the successful development of material systems. Project-wide communication and data integration serve as the two core concepts underlying the data integrability sub-attribute of characterizability. It is the responsibility of the project lead to hold the project team accountable for learning about characterization techniques (i.e. strengths, weaknesses, limitations, etc.) and material properties, as well as requiring the characterization specialists to serve as educators on their fields of expertise. Keeping experts in silos, segregated from research teams upstream and quality engineering groups downstream robs the project team of valuable materials insight throughout the lifecycle and leads to rework, inefficiency, and waste.

When dealing with complex systems, attention must be paid not only to individual subsystems and components, but also to the interactions amongst these constituent parts. Guariniello and DeLaurentis, 2014 speak at length to the interconnectivity of system nodes in both functional and developmental dependencies. A functional dependency exists where one node requires input from another, without which it cannot operate, while a developmental dependency exists where one node’s development is hindered without the development of another node. This study highlights the importance of relationships amongst systems and systems-of-systems where the strength (closeness) and criticality of relationships dictates the success of the system.

Lin et al., 2018 stresses the importance of efficient integration within systems to minimize risks, constraints, and costs. The work breaks down integration into three distinct components (1.) transition, (2.) adoption, and (3.) diffusion. In the transition phase, a technology is installed, validated, and any complimentary systems required for the functionality of the system are put in place. In the adoption phase, the technology is put into operational use. And in the diffusion phase, the technology is extended beyond its original user to other areas of the organization. A similar method can be applied to the integration of knowledge throughout an organization during the development of systems requiring materials characterization. Regardless of where in the organization a material is characterized, that data can be used to solve the initial problem for which it was gathered, and thereby become fundamental to the system process in that part of the organization, and then diffuse throughout the organization, such that the system as a whole becomes stronger.

System architecture consists not only of the preliminary design and needs analysis but also focuses on the entire structure of the project, the vision behind the stakeholders’ intentions, and the translation of functional elements into physical elements (Kossiakoff et al., 2020). The architecture of a system focuses as much on the relationship among structural elements as the quality and content of the elements themselves. While system design focuses on the translation and realization of needs into requirements and, subsequently, functionality, the system architecture focuses on the use of an architectural framework to standardize the structural approach to the system development and track the complexity being developed. As material systems grow in complexity, and, likewise, the integration of these material systems into larger systems-of-systems endeavors becomes more complex, incorporation of a rigorous and more specific architectural framework for material systems becomes a valuable tool within the product development lifecycle. By instituting a characterizability attribute into architectural considerations, engineers can more capably track structural relationships, decision analyses, and test imperatives.

Model-based systems engineering (MBSE) is increasingly made a ubiquitous tool within systems engineering efforts, and is particularly valuable when strong architectural principles are coupled with well-informed design (Kossiakoff et al., 2020). This structure, and its associated data, can quickly and efficiently be shared with collaborators as the requirements baseline is continuously improved and the functionality of the system is built, tested, and validated. Using this approach, interactions amongst different materials, components, and subsystems can be made traceable as requirements and priorities shift over the course of the system’s lifetime. More scalable and evolvable applications can be considered using the modern MBSE tools informed by the most current and applicable data.

2.2.4. Metric formulation

Assigning proxies for these sub-attributes such that a metric can be devised will allow for the direct comparison of design alternatives based upon characterizability. While many attributes and system requirements are of value during decision analyses and trade studies, for the purpose of this study, the evaluation of characterizability will serve as the paramount factor to decide between design approaches.

Material novelty can be approximated with maturity of the material. Materials with lengthy and well-documented histories in research, development, manufacturing, and operation tend to be well characterized. Property-structure-process relationships as understood and planned for as early as the concept development and design phases and typical failure modes are accounted for in risk assessments. The opposite is true for immature materials, or materials that are particularly novel. Complete characterization work, especially within systems containing novel interfaces and processes, is rarely completed to the level required for informed design decision making. Maturity (in years) can serve as a factor in the calculation for characterizability with mature (many years since development) being more characterizable than immature (few years since development).

Technique accessibility is a complex issue. Just because a technology exists that properly characterizes a material that is being evaluated for a system, does not mean that that technology is readily available, that lead times are reasonable for the scope of the project, or that the skill set required to use the instrument will be available or affordable along with the instrument itself. To best approximate this factor, technique accessibility can be grouped into one of four discrete categories: minutes, hours, days, or months. For example, if a piece of equipment in a fabrication laboratory can be used immediately upon creation of a part by the technician typically available in that laboratory, this would qualify as a technique accessible within "minutes" for this process. If, however, a piece of characterization equipment is only available through an outside contract laboratory with a limited number of alternatives laboratories capable of performing the technique, the accessibility may only qualify as "days" or "months". While these categories are not the only manner in which data can be defined and binned, it is useful for the consideration of characterizability to determine typical characterization tasks and associated timeframes.

Data integrability can be most closely approximated by data type. For example, a surface roughness measurement is simpler to understand and communicate than an image from a microscope. While both data can quickly be obtained, defining and communicating a number rather than an image that must be interpreted is a more valuable prospect for a system development endeavor. Data integrability can be approximated as binary, quantitative, or qualitative, with binary being the simplest to determine and constrain (e.g. presence vs. absence) and qualitative being the most difficult to translate across all phases of the system development (e.g. interpretation of imaging without appropriate image analysis software).

Table 2.1 describes the point values associated with the characterizability metric factors. These are loosely grouped to keep the metric valid amongst the broad spectrum of characterization efforts possible depending upon project priorities and specific properties being targeted. Augmentation and tailoring of the metric could be possible depending on the situation.

Table 2.1: Characterizability sub-attribute scoring chart

Material Novelty	Technique Accessibility	Data Integrability
Material maturity (in years)	1 = Minutes	1 = Binary
	2 = Hours	2 = Quantitative
	3 = Days	3 = Qualitative
	4 = Months	

Equation 2.1 describes the calculation required to evaluate characterizability for a material, where C = characterizability factor, M = material novelty score, T = technique accessibility score, D = data integrability score, n_m = number of materials, n_t = number of techniques, and n_d = number datasets.

$$C = \frac{M}{\left(n_m \cdot (T \cdot n_t) \cdot (D \cdot n_d)\right)}$$

Equation 2.1: Characterizability metric

2.2.5. Risk and Trade-off

With the implementation of characterization on a system-wide scale and the integration of that data into the core objectives of the system, there is an increase in both risk and opportunity. The opportunities associated with designing for characterizability have been covered thoroughly in this document, but a moment should be taken to understand the risk involved and how to mitigate that risk. Characterization efforts are usually costly, time-consuming, and can be technically challenging. This is a field of engineering that is actively developing, in its own right, to provide new sources of data and/or better quality data as new frontiers of science are explored and new technologies provide enhanced capabilities for this characterization equipment. With novelty always comes risk and opportunity. Project teams that are working on a particular characterization-heavy project must include events such as equipment failure, alternative equipment sources, departure or addition of characterization personnel, and multiple projects competing for characterization priority (i.e. workload backlog) in their risk assessments.

System attributes have been used to proactively limit uncertainty in the design phase and mitigate risk (Chalupnik et al., 2013). The process here would be to use characterization itself to mitigate some of the risk turning known-unknowns into known-knowns thereby minimizing the extended failure domain (EFD) and reducing ambiguity in product development. Not every characterization effort must involve newly developed equipment with unknown strengths and weaknesses. Plenty of well understood tools and techniques are available to give the project team a jumping off point to better define their system and schedule their project. It is important, therefore, to conduct thorough trade-off analyses based upon the customer needs and organizational capabilities.

Decision analysis considers not only the project goals and stakeholders but also the context and pertinent data for the decision being made (Kossiakoff et al., 2020). By elevating the role of materials characterization in the decision-making efforts within the product development lifecycle, technical personnel responsible for gathering data on materials can weigh in on important challenges, project strategy, and intellectual property opportunities. By Making the creation of the most informed team possible, more informed decisions can be made and the risk associated with a lack of understanding of materials characterization can be avoided. Furthermore, analysis of alternative solutions or alternative methodologies can be better defined such that selection criteria can be better navigated during concept selection. Tools, such as Quality Function Deployment (QFD), can become more valuable for assessing stakeholder priorities when highly informed at the earliest stages of the project and especially in the design development effort. Figure 2.2 outlines the workflow by which characterizability can be integrated into the design phase for a project.

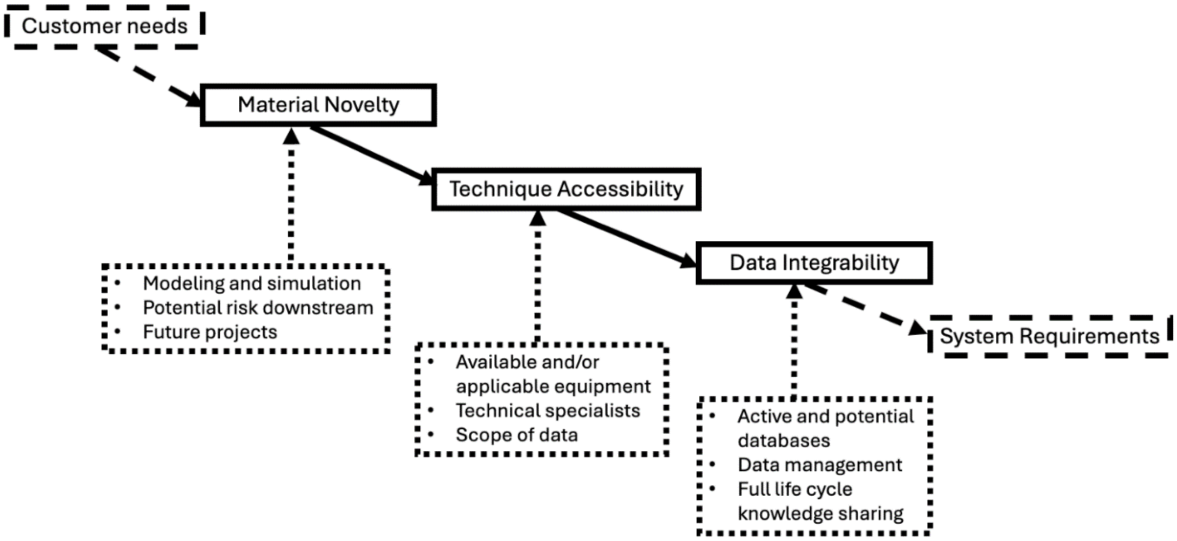


Figure 2.2: Diagram describing the process of designing for characterizability

2.2.6. Testing

Now that the definition of characterizability has been refined, a test scenario can be developed to showcase the degree to which problematic situations can be avoided or mitigated in a materials-intensive system design. Electromagnetic interference (EMI) can be considered a risk-prone arena as more and more electronics become integrated into the lives of the average human. EMI can impede the function of electrical grids (Foster et al., 2008), personal medical devices (Rao et al., 1999), and information technology systems (Bohl et al., 2005) (among others). Due to the criticality of modern electronic devices, it has become an increasingly valued customer need to incorporate EMI shielding into the system being requested and engineered.

The most effective method for shielding a device from electromagnetic interference is to encase the device in metal. Conducting materials with mobile charge carriers reflect electromagnetic waves well, and a portion of the waves that are not reflected can be neutralized by interaction with the dipoles within the metal itself. Porous materials have also been investigated for electromagnetic shielding purposes due to the high number of wave reflections that they generate, which limits the impact of the EMI (Wanasinghe and Aslani, 2019).

While metal is an effective solution, metal casings incorporated into a system have weaknesses such as corrosion, bulkiness, and limited formability (Liu et al., 2016) especially considering the increasing number for form factors being requested by the modern consumer. Furthermore, susceptible aspects of the shielding design limit the shielding's effectiveness, including conductive penetrations, apertures, and material composition (Wanasinghe and Aslani, 2019).

To illustrate the use of designing for characterizability, a test scenario will be analyzed to demonstrate the utility of the system attribute. This scenario will involve the design and implementation of an EMI shielded room with a series of stakeholder needs including:

- The room will need to be equipped with electrical and communications wiring. Therefore, one penetration in the shielding will be required to run the cabling.
- The room will need a transparent section of wall to view an observation area outside of the shielded area.
- As with many modern systems, data gathered during construction will be used to inform decisions on repairs, improvements, and next-generation projects.

It is important to note here that not all stakeholder needs are listed. For the purpose of this document, relevant needs will be considered to demonstrate the designed system attribute. Further evaluation of conflicting needs would prove useful for a more elaborate test model but is outside of the scope of this study. More traditional systems engineering approaches would certainly provide value in this system design, however these will be discussed tangentially to simplify the demonstration.

If we assume, for the purpose of this scenario, that the below mentioned options are functionally equivalent, we can use characterizability to investigate their advantages and disadvantages and select one over the others.

2.3. Results:

2.3.1. Wall Penetration

Current challenge: Apertures and wall penetrations provide an opportunity for electromagnetic waves to leak through the shielding thereby lowering shielding effectiveness. While the bulk shield material can have outstanding electromagnetic shielding properties, a common limiting factor for these designs is the number and size of penetrations and apertures. These can include, for example, holes in the structure for electrical conduit or seams between paneling as the chamber shielding is being installed.

Evaluation: Most typically, a gasket or sealant is used to secure the penetration and reinforce the electromagnetic shielding of the unit as a whole. One approach that should be considered is a foam-based material delivery with acceptable shielding properties to more completely seal the anticipated penetration while limiting the amount of weight added. Foam materials also increase the number of internal reflections for electromagnetic waves due to their inherit porosity. Options include:

1. Electrospun Silver-Ferrite Polyvinyl alcohol fibers (Kim et al., 2012)
    a. Ferrite mixed with Polyvinyl alcohol and electrospun
    b. Resulting fibers physical vapor deposition coated with silver
2. Aluminum foam (Xu and Hao, 2014)
    a. Melt foaming method of aluminum processing
3. Copper-Nickel coated Polyurethane foam (Ji et al., 2014)
    a. Polyurethane serves as a substrate
    b. Electroless Copper coating
    c. Electroplating Nickel coating
    d. Thermal process removes the polyurethane foam leaving a metal compositive microstructure
    e. Electrophoretic deposition of carbon nanotubes

If these options are evaluated using the characterizability metric (shown in Equation 2.1) their scores are as follows:

$C = M/(n_m*(T*n_t)*(D*n_d))$

$C_1 = (100)/((3)*(3*3)*(3*3)) = 0.4$

$C_2 = (174)/(1*(3*2)*(3*2)) = 4.8$

$C_3 = (33)/(4*(3*3)*(3*3)) = 0.1$

Selection: By this evaluation, option two would be the most viable from a characterization standpoint.

2.3.2. Transparent Section

Current challenge: Visible light is a frequency of electromagnetic wave, however maintaining visibility outside of the design chamber while shielding the chamber from most electromagnetic waves is an imperative for this scenario. Since most EMI is induced by wavelengths of lower frequencies than visible light, the opportunity exists to achieve adequate electromagnetic shielding while maintaining the transparent property of the material.

Evaluation:

1. Layered composite of Silver and Indium-Zinc Oxide (Kim et al., 2005)
   a. Radio frequency magnetron sputtering of each layer
2. Stainless steel fibers (Jin et al., 2014)
   a. Dope silicon matrix with stainless steel fibers

If these options are evaluated using the characterizability metric (shown in Equation 2.1) their scores are as follows:

$C = M/(n_m*(T*n_t)*(D*n_d))$

$C_1 = 25/((2)*(3*4)*(3*4)) = 0.09$

$C_2 = 25/(2*(3*3)*(3*3)) = 0.15$

Selection: By this evaluation, option two would be the most viable from a characterization standpoint.

2.4. Discussion:

While several variables were held constant or assumed for the sake of this experiment, the scenario does demonstrate the utility of the characterizability attribute based upon the stakeholder needs, organizational strategy, and risk tolerance. In the wall penetration segment of the scenario, the aluminum foam approach was preferred, and in the transparency segment of the scenario, the stainless steel fibers approach was preferred. These two selections were evaluated as the most characterizable via the metric; however, the consideration of broader strategic implications or decision drivers was not evaluated here. This is a typical consideration and contributing factor to project design, including technological pathways to which the parent company has already committed (e.g. internal product advancement), intellectual property areas particularly of interest to the research or legal teams, or subjective preferences implicit to the project team and associated engineers.

The values being generated by this calculation do not necessarily scale with technical performance metrics, making them difficult to validate. In a perfect scenario, their characterizability would be measured directly, with agreed upon proxies such as time or cost. This is especially difficult given that the scientific and technical priorities with respect to characterization investment and output can vary wildly from one company to another. Direct testing specific to a particular company or industry may be possible and internally consistent, however further application without understanding stakeholder priorities may prove to be difficult.

It is important to note here the interconnectivity of equipment, techniques, and personnel. This relationship can add an additional layer of complexity to this decision-making process and should be tailored to the specific system and engineering organization. It cannot be taken as a given that the appropriate equipment, techniques, and personnel will be available to an organization internally or within a reasonable timeframe. Frequently, internal characterization equipment suites may not be suited for every conceived application, leaving project teams with a limited set of options for characterization scheduling in-house. Equipment, knowledge of techniques, and experienced personnel can be costly to the operating budget of a company, and the expenses associated with these resources may not be justified on a permanent, internal basis, giving rise to the prevalence of outside characterization laboratories for analysis of sample backlogs and small-scale project work. While these laboratories bring a certain amount of expertise and flexibility, in-depth knowledge of the project and institutional knowledge of the company is not usually shared, leading to a less integrable data product and a limited perspective as to the implications and value of the characterization work being completed. Systems engineers can justify integrated characterization staff as a value-added development as companies seek to develop complex material-intensive systems.

The incorporation of dedicated characterization staff also aids in the ability of the project team to communicate and educate, as data is dispersed through the full system lifecycle. As has been discussed, the collection of high-quality data has limited value if these data are not put to work appropriately within the system development. Upstream researchers can educate manufacturing teams on probable areas of risk and foreseen production issues, while manufacturing teams can direct quality engineering refinement and inform research teams on redesign efforts and next-generation products.

The characterizability metric does not consider every variable that a project team may wish to consider. Several terms have been approximated or abstracted, to a degree, to make the metric more usable and interpretable. For example, more specificity as to the maturity of a material may be required. During use, this factor may begin to mean the maturity of the material as used in this particular application or a sufficiently similar application. Where the distinction should be made for material maturity may require further research. Technique accessibility may need additional specificity given that some equipment scientists do not have full mastery of every technique associated with their instrument. Likewise, some equipment, while available to the company, make not be capable of performing a specific technique due to the age of the equipment, recent capability upgrades, or lack of capital improvements to the equipment and laboratories. Sample preparation techniques should not be discounted as a relevant and specific component of most characterization efforts. Not all personnel are equally capable of performing sample preparation work at a high-quality level, which can limit the quality of the characterization data overall. Further refinement of the data integrability metric may require more input from data engineers and software specialists as the characterization-associated datasets become larger and more complex.

There is certainly an opportunity to refine the characterizability metric overall by making the terms more process-specific and by making the resolution of the assessment more granular, but many of the decisions associated with that refinement would require a more specialized approach given the content of the system under development. During the evaluation of alternatives using the characterizability metric, project teams can review the assessment term by term for proactive improvement of the value. For example, if a project team is particularly tied to a substrate material that their company manufactures (and thus can provide input on supplier quality considerations), the team may be comfortable with using this material, even if it is less characterizable than the alternatives, because the characterization process is internal to the company, and the company personnel are already familiar with the associated datasets for this material.

2.5. Conclusion:

Through the course of this study, an attribute has been defined to evaluate system design via characterizability (i.e. the ability of a material system or material components to be characterized). Through the use of a test scenario, the potential value of the attribute has been demonstrated; however, further research will need to be conducted to expound upon this line of inquiry. More quantitative work can be conducted regarding real-world projects with the collaboration of industrial partners and business units in working companies. The evaluation through the test scenario highlighted the importance of stakeholder involvement for the sake of prioritization during trade studies, and, likewise, the importance of educating stakeholders on the potential value and risk of certain development pathways.

As systems increase in complexity, a more rigorous approach to design attributes in material systems development is becoming necessary. By understanding the materials, gathering data, and informing the development process, the project team can leverage the data produced by materials characterization equipment and characterization subject matter experts. These data can be quickly and completely applied to associated models and simulations to limit the need for exploratory experimentation and direct decision-making proactively.

The complexity and specificity of the field presents a potential problem. Quite frequently, for more intensive techniques, characterization specialists train for years through education and working experience to serve as a subject matter experts in their discipline. Many characterization techniques require more in-depth analysis and explanation as to the subtlety associated with the data generated. For example, time-of-flight secondary ion mass spectrometry (ToF-SIMS) typically requires several hours of data analysis and interpretation, which, even when completed, cannot simply be entered into a model free of caveats or stipulations.

It is interesting, however, to consider the utility of the more basic characterization approaches to the proposed attribute. Easily available and interpretable techniques can efficiently be compared to one another, entered into models and simulations, and used to track progress and problems as the product development continues. This seems to indicate an undervalued potential for characterization techniques as they become more readily usable and translatable to a quantitative metric. These processes are frequently associated more with the testing that takes place downstream in quality engineering laboratories but can be translated upstream for more complete research. Engineering efforts dedicated to making more complex equipment and techniques simplified for technician usability and more interpretable results could be worth the technical investment up-front, during the concept development phase. As equipment and state-of-the art techniques are constantly changing and improving for research-based characterization efforts, accommodating data interpretability will require a concerted effort and should be planned for during project scheduling.

Chapter 3: Applications for the integration of materials characterization into systems testing and evaluation planning

3.1. Introduction:

By testing materials, engineers clarify the property-structure-process relationships inherit to the material with which they work and confirm design decisions such that the fully composed system can meet the defined performance requirements. Allowing for a testing plan specifically tailored to materials characterization efforts constrains the complexity within material systems and enforces the rigor typical of test engineering processes for broader systems and systems-of-systems. By applying systems engineering test and evaluation techniques to materials characterization efforts, systems engineers can mitigate risk, leverage acquired data, and proactively plan characterization activities. Producing and evaluating scheduling and budgetary schematics alongside characterization activities can assist systems engineers in resource allocation and project management endeavors.

While materials characterization can be associated with a more multi-faceted approach to the evaluation of material properties, materials testing tends to be associated with a more rigid protocol to ensure compliance with the intended system's utilization and performance requirements. By reducing the lack of specificity with the term and concept of characterization, an improved and more efficient evaluation methodology can be implemented, tracked, and validated during the development of complex systems using material components.

In general terms, testing is used to confirm system status or understand system limitations. It is used to answer questions such as the following:

- Does the system perform according to the requirements?
- Is there a discrepancy between the expectations, according to the design, and the performance, in reality?
- Do unexpected variations or inconsistencies exist within the system?
- How does the system fail, both qualitatively and quantitatively?

By designing test protocols to better understand the system under development, the project engineers can more realistically consider the implications of the system deployment and gather information on the system's behavior for improvement endeavors, redesigns, and future projects. Herein lies an opportunity to apply test engineering principles to materials characterization. In a very similar way, characterization efforts seek to better understand the discrepancy between design and reality and profile the limitations of the material to build a failure mode knowledge base.

While test engineering in a classical systems engineering approach is typically considered a more predominant aspect of the test and integration half of the systems engineering Vee diagram, applying testing activities into earlier concept exploration phases can more adequately address the materials selection steps of research and development-based projects. This is not to say that test engineering is not a full system process in conventional contexts. On the contrary, test engineering and planning has been shown to be a productive and valuable process as early as the needs analysis phase and as late as the retirement and disposal phases. By more holistically testing systems, engineers can gain robust and comprehensive datasets on system behavior and responses to changing conditions.

As novel materials, or materials integrated into larger systems in novel ways, become more prevalent, proactive test planning approaches can provide a breadth of information when conducting upstream research and development efforts and a depth of clarity when analyzing downstream manufacturing quality information. Moreover, proper cataloguing, evaluation, and utilization of these datasets can be applied across the system lifecycle to more efficiently address design concerns and production improvements (Yang et al., 2022).

As material systems become more complex in their own right, more rigorous and complete test planning needs to be incorporated into these system developments. By addressing this complexity proactively, project engineers can ensure functional material components and successful systems (Graics et al., 2023). Furthermore, by building a base of knowledge in material systems testing, more complete test procedures can be developed for future products and more valuable datasets can be generated for modeling and simulation efforts (Siegel et al., 2010).

Failure analysis has been a long-standing component of materials testing. By creating more complex materials, engineers are provided with the opportunity to leverage the institutional knowledge on material failure with the wholistic approach afforded by systems engineering principles to more capably predict material system failure modes, to manage risk, and to limit performance variability.

Materials characterization is a testing process at its core. By evaluating materials through characterization equipment, engineers can measure properties, define the achievement of success criteria, and ensure selected materials are delivering the performance required of the planned system. By applying test engineering principles to materials characterization, a more rigorous and complete approach can be employed to organize and execute the needed materials characterization effort. Integration, testing, and evaluation from a bottom-up approach delivers an effective workflow while using resources efficiently.

System testing consists of a series of typical phases that ensure a comprehensive determination that the system meets the engineering specifications, and that the system truly fulfills the customer needs. These phases include, but are not limited to:

- Test planning – Engineers will consider the functional requirements, key technological linkages, and least understood elements of the system design. Testing protocols will be developed to understand the behavior of the system to ensure that the system meets the designated requirements when completed.
- Element testing and integration – Engineers will test system elements in a bottom-up fashion as the system is integrated. Higher levels of integration and a more materialized system will require more complex testing.
- Developmental testing – Engineers will test the system under a variety of operational conditions and use-case scenarios. System capabilities that fall short of the requirements will be analyzed and improved upon until the system is compliant.

- Operational testing – Engineers will test the system in a realistic operating environment. Readiness of the system for production and deployment will be evaluated.

It is important to remember that every system is different. System testing is unique to each system, but certain commonalities apply across technological disciplines and engineering imperatives. For example, a glass fiber reinforced polymer composite selected as a component material may not be identical to previously used component materials, but certain material behaviors will be expected, and corresponding test protocols can reasonably be developed given the implied challenges (e.g. non-destructive testing in service for fiber warping).

Test planning for material systems presents a unique challenge in that the range of technical disciplines needed to understand some materials characterization efforts can require expansive technical breadth, depth, and knowledge of adjacencies. Systems engineering, likewise, is uniquely suited to address this issue as it is a disciple based upon the design, development, and production of the system beyond the component level. Component owners and technical specialists can develop components according to the designated requirements, while systems engineers can focus on the integration of those components such that the system, as-a-whole, functions soundly. Systems engineers frequently serve as a technical resource able to communicate and coordinate among the various engineering disciplines. By treating materials as a systems-type problem, a more comprehensive solution to test planning and execution can be devised.

While the engineers responsible for building complex systems typically dedicate a substantial amount of effort to integration, and its associated testing and evaluation, material systems, as a class of production unit, can be particularly integration intensive. Increasingly, material systems are being engineered with novel materials, novel joining methods, novel processing techniques, and novel applications, leading to a higher than typical failure rate for a component-level system element. This failure rate stalls progress and leads to redesign and rework. By emphasizing the criticality of the integration of material systems within larger systems, project engineers can more adequately address development challenges.

Test engineering within system development consists of an iterative process of verification and validation as the system elements are produced and integrated. Verification is the process by which a system is tested to ensure compliance with the established specifications. Validation is the process by which a system is evaluated to ensure that it meets the customer needs.

With respect to materials verification and validation, it is important to consider not only the material properties, dimensions, and measurements, but also the successful integration of those material components into a product that serves the customer needs. Approaching material systems with a systems perspective can allow for the evaluation and selection of appropriate materials, comprehensive test protocols to ensure full system integration, and a final system production that directly addresses the customer needs. As test engineering activities can sometimes become limited due to schedule and budget constraints, successful test and evaluation addresses the full life cycle requirements of concern to the stakeholders and should be planned for from the earliest stages of the project.

It is important to treat test and evaluation as a full life cycle task, and, similarly for the purposes of this investigation, materials characterization and testing should be considered through all phases of the system life cycle. As such the testing effort should begin in the earliest stages of planning, needs analysis, and design and should extend through to the system retirement and disposal. This is especially important when considering the sometimes-emergent failure modes of complex materials and the changing regulatory environment governing waste, recycling, and reuse. While conventional aspects of test engineering focus on the production of a functional system, customers and stakeholders are increasingly concerned with the longevity, reliability, and successful termination of requested systems.

The use of digital twins can significantly limit the cost associated with concept exploration and testing (Xie, et al., 2022); however, these models of system element behavior must be accurate, precise, and representative of the phenomenon of interest. Using empirical and experimentally verified information to quantitatively define behavior and develop a representative model provides a high degree of utility to a product development team. Models, in this context, can be used to guide decision making and limit the number of exploratory experiments required to make critical design and development choices. Likewise, testing efforts can be made more efficient when the behavior of a system phenomenon is appropriately defined (Zhu et al., 2021).

Simulations provide a mathematical representation of dynamic system behaviors. These allow the project development team to more quickly and efficiently evaluate more complex system behaviors and guide development efforts throughout the system lifecycle (Botocan et al. 2022). Simulations simplify the test and evaluation process by allowing a more targeted approach to designated developmental and operational test scenarios and can limit the time and resources allocated to well constrained system behaviors that are adequately represented by this mathematical characterization.

The use of models and simulations provide an opportunity for project teams to streamline the concept development phase and choose the most necessary testing protocols to determine system compliance with the designated design requirements and customer needs. However, to inform these tools appropriately, an initial and proactive approach must be utilized to build representative models and simulations for the desired system (Eriksson et al., 2002). This shifts the test design and implementation effort to a full system approach and an iterative, proactive strategy. Instead of selecting a concept and then designing a testing regime to confirm the system's capabilities, an effort needs to be made to consider what test information will be valuable to future projects and to incorporate these data proactively into next-generation system models to aid in concept exploration, analysis, and decision making.

While mathematical models of system behavior are not the only kinds of models (e.g. physical models, schematic models, etc.), they are becoming increasingly relied upon to minimize the resources dedicated to the analysis of alternatives and the planning of test regimes. The risk with relying too heavily upon mathematical models lies in the overconfidence in the model accuracy without adequate input data to teach the model. Poor data quality will not produce an accurate model and can lead to poor decision making for an unwary systems engineer. With increasing access and availability of modeling tools and techniques, engineers must remember to train models appropriately for the desired application. Good quality datasets can be derived from previous testing on similar systems and institutionally developed engineering datasets based upon adjacent technologies.

Wang et al., 2022, evaluated the consistency of a power battery pack for automotive applications using a virtual model. The investigators used the data acquired from a thermal effect and electrochemical performance test and evaluation unit to train a neural network model. The model was able to evaluate battery consistency to improve safety and efficiency of the unit and to predict battery behavior in future endeavors.

Karomoddini et al., 2022, devised an automatic test and evaluation process for autonomous systems where simulations using fuzzy logic were used to replace manual review of all test scenarios by test engineers. Instead, a flagged subset of scenarios was reported for the engineering team to review, so that while many scenarios were evaluated by the test system, the engineers' time was spent on scenarios of interest where further consideration may be needed. The toolkit was successfully used for testing and evaluation of an Unmanned Aerial System's perception subsystem.

It is especially important to consider material interfaces when developing material systems and integrating these functional elements into larger, and more complex systems and systems-of-systems. By elevating materials engineering and materials characterization efforts to a systems engineering task, a more comprehensive effort can be made from the earliest stages of the product development to manage complexity, plan for integration, and conduct rigorous testing to ensure that the customer needs are met. Gathering materials characterization and testing data from material systems can propel intellectual property exploration forward and reduce the amount of uncertainty associated with downstream production efforts.

Efatmaneshnik and Ryan, 2015, proposed a “System of Interest” model to address complexity management. The System of Interest model consists of a series of system elements that interact amongst each other and a defined boundary between the elements inside of the System of Interest and the elements outside of the System of Interest. The system complexity can be broken down into two components: the objective component and the subjective component. The objective component of complexity consists of the number of system elements and their relationships to one another. The subjective component consists of the deviation of the system being developed from some idealized reference model. By defining a system in this manner, complexity can be better accounted for both in a context-independent (or absolute) manner and a context-dependent (or relative) manner. While complexity within systems tends to be context dependent, the authors in this investigation attempted to devise a generic categorization that could be applied to a variety of scenarios independent of the situational circumstances.

Padhee et al., 2023, addressed complexity through innovation team compositions during the product development lifecycle. The investigators used computational simulations to model group dynamics within an innovating community. Agent roles were either defined as explorers or exploiters. Explorers preferred autonomous exploration of potential solution spaces, while exploiters preferred communicating with other agents in their network to develop the best available solution. The study found that teams with a higher proportion of explorers performed better in high-complexity spaces, such as early lifecycle tasks (e.g. concept development) and that teams with a higher proportion of exploiters generally performed better in the later stages of the development lifecycle, although explorer majority teams were eventually able to catch up to them.

The discussion of test engineering within the materials engineering space should not be held without consideration of the related human factors engineering efforts. The production of adequate materials characterization and quality testing workflows requires the simultaneous consideration of human capabilities, limitations of the current workforce, and opportunities for task efficiency. The scientific sub-disciplines within materials characterization are typically specialized within technology groups and further specified to distinct industrial contexts and institutional histories. For example, a project may require not just electron microscopy, but scanning electron microscopy of porous metal structures with a feature-scale on the order of single digit nanometers. This makes characterization scientists and engineers with a background in products similar or adjacent to the proposed project incredibly valuable to its success and critical to the garnering of data of worth for system development.

3.2. Materials and Methods:

To adequately address the amorphous issue of conventional materials characterization approaches and define them more rigorously as a testing methodology, a series of core principles need to be defined to guide the design of a quantitative evaluation and test approach. These principles consist of (1.) understanding the current capability, (2.) understanding the required capability, (3.) allowing for emergent behavior and flexibility, and (4.) considering the full life cycle. By addressing these principles, a test planning methodology can be designed and deployed to create a more efficient workflow for material system development efforts.

3.2.1. Evaluate the current capabilities

The project engineering team will first be required to understand the current characterization capability. This is quite frequently a planning step that is missed by design engineers. By recognizing the value provided by materials characterization and the associated cost (i.e. budget and schedule) associated with proper characterization efforts, project teams can plan for the necessity of these analyses and coordinate efforts to access equipment and schedule the time for specialists. Because characterization planning is a multicomponent problem, requiring not only equipment time but also data analysis and interpretation, it is important to account for its labor-intensive nature as early in the system development lifecycle as possible.

For example, a system under development may require the use of field emission scanning electron microscopy to characterize a thin film layer adhesion and thickness. This tool is available to the team internal to the company, but the ion mill preparation tool required to appropriately reveal these features of interest at the scale required is only available externally. The design team in this scenario understands a characterization requirement for the project and understands the type of tool needed to conduct this analysis but is unaware of the preparation requirements or alternatives available. This example illustrates the utility of incorporating characterization specialists into the design and planning phases of the system development process. Clear definitions of the analysis required for critical technology investigations provides the design team as a whole with a more complete understanding of the project milestones moving forward.

Shabi and Reich, 2012, address system verification, validation, and testing (VVT) as a function of complexity. By sub-dividing VVT into task categories including stakeholder requirements, engineering requirements, VVT strategy, VVT activity, and method, the investigators were more able to organize VVT conceptually and define the building blocks of successful VVT in complex systems with a high interconnectivity of competing requirements. Risk was also calculated during this evaluation to capture the volatility inherent to complex system planning and the potential cost associated with inadequate VVT processes.

An emphasis should be placed on understanding the current tools and techniques available and the best way in which they can be applied to the current project challenges. Understanding the current inventory of equipment and expertise can streamline the test planning process and produce a wider array of test data on which future elements of the project can be informed. Leveraging the current characterization capabilities can also dictate the direction of future characterization equipment upgrades as well as guide technology road mapping for company capital planning and institutional knowledge growth in scientific fields of interest. This iterative and continuous improvement can fuel ongoing innovation growth within the company for system upgrades and future projects.

Furthermore, understanding resource timelines, equipment lead times and backlogs, personnel schedules, and competing company priorities are critical to the planning and management of materials characterization resources and test planning. Without a clear vision of characterization resource management, a test and evaluation master plan cannot be detailed with any accuracy, nor can a complete list of testing requirements be conceptualized or scheduled, making knowledge of the materials characterization sciences a limiting factor for the project overall.

3.2.2. Evaluate the required capabilities

With a constantly advancing state of technological innovation and system design options, it is critical to understand the required characterization capability not only for the project under development but also for relevant and expected advances required for next-generation products. By valuing the characterization data for both current and future projects, more efficient development pathways to novel products and technologies can be evaluated and deployed. These datasets can be used to train models and simulations, calculate risk and opportunity, and streamline design and redesign decision making.

While evaluating current capabilities is, in essence, a bottom-up process (e.g. we have these tools and techniques, can these address our requirements?), the evaluation of required capabilities is much more of a top-down process (e.g. this information is required, how do we achieve understanding of this information?). In some circumstances, this shift is rather straightforward, such that a new characterization technique needs to be applied, but the characterization specialist and tools required are available internally. In other circumstances, development of new characterization capabilities can be quite challenging, such that tools, techniques, and personnel are not available internally and not easily obtained externally.

The investigation and evaluation of new characterization capabilities can be a challenging and technically complex task within the broader system development. These technology groups, themselves, are rapidly evolving to meet the challenges of advances to the frontiers of science and engineering. New equipment and techniques are actively being developed that require continuing education for characterization specialists and retraining for equipment operators. Frequently, new equipment needs to be further tested and validated within the purchasing company to understand the capability and ascertain its application to ongoing and future projects. Purchasing and procurement of these equipment and techniques requires capital proposals sometimes evaluated as infrequently as annually, and the most novel techniques may require hiring of new personnel, which can take even longer.

It is also important to note that the time and cost associated with the invention and development of new characterization techniques are extensive. Even internal efforts conducted by well-funded and well-staffed characterization teams require a period of research, experimentation, and validation. These tools and techniques then need to be verified for the specific product under development, and, quite commonly, a process control or quality testing equivalent will need to be designed to maintain the product quality standard downstream, which will require more testing. In some circumstances internal characterization resources may be weighed against external characterization resources in a trade off analysis to determine the best path forward for a particular project. While external resources may offer enhanced specialization, internal resources will have a stronger command of the institutional history, current company product portfolio, and future company technological ambitions. In short, using an internal characterization team, while costly initially provides a stronger engineering resource for the long term.

3.2.3. Allow for emergent behavior

As with most systems engineering endeavors, the complexity inherent to the project drives emergent behavior within the system which introduces a degree of unknown variability. This phenomenon, therefore, drives systems engineers to consider flexibility as a valuable system attribute. By maintaining a flexible approach, the project engineering team and their associated characterization specialists can more quickly adapt to changing circumstances, develop new or more appropriate test protocols, and ensure that the customer needs are met.

Haugen et al., 2023, investigated the detection of emergent behavior in engineered systems. They define emergent behavior in complex systems as dynamic behavior that can be observed at the macro level but cannot be traced to the micro level. A system with a high degree of complexity requires increased testing to predict emergent behavior and limit the quantity and criticality of technological pitfalls. The authors further subdivide system complexity into four categories: (1.) simple, (2.) complicated, (3.) complex, and (4.) chaotic. A recommendation is provided to establish test suites when designing complex systems to trigger emergent behavior within the system and use models and simulations to test a wide variety of system conditions. These procedures can increase the likelihood of detecting emergent behavior and lead to the production of more complete test protocols as system complexity continues to increase.

It is important to note here that flexibility for the unknown is a key strength to successfully designed complex systems. By valuing flexibility as a system attribute, emergent behavior can be detected, accounted for, and absorbed by the system under operation. Engineers responsible for designing complex systems can introduce flexible elements by elevating resiliency, reliability, and redesignability at a prioritized level. Walker, 2020 uses agile engineering processes to develop more comprehensive testing regimes such that model-based systems engineering, test automation, and agile stakeholder communications produce more efficient, proactive, and complete testing. This approach is especially valuable as the system integrates, evolves, and exhibits unexpected emergent behavior.

3.4.4. Consider the full life cycle

It is critical to consider the full system life cycle when developing and testing systems involving complex material components. This includes evaluation of stakeholder needs, detailed design, production, operation, support, and retirement. This consideration is especially important as system developments increasingly shift to the concurrent manufacturing perspective, where a systematic and wholistic approach is taken for the system development effort where all phases and aspects of the development are considered simultaneously (Blanchard and Fabrycky, 2011).

Designing for testing of materials requires this wholistic perspective. Materials being evaluated for specific properties and functionality under research and development efforts should, likewise, be evaluated for manufacturability, producibility, and operability. Testing systems should be put in place that adequately confirm that the material meets the design specifications and subsequently satisfies the customer needs.

Planning for full life cycle is not a trivial endeavor. In terms of testing, while destructive examination and more complex, comprehensive characterization may be warranted and even necessary for upstream activities, limiting the amount of destructive testing downstream allows for adherence to the quality standard while maintaining production throughput. This is especially true of more complex systems where destructive testing of high-valve components and subsystems significantly limits the profitability of the product line. This initiates the imperative to shift testing to non-destructive alternatives as soon as is possible. In circumstances where destructive testing is the only option, non-destructive alternatives should receive time and funding to limit waste and improve yield while maintaining system quality.

Wang et al., 2020, researched non-destructive testing methods as applied to composite materials. Non-destructive techniques address safety concerns and maintenance costs while improving the quality assurance process. By detecting defects non-destructively, rapid feedback can be provided to process engineers to minimize process variability, drive root cause analysis, and prepare corrective actions. The researchers also acknowledged the necessity for multiple testing techniques to fully characterize the material under evaluation and the shifting of testing techniques to automated inspection systems to increase accuracy and make data processing and integration more efficient. While this investigation was mostly concerned with the structural integrity of composite materials, similar techniques and evaluations can be applied to other material properties as the stakeholder needs apply to each project specifically.

Yang et al., 2016, apply a similar evaluation of non-destructive testing technologies to composite wind turbine blades. They argued that the availability and reliability of wind turbines is directly related to the ability to non-destructively inspect wind turbine blade composite materials in the field. This technology advancement is a catalyst for the continued development of the wind turbine and the economic position of alternative energy sources. The inspection technologies can also be used for manufacturing quality control efforts to more quickly trace defects to their root causes and eliminate process deviations at the source. This is a critical component to production efficiency and economic viability as material systems, upon which novel technologies are built, become more complex and more expensive (Schicks et al., 2020). The broad spectrum of non-destructive testing technologies can also be further developed and applied across adjacent technology sectors such as solar energy (Botteon et al., 2022), renewable energy (Sheehan et al., 2010), and building inspection (Sfarra et al., 2021).

3.2.5. Characterization management

For all characterization efforts, there is inherently a problem of scale. Techniques and equipment that provide the appropriate resolution for the sample size are required while being able to analyze the sample efficiently. This balance between resolution and sample size drives the development of new characterization tools, which in their own right serve as complex systems with specific requirements for stakeholder satisfaction. It is entirely possible that novel testing equipment and methodologies that require their own budget, schedule, and technical resources may be necessary for a new system development to be verified and validated.

For example, the tools and techniques to characterize two material phases on the order of 5 nanometers may exist internally but adequately charactering the interplay and distribution of those two phases throughout a one meter cube of material may prove to be quite difficult. This is an interesting and unique challenge in that a sample of the material is representative of certain information (i.e. characteristics of the material) but understanding the variation of those properties by direct testing of the material structure is logistically difficult. A new technique could be developed to characterize the one-meter cube in its entirety, or a series of subsamples could be analyzed that the scientist responsible for the characterization calculates is adequately representative of the whole. In the former case, a sufficient technique may not be devised at an acceptable cost or timeframe, or the technique may not be able to analyze quickly enough to make the technique worthwhile in an iterative system development project format. In the latter case, the assumption is being made that a number of subsamples will be representative of the whole throughout the experimentation and development process, and furthermore that an adequate manufacturing control or inspection can later be devised to ensure product quality downstream.

This issue is illustrated in Figure 3.1 below, which describes the size of the features of interest with respect to the broader sample size and complexity of the characterization effort. While the diagram simplifies a wide range of material technological capabilities, increasingly, stakeholder demands and engineering technical requirements push engineers to innovate, integrate, and test toward the more challenging quadrants of the chart, where it is required that the distribution and interactions amongst small features be characterized on a large scale.

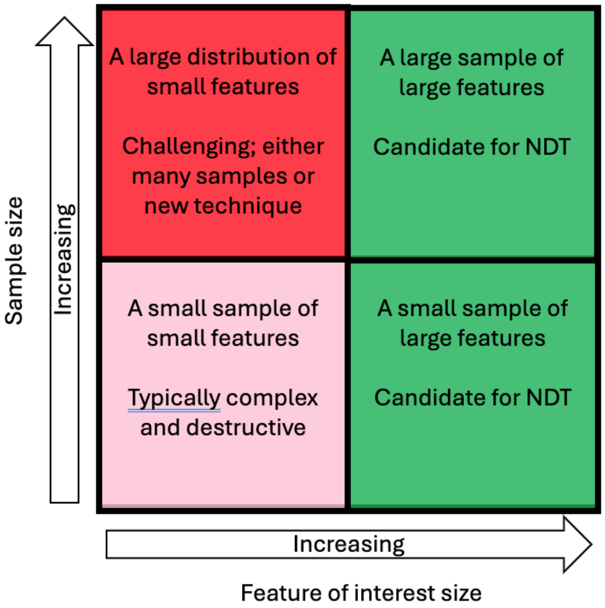
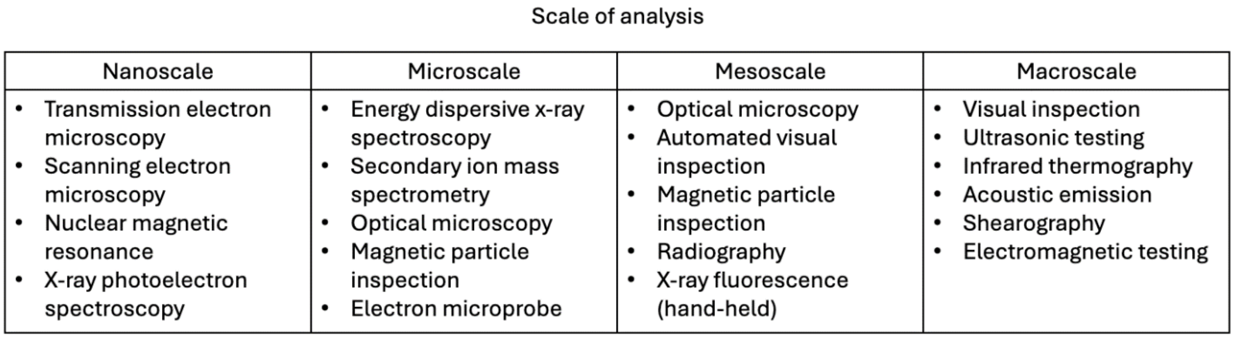


Figure 3.1: Chart describing the difficulty of characterization techniques as feature size and sample size increase (red quadrants is technically challenging, while green quadrants are technically straightforward; pink quadrant is intermediate)

It is also important to note here that, along with most engineering activities, engineering challenges that are overly large require special attention. This is especially true when it comes to characterization activities. Even relatively easy-to-define defects become difficult to test for when the sample under evaluation is an extremely large component of a system. For example, understanding the distribution of corrosion under visual inspection of a component may be rather straight forward; however, scanning and entire in-service oil pipeline for evidence of corrosion becomes a more difficult task.



Scale of analysis

Nanoscale	Microscale	Mesoscale	Macroscale
• Transmission electron microscopy • Scanning electron microscopy • Nuclear magnetic resonance • X-ray photoelectron spectroscopy	• Energy dispersive x-ray spectroscopy • Secondary ion mass spectrometry • Optical microscopy • Magnetic particle inspection • Electron microprobe	• Optical microscopy • Automated visual inspection • Magnetic particle inspection • Radiography • X-ray fluorescence (hand-held)	• Visual inspection • Ultrasonic testing • Infrared thermography • Acoustic emission • Shearography • Electromagnetic testing

Figure 3.2: Chart depicting characterization techniques and scales of analyses

As engineers consider processes and engineering efforts later in the system development lifecycle, an emphasis of non-destructive testing should be made over conventional materials characterization in more respects. While characterization can be useful in downstream phases, implementing process controls to eliminate issues that would require more elaborate characterization becomes more economically efficient, in terms of both time and cost. Producing systems that can be non-destructively tested and inspected provides more direct feedback on a part-to-part basis and reduces the scrap rate of good quality parts.

In Figure 3.3, a process workflow is detailed for a test engineering approach to materials characterization. The workflow describes a four-part process that converts a clarified concept into a system containing validated functionality. Critical activities for this procedure include evaluating current inventories, capital planning, and designing for flexibility and testing.

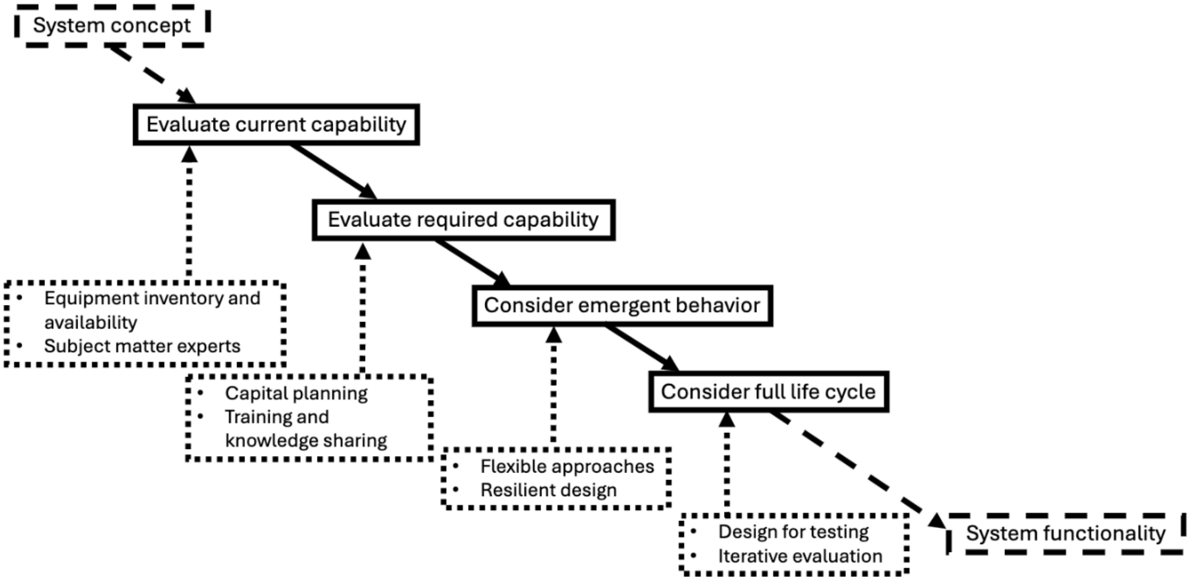


Figure 3.3: Diagram describing the process of materials characterization as a test and evaluation protocol

A routine problem encountered during characterization work are sample backlogs and scheduling challenges. These techniques frequently require equipment time as well as data analysis and interpretation. While ideally materials testing data would be immediately available, easy to understand, and automated, these datasets are not always available during the development of novel materials. There is an opportunity, however, to make materials characterization efforts more streamlined and more understandable to project engineers by applying queuing theory to characterization scheduling efforts.

3.2.6. Queuing theory

Queuing theory describes a method of analysis where a facility is required to meet a demand for service created by a population. This population forms a queue, and receives service according to their arrival time, servicing time, and quantity of population demanding the service (Blanchard and Fabricky, 2011). By considering characterization as a service, and understanding the bottleneck created by analysis of variable feature sizes and sample sizes, an evaluation of this waiting-line system for materials characterization can be conducted. Several components of queuing theory are detailed in equations 3.1 through 3.3. For these equations, λ is equal to the expected number of arrivals per period, and μ is equal to the expected number of service completions per period.

$$n_m = \frac{\lambda}{\mu - \lambda}$$

Equation 3.1: Mean number of units in the system

$$m_m = \frac{\lambda^2}{\mu(\mu - \lambda)}$$

Equation 3.2: Mean length of the queue

$$w_m = \frac{\lambda}{\mu(\mu - \lambda)}$$

Equation 3.3: Mean time an arrival spends waiting for service

It is quite typical, within materials characterization equipment suites, to have backlogs of samples for analysis. Depending on the style and format of this analysis, results and interpretation of the data could be required as soon as possible, (e.g. production upset failure analysis), or could be a topic of discussion with broader system implications (e.g. product development steering). Also, it is common for materials characterization scientists to manage a series of project priorities depending on shifting organizational goals. This leads to variable wait times for analysis unless a prior arrangement has been made with a project engineering group to guarantee certain analyses on a regular basis. Again, these arrangements can be altered depending on company priorities. While this is a complex test engineering problem, for the purposes of this foundational study, sample backlogs and analysis capabilities can be abstracted to sample quantity and processing time in this queueing model.

For the purposes of this study, three scenarios will be considered. In scenario #1, a suite of scanning electron microscopes is being used to analyze samples critical to a product research and development effort, and a rapid turn-around time for the testing, data analysis, and interpretation is requested. The instrumentation and associated analyst are able to process samples at a rate of 0.6 per hour and samples arrive at the characterization facility at a rate of 0.4 per hour. For scenario #2, the suite of instrumentation is assigned to a more aggressive analysis schedule for a later-stage product development and production support effort. The analysis required is simpler to conduct and interpret, however, the turn-around times requested for more direct product processing feedback have been requested to be shorter, and samples are arriving more quickly for analysis compared to scenario #1. In this scenario, the analysis occurs at a rate of 0.9 per hour and samples arrive at the characterization facility at a rate of 0.8 per hour. In scenario #3, the instrumentation suite is assigned to a production support role and an accelerated analysis regime is implemented to shorten the expected turn-around time for the data. The values associated with these scenarios are listed below:

- Scenario #1: $\lambda = 0.4; \mu = 0.6$
- Scenario #2: $\lambda = 0.8; \mu = 0.9$
- Scenario #3: $\lambda = 0.8; \mu = 0.95$

By evaluating these scenarios, an application of queueing theory-based test planning can be illustrated to provide context for the potential utility of test engineering practices to materials characterization activities.

3.3. Results:

The critical queueing theory values are calculated below. Each scenario represents a different style of analysis, with an augmentation of the required turn-around time detailed in the shift between scenarios #2 and #3.

3.3.1. Calculation for the mean number of units in the system

$$n_m = \frac{\lambda}{\mu - \lambda}$$

- Scenario #1: $n_m = \frac{(0.4)}{(0.6-0.4)} = 2$
- Scenario #2: $n_m = \frac{(0.8)}{(0.9-0.8)} = 8$
- Scenario #3: $n_m = \frac{(0.8)}{(0.95-0.8)} = 5.33$

3.3.2. Calculation for the mean length of the queue

$$m_m = \frac{(\lambda^2)}{\mu(\mu - \lambda)}$$

- Scenario #1: $m_m = \frac{(0.4)^2}{(0.6)(0.6-0.4)} = 1.33$
- Scenario #2: $m_m = \frac{(0.8)^2}{(0.9)(0.9-0.8)} = 7.11$
- Scenario #3: $m_m = \frac{(0.8)^2}{(0.95)(0.95-0.8)} = 4.49$

3.3.3. Calculation for the mean time an arrival spends waiting for service

$$w_m = \frac{\lambda}{\mu(\mu - \lambda)}$$

- Scenario #1: $w_m = \frac{(0.4)}{(0.6)(0.6-0.4)} = 3.33$
- Scenario #2: $w_m = \frac{(0.8)}{(0.9)(0.9-0.8)} = 8.89$
- Scenario #3: $w_m = \frac{(0.8)}{(0.95)(0.95-0.8)} = 5.61$

These scenarios cover a range of operational conditions. These include a research phase, a development phase, and a reassessment of the development phase analysis to decrease the time an arrival spends waiting for analysis to below 8 hours per sample. In scenario #1, on average, there are 2 samples in the system, with a queue of 1.33 samples, and a mean sample wait time of 3.33 hours after arrival. In scenario #2, on average, there are 8 samples in the system, with a queue of 7.11 samples, and a mean sample wait time of 8.89 hours after arrival. In scenario #3, on average, there are 5.33 samples in the system, with a queue of 4.49 samples, and a mean sample wait time of 5.61 hours after arrival.

3.4. Discussion:

Through the test scenarios, it is demonstrated that queueing theory style test planning can be applied to materials characterization activities. This approach provides scheduling and cost information for the project development team related to resource utilization, sample backlogs, analysis timeframes, and potential areas for process streamlining. By calculating the mean number of samples in the system, average length of the sample queue, and average wait time for newly arrived samples, systems engineers can more adequately understand the flow of samples through a characterization system and evaluate the need for additional characterization resources. Further investigation into more complex test planning tools, including multi-channel queueing theory could be conducted in the future to consider the characterization analysis suite more comprehensively. Adjacent applications for the technique could include in-line inspection, expert evaluations of ongoing issues, and regulatory compliance scheduling, and are a topic for further research.

It is important to note that several key determining factors of materials characterization were abstracted for the sake of simplifying and clarifying the proposed queueing model. Materials characterization, in most contexts, requires a significant amount of time for sample preparation, instrument operation, data analysis, interpretation, and reporting. For the purposes of the evaluated scenarios, these factors were simplified to an analysis time metric. Likewise, samples being generated for materials characterization purposes can be produced specifically for experimentation purposes with variable analysis interests. The quantity of samples and their associated datasets are very much dependent upon specific engineering questions related to property-structure-process relationships, and these questions change as the system development lifecycle progresses. For the purposes of the aforementioned scenarios, these sample quantities and arrival consistencies were abstracted to an arrival rate metric.

In the broader consideration of materials characterization within product development, the project focus shifts as the product becomes more well-defined and understood from characterization activities to measurement and inspection activities. Materials characterization, while critical for providing in-depth analysis of material properties and more complex datasets that can educate models and simulations, are resource and labor intensive. It typically becomes prohibitively expensive to use traditional characterization equipment and techniques when a more simplified and targeted analysis can be developed. This results in the development and installation of measurement and inspection equipment and personnel that can be involved both with in-line product testing (i.e. as the product is being manufactured) as well as post-production quality testing (i.e. sub-sampling and testing of product). The changing context for the type of analysis, speed of results, and impact to the broader production efforts is critical to account for during test planning calculations.

More amorphous and exploratory characterization may require a less constrained scheduling estimate, while downstream inspection efforts can be more accurately predicted. This is especially important for the evaluation of process control and the eventual reduction of inspection efforts, entirely, as the controlled product production no longer requires intensive inspection activities to maintain the quality standard. This type of inspection reduction should be evaluated with the utmost care and an iterative risk evaluation.

It is particularly difficult to plan for the analytical resources required for failure analysis. This can include investigation of parts and components that have been tested-to-failure as well as products that have failed in-service. With any failure analysis, scheduling becomes difficult due to the nature of the problem and the questions being asked of the analyst (e.g. How has the product failed? Why has this occurred? How can this be corrected?). Due to the uncertain nature of the problem, failure analysis can take a significant amount of time, require additional characterization equipment, or necessitate follow-up analysis on additional, similar failures. The proposed approach can more rigorously plan for characterization activities such that well-constructed data sets and complete testing regimes can be drawn upon for failure analysis activities.

Shifting stakeholder priorities, with respect to product properties and specifications, require an iterative approach to test planning evaluations. While test and evaluation planning should be a proactive and full-system process, it is important to remain flexible as priorities change and resources are reassigned based upon broader organizational needs. By using the process workflow coupled with more conventional test engineering planning tools, iterative assessments can be prepared to manage test activities and ensure verification and validation milestone completions. This can limit the uncertainty associated with materials characterization, measurement, and inspection, as well as product requirements analysis, adjustment, and modification. The challenge remains, however, when dealing with novel or limited-access characterization techniques where the characterization objective is simple to understand and define, but the actual acquisition of the required datasets are difficult or impossible. These situations may require analysis via proxy techniques, representative sub-sampling, or invention of new characterization methodologies to generate the material information.

3.5. Conclusion:

The investigation detailed in this document demonstrates the potential value of a test engineering approach to materials characterization efforts. Utilizing test scheduling calculations and resource management workflows can constrain the variability associated with materials characterization, measurement, and inspection, while allowing for a proactive understanding of project task requirements. By considering, in advance, the current characterization capability, the capability required for the project, emergent behavior, and the full system life cycle, the potential risk and volatility associated with materials characterization can be minimized, and verification and validation activities can be accounted for and conducted in a complete manner.

Future work into these concepts would include more complete real-world testing of the workflow and associated test planning tools. By evaluating this approach against conventional approaches, the value added to the project in question can be appropriately calculated. Furthermore, additional test and evaluation tools could be evaluated for their utility within this intersectional domain of systems engineering and materials engineering workspaces. These could include liner programming approaches to project optimization, economic evaluations and break-even analyses, statistical process control analyses, and system attribute trade-off analyses.

Chapter 4: A process for evaluating materials characterization risk in post-development phase systems

4.1. Introduction:

As materials become more complex, the manner in which they are incorporated into larger systems produces significant challenges. These challenges can include upstream, research and development type problems related to fundamental scientific questions of material applicability and selection and can extend well into the later stages of the system development lifecycle to include downstream manufacturing, production, and operational issues. Furthermore, as the complexity of systems increases, the value of systems, in terms of cost, time, and technological investment increases. This leads to an enhanced risk associated with late-stage failures in system operation and an increase in the scrutiny required during quality engineering efforts. An emphasis on quality engineering, risk assessment, and failure analysis, throughout the full system lifecycle can limit the potential for high-cost incidents. With high-value systems containing complex materials, materials characterization can be used to enforce the quality standard, drive root cause analysis of component failures, and carry out emergency response procedures in the event of system failures.

By applying systems engineering risk and quality assessment tools to materials characterization activities, systems engineers can mitigate characterization risk directly while leveraging accumulated material data. Using these tools to proactively plan for emergency, or otherwise unforeseen, circumstances can allow systems engineers to quickly and effectively respond to post-production incidents or quality issues.

Emergency response and preparedness is frequently seen in the military and defense sectors (Paturas et al., 2007), as well as utility networks (Mohammadi et al., 2019), information technology systems (Huang et al., 2020), and the biomedical industry (Johnson and Vindrola-Padros, 2017). The concept being that the system owners need to assume the system will fail in a catastrophic manner and draft an appropriate response plan, which needs to be prepared, implemented, and rehearsed on a continuing basis. Iterative improvements to the response plan should be made based on the results of the practice drills via after action reporting or other evaluation schema (e.g. What went well?, What did not go well?, How can we improve the plan based on these observations?). While these activities are commonplace for the above-mentioned systems, applying these approaches to material systems has not been transferred on a wide scale. Part of the argument against incurring this added cost and time would be that the criticality of these material systems does not warrant the expenditure, however as materials become more complex, cost-intensive, and critical to system and system-of-system functionality, the imperative exists to proactively plan responses for material system failure emergencies.

When discussing emergency preparedness and emergency responses, it is important to also discuss the broader topic of risk and risk management. The identification and mitigation of risk has been a core systems engineering process since the birth of the discipline (Kossiakoff et al., 2020). The fundamental challenge for systems engineers is to create technically advanced systems, sometimes containing significant novelty, while minimizing unknown outcomes, adverse effects, and the criticality of those negative events. This requires advanced knowledge of the system while it is still being conceptualized, under development, and not yet completely understood.

4.1.1. Risk

Risk management is a full system lifecycle endeavor. While the program risk typically decreases through the development of the project (i.e. as the system becomes more known and understood), risk can occur due to late-stage emergent behavior, changing regulatory conditions, or shifting stakeholder goals. This is especially true of materials engineering, where novel material interfaces, operational use-cases, or disposal options may be implemented or modified late in the system development lifecycle that had not been accounted for earlier in the program. These sorts of considerations, while typically planned for during the earlier stages of the project, are becoming increasingly difficult to constrain during concurrent engineering activities and a rapidly changing technological and economic environment.

The concept exploration and advanced development phases are associated with the greatest reduction in risk for a system under development. These phases correspond to activities such as system architecture, feasibility studies, and experimentation and prototyping of immature components. The goal for risk reduction in the early stages of the system development life cycle is to limit the risk and uncertainty as much as possible, prior to production, to maximize the likelihood of delivering a successful system. Late-stage issues, such as in-service failures, customer unit returns, and warranty claims, are typically dealt with on a responsive, ad hoc basis, where an issue occurs, a team is assembled to investigate the matter, and a responsive correction is issued to eliminate the production problem and satisfy the customer.

However, as late-stage issues in material systems become more complex and require substantial materials characterization efforts in coordination with quality engineering, manufacturing, and development personnel, a more proactive and organized response is required.

Risk management can be broken down into two components: risk assessment and risk mitigation (or remediation). Risk assessment includes risk identification, planning, and organization, while risk mitigation includes the design of preventative measures, responses, and monitoring (Kossiakoff et al., 2020). The goal of these activities is to minimize or eliminate uncertainty, and, in cases where uncertainty remains, to understand the likelihood and criticality of the risk to the most complete degree possible given the context. A failure to understand or evaluate risk proactively threatens to damage, or otherwise render inoperable, the system being designed, developed, and deployed. In a similar manner, risk can also be treated as a system attribute, where more risk-prone solutions may be selected to accomplish certain project deliverables, as long as sufficient mitigation efforts are used. Accepting an excessive amount of risk can usually be translated into a high cost associated with this uncertainty given the probabilities of the risk event occurring.

By managing the likelihood and criticality of system failures, risk can be more adequately measured, interpreted, and accounted for. In this manner, the risk probability can be evaluated alongside the cost of the system failure to determine the stakeholders’ exposure to the risk event. In a material system, for example, a dimensional production defect at the interface joining several components may prevent those components from integrating properly in the manufacturing facility or could cause them to fail during use. Without accounting for these scenarios, both in terms of likelihood and criticality, an appropriate cost of this risk factor cannot be quantified. While novelty, innovation, and iterative design changes are inherent to systems engineering as a discipline, it is important to evaluate risk factors iteratively as the system is being developed and deployed.

While conventional risk management tools, such as failure mode and effects analysis (FMEA) or failure mode, effects, and criticality analysis (FMECA), provide value to product development teams seeking to understand and account for the risk condition of their system, a more tailored approach to materials-intensive systems is required that more appropriately considers materials research efforts, characterization analysis, and production upsets during the manufacturing ramping processes. As these sorts of process elements typically result in uncertainty with respect to budgets, schedules, and technological capabilities, a certain amount of risk is assumed by the project engineers prior to the project even beginning. Furthermore, as complex systems fail in-service, stakeholders will have the expectation that the project development team will address the failure and drive a root cause analysis. Preparing a response plan proactively can produce a more efficient workflow for this response, inform product recalls and corrective actions, and eliminate the cause of the problem in the fastest manner possible.

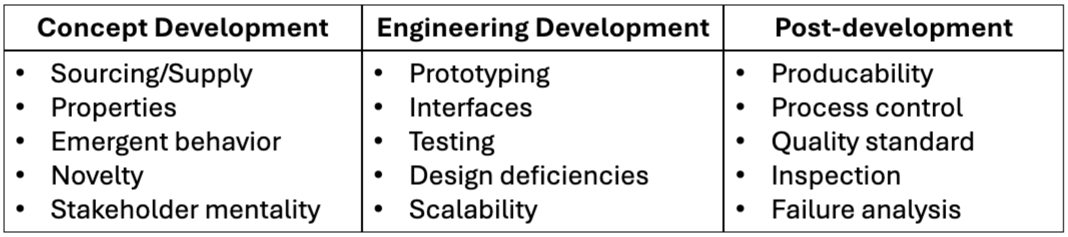
4.1.2. Quality

Quality engineering consists of the activities performed to ensure that the product, as manufactured, adheres to the customer's requirements and established methodologies (Walden et al, 2015). It is concerned not only with the accurate production of the system, but also the consistency of the production, assembly, and operation. The broader objective of quality engineering is to control variation in the product by controlling the process. This is achieved by measurement and inspection protocols, direct sampling and analysis, statistical control, and strict documentation procedures. These activities ensure that the product has been produced as requested and meets the agreed upon specifications. They also provide traceability of products and understanding of process changes and improvements. By monitoring the quality of the product being shipped to the customer, a great deal of data can be gathered to ensure product operability, manage manufacturing consistency, and provide potential avenues for process refinement and system redesign.

It is common to tune quality engineering activities to the system application, stakeholder preferences, and technological criticalities of the product. For example, if a failed product results in nothing more than a warranty claim and replacement unit at a rate that the stakeholders find acceptable (e.g. mobile phones), a looser quality standard may be enforced than for a system, for example, whose failure results in loss of life, high-cost system damage, or substantial loss of technical data (e.g. space craft). The more complex the system, the more rigid the quality engineering activities tend to be in order to ensure the system’s successful production and operation. High criticality incidents are less tolerated, and the time and cost associated with comprehensive and proactive quality engineering efforts are encouraged. Scenarios where quality engineering is not emphasized in these complex systems can lead to disastrous outcomes; therefore, it is critical to implement quality engineering efforts iteratively based upon the risk incurred by the materials' research, development, integration, and implementation.

As material systems become more complex, a more complete evaluation of the risk associated with these materials and their interfaces is required. The risks associated with the materials used for a system development span the lifecycle from concept exploration and selection to system operation and disposal. These can include material properties, cost and sourcing, integration with other elements of the system, manufacturability, adverse in-service reactions, and disposal requirements. With every new material or new material application, real world deployment will find weaknesses and failure modes that were not apparent during testing. The reasonable expectation moving forward, from a risk perspective, is that products will fail in service and that the development team responsible for deploying the product will be asked to respond quickly and efficiently to eliminate the problem.

Figure 4.1 describes some of the risks areas associated with materials within systems. It is important to remember that, in many cases, complex systems require novel, or sufficiently complex, materials to meet the engineering requirements and customer needs. New manners of supplying, producing, and analyzing these components may be needed in each one of these risk categories, whereas other components may be more technologically understood and constrained. For example, the raw materials for a new synthesized material may require a completely new supply chain, vendors, quality inspection system, and logistical support network.



Concept Development	Engineering Development	Post-development
• Sourcing/Supply • Properties • Emergent behavior • Novelty • Stakeholder mentality	• Prototyping • Interfaces • Testing • Design deficiencies • Scalability	• Producability • Process control • Quality standard • Inspection • Failure analysis

Figure 4.1: Examples of risks associated with materials at each phase of systems engineering lifecycle.

4.1.3. Emergency preparedness

While many industries and fields of engineering participate routinely in emergency preparedness planning, drills, and reviews, the mobilization of resources for material systems, post-incident, are not prepared so proactively. Usually, a team of engineers is informed that a failure has occurred in the field and the task of determining root cause and eliminating the problem is added to these engineers' lists of priorities. In this circumstance, it is possible for the initial development team for the product not to be notified. Instead, commonly, a team is assembled of the manufacturing and quality engineers that currently produce the product. While in-depth knowledge of the product, as-manufactured, is absolutely valuable, a complete understanding of the development process of the material-in-question and the problems encountered during that process also holds merit. It is additionally valuable for these original development engineers to observe in-field failures to understand future design modifications, next-generation products, and possible augmentations to the risk analysis previously conducted given the expanded, real-world testing data provided by in-service issues.

The Department of Energy (DOE) and the National Nuclear Security Administration (NNSA) have site-specific emergency response plans for biocontainment facilities (Roberto et al., 2011). These response plans must comply with the codes and standards of several regulatory agencies, require the establishment of an internal safety committee, and include preparations for site-specific and situation-specific contingencies. These measures are taken to properly mitigate the safety risk to the site employees, the public, and the environment. Their readiness assurance programs include emergency planning, protective action (PA) implementation, and training exercises. Evaluation of these exercises provides direct feedback for improvement of the process and improves the site readiness level. While not all of these sites rely upon novel materials and complex materials systems, it is certainly conceivable that in a rapidly evolving technological landscape, complex materials will be more intensively integrated into broader systems and relied upon for increasingly critical functions. Applying emergency preparedness measures as have been institutionalized by many government agencies can provide a more adequate level for risk understanding and threat preparedness for safety assurance.

Within the methodology of emergency management, several overarching risk categories tend to provide a useful backbone for conceptualizing threats to the system under development. These categories include (Blanchard and Fabrycky, 2011):

- Technical risk – The possibility of the project failing to meet performance requirements or technical objectives, including a failure to consider critical technological linkages.
- Cost risk – The possibility of the project exceeding its allotted budget, risk costs, and operational financing over the course of the full system lifecycle.

- Schedule risk – The possibility of the project failing to adhere to its schedule, reach technical and operational milestones on-time, or maintain its critical path scheduling.
- Programmatic risk – The possibility of the project being impacted, as a whole, by external factors outside of the control of the program engineering team.

These risk categories are interconnected and related via schedules, funds, and technical demands. With increasingly complex program suppliers and program deliverables, a greater and more multi-faceted level of risk is associated with the project. As the systems engineers prepare the systems engineering management plan (SEMP), a significant emphasis should be placed on risk planning, identification, assessment, analysis, and mitigation (Blanchard and Fabrycky, 2011).

Within the field of cyber security, risk management and emergency planning are quite common and a critical component of project development and operational continuity. Active projects typically have a recovery strategy in place prior to an emergency, where, in the event of a product disruption, a fast, efficient, and effective plan for restoring the service is devised, documented, and rehearsed (Cyber book REF). Methods for ensuring adequate system recovery include backups and alternatives/replacements for the current system. Throughout the testing cycle, personnel are trained for the emergency event and exercises are conducted to evaluate the recovery strategy as-a-whole. While the technical objectives for information technology systems are not entirely transferable to materials engineering systems, there is a certain amount of inspiration that can be drawn from the dedication, discipline, and proactive nature of cybersecurity planning when it comes to tailoring risk and emergency management to materials characterization efforts.

Aygun et al., 2022, examined cascading failures and risk associated with complex systems being affected by component malfunction and operational anomalies. They pointed out that natural events, malicious attacks, and component failures can cause a system-wide failure requiring significant time, capital, and technical resources to bring the system back to an operational state. It is critical, therefore, to consider not only the risk factors affecting each component but the potential for cascading failures affecting larger sections of the system or system-of-systems. By assessing these chain-reaction prone assemblies, a more realistic risk assessment can be prepared, and a more complete mitigation and recovery plan can be engineered. The researchers proposed a mitigation strategy that reduces the system risk by increasing edge capacity and integrating enough reserve resources into the system to avoid systemic failure propagation and system-wide collapse.

Rodriguez et al., 2017, devised a specialized selection process for risk assessment for the information technology sector. They acknowledged that while a number of risk assessment and analysis tools have been designed, a need existed to develop a specialized risk analysis selection tool for the challenges encountered within the information technology sector including risk areas such as hardware, software, human error, and cybersecurity. The myriad of component types leads to complex systems and, likewise, complex risk assessments. The authors propose a multi-criteria decision model, using fuzzy logic, to address the risk complexity, which more adequately addressed the uncertainty and multidimensionality of risk associated with the information technology sector.

Sun and Dave, 2022, commented on the intersection of materials science and pharmaceuticals. The complexity entailed with the chemical synthesis, product manufacturing, and regulatory environment, produces significant challenges. Pharmaceutical companies are beginning to invest more heavily in materials engineering processes to ensure product quality while manufacturing at scale with high yields. More than ever, pharmaceutical engineers are focusing on raw material properties, proactive inspections, and materials characterization analysis to ensure active pharmaceutical ingredients exhibit the appropriate performance metrics and are processed in the most efficient manner possible. Structure-property-performance understanding of pharmaceutical raw materials is a multi-disciplinary effort with a complex risk network. By investing in comprehensive materials characterization, a solid scientific foundation can be established to eliminate uncertainty, manage risk, and improve ongoing processes. Furthermore, quality standards and regulations in the medical field are extremely rigorous. By devoting resources to understand the processing of the material itself, quality discrepancies downstream can be reduced or eliminated. This highlights the potential value for a materials characterization-based risk management and emergency preparedness approach.

Filz et al., 2021, used a data-driven failure mode and effects analysis for maintenance planning in manufacturing. The goal with this approach is to make the assessment quantitative and predictive. By leveraging the amount and quality of manufacturing data available, engineers can more adequately, and proactively, improve production processes, perform maintenance activities, and predict failure behavior.   in certain cases, this could even be tracked back directly to a specific component or process step thereby significantly increasing the efficiency of root cause analysis. Decision support through manufacturing data analytics can better control process variability, reduce the amount of engineering rework, and limit the number of incidents requiring an emergency response. Using manufacturing and product data to determine risk factors can drive the risk management process in a more qualitative direction and can limit the amount of subjective risk assessment based upon engineering experience and institutional knowledge.

Figure 4.2, below, depicts a critical function analysis of the materials characterization efforts associated with a system development. The diagram notes several of the key components for each critical function that spans the full lifecycle of the system. While this is not a comprehensive listing, it does illustrate the efficacy of applying risk management procedures to materials characterization. Maintaining reserve resources, redundant capabilities, and safety systems provide a manner in which to respond to a collapse within the system and a fast and efficient manner in which to address post-development emergencies. While systems engineering provides substantial guidance for managing risk, analyzing decisions and tradeoffs, and responding to emergencies, it is not tailored specifically for the complexity associated with materials characterization without further adaptation and augmentation. By treating in-service system failures as an emergency, engineers can respond more adequately to the crisis, conduct failure analyses and drive root cause investigation.

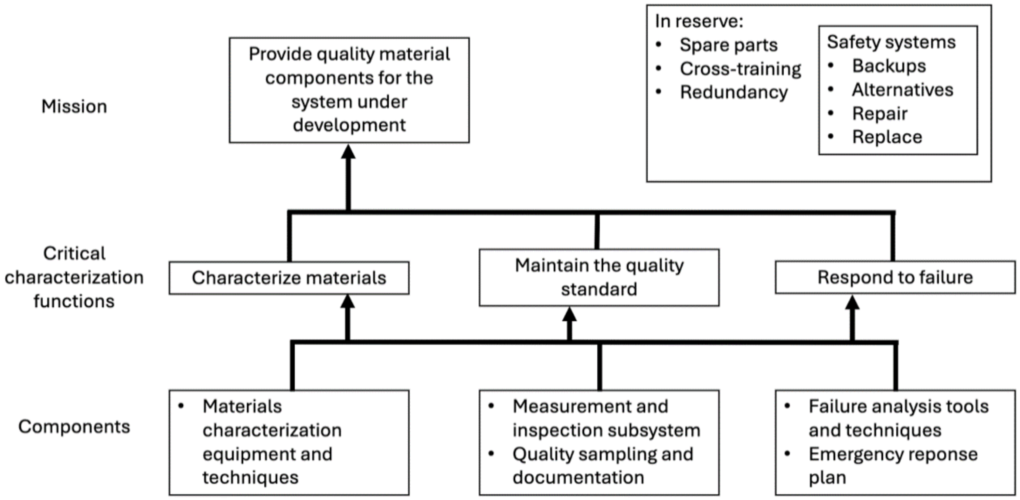


Figure 4.2: Critical function analysis of materials characterization

Root cause analysis is defined as a method of problem solving designed to address the underlying causes of defects and anomalies (Walden et al, 2015). Several commonly used techniques include Ishikawa diagrams, the five why's method, fault tree analysis, and the eight disciplines (8D) quality approach. While these approaches are broadly applicable to a wide variety of issues, they fail to adequately account for and capture the complexity related specifically to materials characterization. These complicating factors include specialized equipment and techniques, equipment lead-times and backlogs, and communication of complex scientific concepts throughout the product development lifecycle. By creating a method of root cause analysis that more closely conforms to the challenges specific to materials characterization and complex material systems, project engineers can more capably calculate risk, respond to emergencies, and conduct root cause analysis.

4.2. Materials and Methods:

To properly address the criticality of in-service failures of material systems, a workflow must be developed that addresses the need for stringent quality control, efficient and well-informed failure analysis, and emergency planning and response. By focusing on the impact of materials characterization on the post-development phase of the system development, the data provided by upstream characterization efforts can be leveraged to eliminate waste and rework. The process will need to include the following:

- Control the process inputs
- Monitor the process
- Plan, train, and respond to incidents

By training engineers to collect data and devise data-driven solutions, they can make decisions more quickly and design solutions more proactively. This reduces the need for subjective experience-driven risk and emergency management, while not eliminating its value, and allows the emergency response system and training to carry the burden of the load during the inciting incident.

4.2.1. Control the process inputs

By minimizing the variability of inputs to a process, the system variability, overall, becomes limited. The engineers are more able to understand the steady state and special cause variation within their system and control production consistency to a stronger degree. Materials characterization can be especially valuable to process input control as a method of verifying raw material properties (e.g. density, grain size, crystallography, etc.), conducting incoming quality inspections, and ensuring that internally derived process inputs are developed appropriately for the intended manufacturing setting and application. Collaborating with suppliers directly to enforce smooth transitions of materials from one manufacturing cycle to another can eliminate production issues and foster a beneficial business relationship for both parties.

There is a specific challenge related to translation of research and development concepts to downstream production settings. Quite frequently, transferring novel materials to manufacturing settings results in redesign of components and modification of existing systems due to the change in scale, production equipment, and characterization equipment. In addition, the regulatory environment is more codified and stringent compared to small-scale experimentations setups. For the “lab-to-fab" translation, in the case of microelectronics, the objectives of the research teams and the manufacturing engineering teams are distinctly different (Luo et al., 2020). Small scale laboratory research is mostly dedicated to technical achievement and small-scale sample production with marginal interest in scalability and per-unit-cost, while mass production is specifically concerned with meeting the technical requirements for as low a cost as possible on a mass market scale. The interest in experimentation and small batch, bench-top sample production is not necessarily of interest to a manufacturing team.

The solution to address this conflict is to consider manufacturability throughout the full product life cycle, such that solid technological materials researched and developed upstream can be quickly, easily, and efficiently adapted for downstream manufacturing. The four stages most typical to product manufacturing are (1.) design, (2.) material supply, (3.) processing, and (4.) integration (Luo et al., 2020). These are considered concurrently with product and process standards, policy, regulation, and governance. By considering these four steps from the beginning of the product development, more products can continue to progress through their development cycles to see the consumer market instead of stalling out due to lack of manufacturability. Product design and materials supply considerations include performance goals, producibility at scale, and synthesis methodology, while processing and integration considerations include cost effectiveness, uniformity, and interface interconnection. By tailoring a systems approach to materials development, valuable technologies can be brought to market, and by gathering good quality characterization data throughout the process, well informed decisions can be made to enhance and deliver the project.

It is also important to note, as generation and translation of inputs from upstream investigation to downstream production becomes more efficient and well documented, the data collected can serve to inform product and process improvements, next-generation products, and digital twins. This serves to enhance the efficiency of innovation and accelerate the product conception-to-delivery timeframe. As the industrial, institutional, and technological databases become more diverse and more mature, models and simulations can further advance and enrich the innovation atmosphere.

4.2.2. Monitor the process

With any manufacturing process, the push to ramp production from pilot studies, to low-rate initial production, and eventually to mass production relies upon the monitoring of the manufacturing process. This can be done via measurement and inspection equipment installed on the manufacturing line, quality control sampling and testing, and, eventually, through process control. By monitoring manufacturing, engineers can better prescribe corrective actions for defective components and ensure that all batches of product meet the quality standard, such that the engineering requirements are met, and the customer needs are satisfied.

Quality Management Systems (QMSs) are used to control process variation, increase consistency, and limit process deviations. While there are many different kinds of QMSs most of their core tenants are interconnected. These tenants consist of standardization, reducing variation, and eliminating waste (Hellman and Liu, 2013). The quality management systems are further specified by industry best practices, the consumer market, and the stakeholders for the product itself. For example, the biomedical industry is highly regulated with governmental, health, and safety regulatory audits while the regulation associated with the consumer goods industry (e.g. ballpoint pens) is fairly lax comparatively. The quality standard for any product is determined by the product specifications, stakeholder needs, and, ultimately, by what the consumer is willing to purchase.

Quality management and monitoring is especially applicable to the processing and manufacturing of material components. Online quality monitoring equipment has been used for traditional materials manufacturing since the advent of the technology and is increasingly being used for novel production methods such as additive manufacturing. These systems are not only being used to detect defects in manufactured parts but also to inform and adjust upstream processes on the line to eliminate the problem causing the defect (Lin et al., 2021). This approach functions by comparing a laser scanned surface of the product with an ideally drafted surface that has been generated virtually. As manufacturing techniques evolve it is crucial to adapt to new measurement and inspection processes and implement new technologies for enhanced production efficiency.

Accurate monitoring technologies also provide the opportunity to gather manufacturing data, train models and simulations, and predict when and how defects can be generated. Bartlett et al., 2020 researched the predictive potential of inspection for micro-structural defects and residual stresses in additive manufacturing systems for metal components. They used three-dimensional digital image correlation to identify and quantify the powder bed irregularities during the manufacturing process and intend to use this process as a preventative measure, in conjunction with more conventional quality screening approaches, to eliminate the production of defects prior to the production of an entire non-conforming batch.

4.2.3. Plan, train, and respond to incidents

Roberto et al., 2011, investigated incident response planning for the Idaho National Laboratory facility to evaluate biosafety and security protocols. The three core tenets of the response methodology included:

- An effective response is the last line of defense for hazards.
- The state of preparedness needs to be specific to and commensurate with the hazards.
- Early recognition is critical to an effective response.

The emergency management plan for the associated hazardous materials program included planning, preparedness, readiness assurance, and response, the specificity and severity of which were directly related to the hazard condition under evaluation. The study further breaks down roles and responsibilities for participants of the training exercises including players, controllers, evaluators, actors, and observers. Exercises were designed to provide a challenging and meaningful training scenario, after which the exercise was evaluated by (1.) controllers assessing players and (2.) controllers and evaluators conducting an assessment of the exercise, in which evaluators report positive and negative areas with respect to the exercise objectives and controllers provide situational context on the actions taken during the event (Roberto et al., 2011). The approach highlights the potential for discipline and rigor to be instilled within crisis response efforts across a wide variety of industries.

Hajibabai and Saha, 2019, investigated patrol route planning for incident response vehicles. Dispatching station locations and patrol route planning directly impact the speed and efficiency of the response to an incident. By more quickly responding to incidents, first responders can reduce the number of secondary incidents, improve the public safety of the region, and reduce the traffic congestion in the area. Advanced planning for incident response involves strategic decisions regarding resource planning, readiness level, and designing for reliability. These preparations allow for a resilient and effective system response while balancing priorities related to personnel management, incident severity, and resource scheduling. The researchers also comment on the importance of infrastructure design as it relates to the response times for incidents given the potential for the route planning strategy to be applied to a variety of cities, towns, and communities.

Rogage, 2018, researched virtual training environments for major incident response planning within the United Kingdom gas infrastructure. The criticality associated with gas incidents is high and can significantly impact individuals, communities, the environment, and the gas distribution network itself. While paper-based incident training provides benefits and allows companies the opportunity to instruct personnel on response, evaluate the current state of readiness, and mitigate the potential for an undertrained emergency response, virtual training was found to better educate regarding the decision-making process. This was especially true regarding auditory and visual cues, which contributed to the realism of the exercise. The author found that the virtual training environment resulted in improved training performance, remote participation, and decision testing.

It is important to note that while eliminating or significantly reducing the potential for incidents by leaving the production system unchanged once established may seem worthwhile from strictly an incident prevention point-of-view, process improvements and value engineering efforts serve as their own imperative when developing and deploying systems within a competitive market. Value engineering seeks to achieve the essential functions and requirements of the system while lowering the total lifecycle cost (Walden et al., 2014). When augmenting, streamlining, or modifying a system, there is always a potential for new risk, and additional iterations of risk assessments must be completed to analyze and mitigate the changing risk environment. Therefore, it is important to understand the risk factors associated with the system under development and plan proactively for emergency response.

Figure 4.3, below, describes the workflow for risk management, stewardship of the quality standard, and emergency response. As material systems become more complex, the likelihood and criticality of their associated risk factors increase. A more stringent, organized, and proactive response is required to design, integrate, and deliver successful material systems.

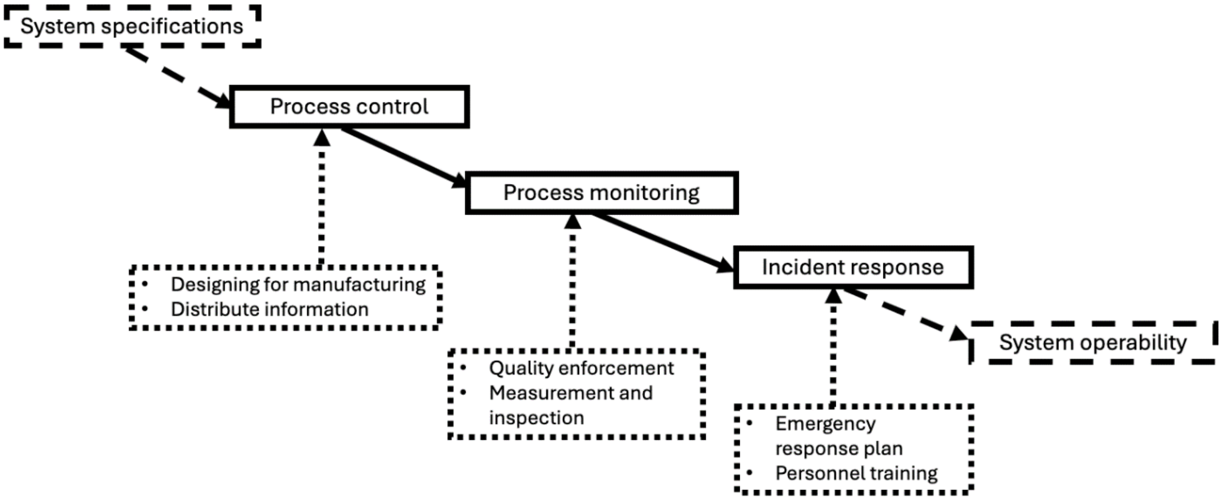


Figure 4.3: Diagram describing the process of risk mitigation for material-intensive systems.

4.2.4. Probability and risk factors

As project engineers begin to assess for risk within their system developments, the risk potential associated with materials characterization and quality assets must be accounted for and quantified to appropriately plan for the project cost, schedule, and technical achievability. Estimating risk by means or probability calculation is a common procedure within systems engineering practice; however, a risk assessment evaluating materials characterization equipment is typically not conducted. This exposes the project to risk based upon materials characterization equipment availability, personnel, technique knowledge, and competing company priorities.

Bayes' theorem calculates the probability of an event based upon prior knowledge of the conditions surrounding that event (Ostrom and Wilhelmsen, 2019). Equation 4.1 details this relationship, where A and B are events, P(A) is the probability of event A occurring, P(B) is the probability of event B occurring, P(A|B) is the probability of event A occurring given event B occurring, and P(B|A) is the probability of event B occurring given event A occurring.

$$P(A|B) = \frac{P(B|A)\,P(A)}{P(B)}$$

Equation 4.1: Bayes' theorem

Bayes' theorem can be used to evaluate the risk associated with characterization equipment in a developing project. By understanding and quantifying this risk factor, project engineers can more appropriately manage the project risk and account for the risk cost associated with characterization variables. This concept will be evaluated using two scenarios that can illustrate the calculation and demonstrate the shifting risk potential within the project.

In Scenario #1, a systems engineer is evaluating a series of scanning electron microscopes that are required to analyze the samples associated with the project. Scope A is assigned to the project for 35% of the workload, Scope B is assigned for 50% of the workload, and Scope C is assigned for 15% of the workload. Scope A typically has 15% downtime for technical issues and maintenance, while Scope B has 5% downtime, and Scope C has 40% downtime. In Scenario #2, the systems engineer reevaluates the risk associated with this group of scanning electron microscopes by considering if they were to allow Scope B to be assigned to another project entirely.

4.3. Results:

The logic tree associated with Scenario #1 is detailed, below, in Figure 4.4. The probabilities for the different events are listed accounting for uptime and downtime for each scope. Scope B has the most time assigned to this project at 50% and has the least downtime at 5%, while Scope C appears to be down quite frequently at 40% downtime but is only assigned to the project at 15%. Scope B is intermediate between the two. The cumulative risk of all scopes being down at the same time would be essentially 0% (precisely 0.007875%), however the risk of any scope going down and delaying the project would be 13.75%.

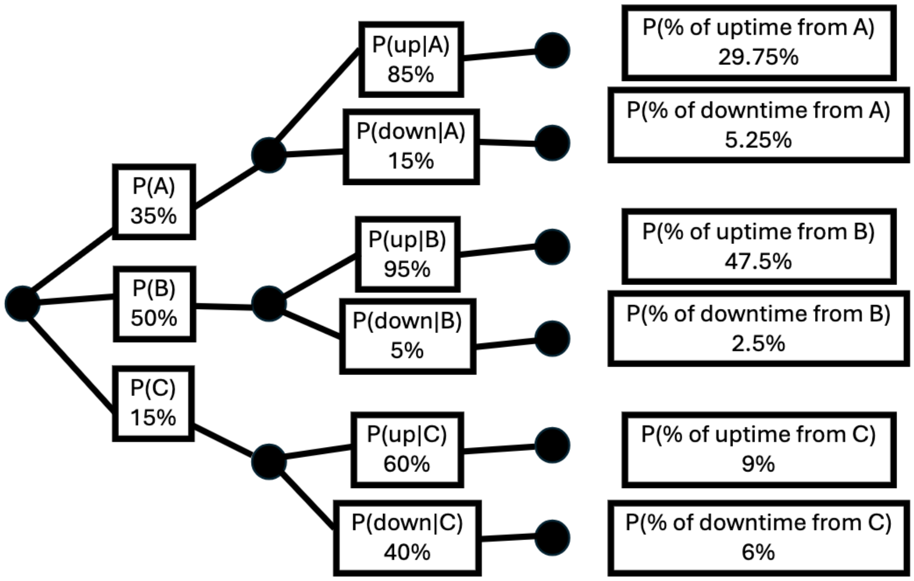


Figure 4.4: Risk assessment of downtime for Scenario #1

The logic tree associated with Scenario #2 is detailed, below, in Figure 4.5. The probabilities for the different events are listed accounting for uptime and downtime for each scope. The scope assigned for the largest percentage of time and the least amount of downtime was tasked to a different project. With the remaining scopes, Scope A must assume 70% of the analysis responsibility leaving Scope C with 30%, assuming the same distribution as was the case in Scenario #1. Given the new analysis paradigm, the cumulative risk of both scopes being down at the same time would be 1.26%, however the risk of any scope going down and delaying the project would be 22.5%. Note that this model can be further specificized and expanded upon to include likelihood and criticality of failure impact, such as the capability of manufacturing, insurance rates, and regulatory compliance and safety costs given a specific equipment failure. The provided model simply illustrates a starting point for this type of evaluation.

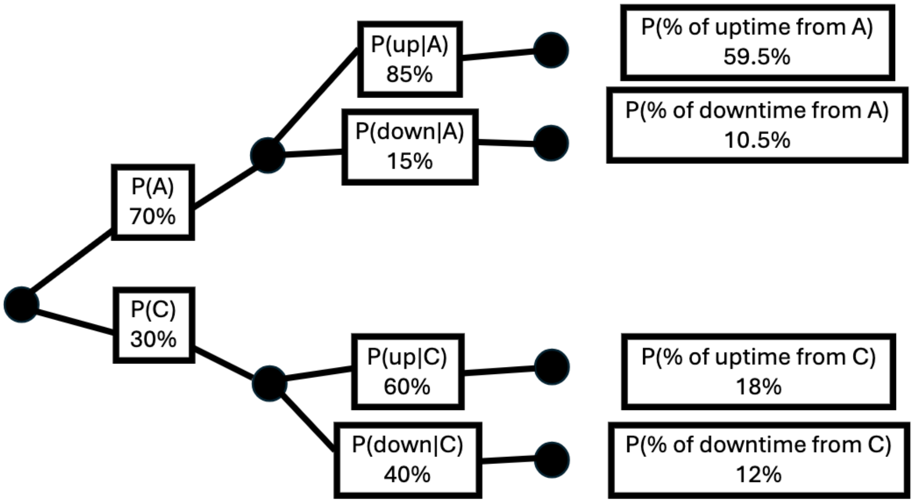


Figure 4.5: Risk assessment of downtime for Scenario #2

4.4. Discussion:

The scenarios used in this investigation are illustrative of the value brought to a project by applying systems engineering principles and tools to materials characterization activities. This approach serves to more adequately evaluate risk, plan for development activities, and calculate risk cost such that systems engineers can more capably address the needs of their system. While applying risk analysis to materials characterization, equipment such as the scanning electron microscopes in the example scenarios is not the only element that can be improved upon or should be considered for complex material system development. However, these scenarios do serve to illustrate a new risk awareness paradigm associated with the materials characterization processes within system development.

Risk assessment and mitigation as applied more diligently to material systems, as described in the aforementioned example, can more appropriately estimate cost when calculating system budgets and can more aptly assist in resource management. In the example, Scope B could be shifted to another project entirely if the systems engineers for the project are comfortable with accepting the 8.75% uptick in risk due to that reassignment. In the event that the presiding company requires the reassignment, the systems engineers can use this evaluation to estimate cost incurred by the decision and argue a legitimate case for additional funding based upon the increased risk.

It is important to note that materials characterization carries a certain amount of incalculable risk, as many complex processes do. Personnel required for specific analysis procedures and by extension project completion may be moved to other projects or may leave the organization for other opportunities. Equipment may fail and require repair by service engineers or replacement with comparable technology. It is important in these cases to remain flexible and develop contingencies and redundancies. Other equipment within the organization should be evaluated to pick up the slack for equipment failure, cross-training should be used to maintain a strong technical base of knowledge within an organization, and external resources should be proactively considered such that sample analysis can continue if the internal methods of characterization prove unusable.

In a broader sense, quality engineering should be considered as a full life cycle process, with respect to the materials characterization efforts being conducted throughout the project. While quality management and engineering practices are mostly associated with downstream activities (e.g. manufacturing, product validation, failure analysis, etc.), the intensive use of materials characterization processes in research, development, and technology transfer should be leveraged to inform quality engineering and preemptively discover and mitigate impending quality issues. By communicating materials characterization science to quality and manufacturing engineers, the downstream technical activities can build a more complete understanding of the materials-in-use allowing for more informed approaches to process control, and thereby quality control. This is especially important during concurrent manufacturing activities and shortened scheduling timeframes.

Emergency preparedness and response should be planned for among the earliest stages of the project. Emergency management plans can be drafted and coupled with live training exercises involving the responding personnel. Improvements can be made iteratively based upon exercise observations to more adequately prepare for an emergency event and mitigate the risk associated with high criticality scenarios. It is valuable to make these training exercises as realistic as possible, incorporating enhanced training techniques (live demonstrations, virtual training, etc.) to illicit a realistic response and understand the weaker points of the emergency plan overall. This is a common strategy in military, biomedical, and hazardous materials industries; however, it is uncommon to apply a response plan of a similar rigor to materials systems or system incorporating significantly novel material components. As materials become more complex and integrated in increasingly system-critical ways, the criticality of material failures should be evaluated realistically given their risk factor to the system and incorporated into the emergency response in high criticality situations using the appropriate planning tools.

Safety systems should be used to reduce the risk level associated with materials characterization. Backup systems can be developed, internal to an organization. For example, using our illustrative example, if a “Scope D” existed within the organization to serve as a backup for any scope of the suite that was not able to perform its analysis, the risk associated with the analysis downtime could be significantly reduced. Furthermore, externally sourced backups could be briefed on the project such that a transition to external analysis, in the event of an internal equipment failure, would be seamless and all scheduled project progress could be maintained.

Alternatives to analysis methods should be devised at the onset of the project. There is a cost associated with redundancy of materials characterization approaches given the expensive nature of the tools, techniques, and personnel. There is, furthermore, a difficulty in replicating or recreating analytical techniques using different sources. For example, a set of analyses could be scheduled to be performed by a certain specialist on a specific piece of equipment that is unique to the industry. Working with that specialist to ensure an alternative procedure provides flexibility in the process, if for whatever reason the primary approach is no longer available. Repair and placement of equipment and personnel should also be considered including time, expense, and potential technological repercussions. This could include standardized testing where a specific piece of equipment had been qualified and calibrated for that particular method against external sources, such as corporate engineering procedures, state mandated regulations, or federally defined sources (e.g. the National Institute of Standards and Technology).

4.5. Conclusion:

Through the course of the investigation a risk assessment approached was devised to assess and mitigate risk factors associated with materials characterization processes within systems containing complex material components. This approach was coupled with a procedural workflow to more proactively address risk, manage quality, and prepare for emergency response within the development of material systems. By treating materials as a high criticality component, in the event of failure, systems engineers can more adequately calculate for and respond to risk events.

Materials characterization is, inherently, a risk prone area of project development with a multifaceted resolution and scope. Materials under research and development require complex analysis procedures, specific investigative processes, and intensive study by highly trained and specialized individuals. As material components evolve through the system lifecycle, engineers should become trained in the initial development efforts to more adequately address manufacturing, quality, and failure analysis concerns. The models, in turn, can be updated and adapted to real-time feedback to events on the ground to enhance their utility. The risk associated with materials characterization can arise from the equipment, techniques, or personnel associated with the analysis but can be mitigated by implementing safety systems and redundancy.

Future work made include more elaborate mathematical tools to assist engineers in calculating risk within materials systems. Risk analysis as a systems engineering procedure is hardly new and has been applied to a wide variety of project activities. Its value as applied to materials characterization activities is only beginning as the risks associated with materials innovation, and the techniques themselves, become more complex. Further testing of the designed procedures from this document in a real-world situation would be invaluable. While the aforementioned approach demonstrates value, a full-scale test regime involving an active and ongoing project would allow for the evaluation of the coverage and efficacy of the approach and provide opportunities for process improvement as well as a quantification of the efficacy of the workflow and associated tools.

Chapter 5: Implementation guide

In an effort to make this document as actionable and applicable as possible, the remaining section of the document will serve as an implementation guide. The implementation guide will serve to tailor this approach more specifically to different material systems, company sizes, and risk profiles. By providing guidance for implementation, working systems engineers can more capably mitigate characterization risk, leverage the value of characterization-generated data, and plan proactively for characterization efforts at the onset of the project while reevaluating risk and opportunity iteratively.

A specifically tailored approach can be generated for the major four material groups, with the understanding that more complex materials, as are being designed and developed to more intricate and advanced requirement levels, may require concurrent approaches depending upon their constituent components. Categorizing materials into major, and most common, groups can help visualize and clarify the application of characterization systems engineering. These groups include (1.) metals, (2.) polymers, (3.) ceramics/glasses, and (4.) composites.

By designing an implementation guide to address material categories, a targeted and highly applicable guide can be derived to assist systems engineers in the field. The CSE method can categorize the possible options associated with the common material families. For each element of the CSE method, questions can be asked to develop core knowledge about material options and characterization capabilities.

Questions for each element of the CSE methodology:

- Compositions:
    - What compositions are available for this application?
    - What is the cost associated with these materials?
    - What are the properties associated with these materials?
    - What are the fundamental scientific challenges associated with the material’s chemistry?
    - Is there a technical strategic benefit to understanding this composition better?
    - What resources would it take to characterize this composition?
- Interfaces
    - What interfaces exist within and without the materials in the system?
    - How well are these interfaces understood?
    - What interfaces will the material encounter during production and operation?
    - Are there known challenges associated with this material interface?
    - Is there a technical strategic benefit to understanding this interface better?
    - What resources would it take to characterize this interface?
- Processes
    - What processes are involved with developing this material?
    - What processes are involved with manufacturing this material?
    - At a fundamental level, what is the process doing to the material?
    - How can the effect of the process be monitored and manipulated for benefit?

    - Is there a technical strategic benefit to understanding this process better?
    - What resources would it take to characterize this process?
- Forethought
    - What characterization equipment is needed to analyze this material?
    - Are those characterization tools and techniques available (internally or externally)?
    - What are the lead-times associated with these characterization tools and techniques?
    - Will fundamental study of the technique have to be completed to develop a more repeatable and representative characterization protocol?
    - Is there a technical strategic benefit to understanding these characterization tools and techniques?
    - What resources would it take to develop and maintain this characterization resource?
- Limitation
    - How many samples can be analyzed in a given characterization instrument?
    - How many personnel can operate a given characterization instrument?
    - What delays are we willing to risk given the need for this characterization tool or technique?
    - If the characterization instrument breaks, are there readily available alternatives?
    - What data is of value?

    - What is the risk involved with using this characterization tool or technique?
- Elevation
    - What can the project gain from good characterization data?
    - What can the company gain from good characterization data?
    - How will materials development, overall, benefit from this characterization effort?
    - What data do we want to collect given the resources being spent?
    - How can we use this collected data to inform models, simulations, and decision making?
    - Would characterization of this material serve to generate material innovations for next-generation products?

It is important to relate CSE methodology elements to the materials that are available or attainable given the needs of the project. While the attributes of CSE seek to develop the systems engineer's understanding of the material itself, the integration and constraint-based elements deliver clarity on the characterization equipment, techniques, and personnel.

CSE evaluation as applied to common material groups:

- Metals:
    - Compositions:
        - Iron, Copper, Aluminum, Titanium, Magnesium, Nickel, Chromium, Molybdenum, associated alloys
    - Interfaces:

        - Crystal structure, phase microstructure, surface, passive layer, magnetism
    - Processes:
        - Hot working, cold working, heat treating, shaping, cutting, joining, etching, coating
    - Forethought:
        - Sub-sectioning, epoxy mounting, polishing, metallography, scanning electron microscopy, energy dispersive x-ray spectroscopy, hardness testing, associated mechanical testing
    - Limitation:
        - Time associated with polished cross-section preparation, time associated with mechanical testing prep (e.g. tensile strength testing)
    - Elevation:
        - Evaluating new alloys for unique properties and intellectual property exploration, dedicating resources to acquire in-situ and in-operando measurements
- Polymers:
    - Compositions:
        - Natural (cellulose, rubber, silk), Synthetic (PVC, EPDM, nylon), additives
    - Interfaces:
        - Monomers, copolymers, surface, coating, cross-linking, crystallinity

    - Processes:
        - Catalysis, mixing, forming, extrusion, molding, curing, machining
    - Forethought:
        - FTIR, TGA, DSC, SEM/EDS
    - Limitation:
        - Time to analyze, contamination/damage
    - Elevation:
        - Testing new polymers to create a body of knowledge surrounding the new technology, intellectual property exploration, in-depth degradation and compatibility analyses
- Ceramics/glasses:
    - Compositions:
        - Oxides, non-oxides, ceramic composites, additives
    - Interfaces:
        - Crystal structure, short range vs. long range order, surfaces, porosity, coatings, textures
    - Processes:
        - Mixing, extrusion, firing, floating, annealing, operational use
    - Forethought:
        - Microscopy, SEM/EDS, XRD, Raman, NMR, SIMS, mechanical testing
    - Limitation:
        - Preparation time, sample damage, sample chemical contamination

  - Elevation:
    - Testing novel ceramics and glasses, pursuing potential advantageous properties, pursuing lower cost facsimiles of other technologies
- Composites:
  - Compositions:
    - Metal matrix, ceramic matrix, polymer matrix, carbon matrix, hybrid, additives
  - Interfaces:
    - Matrix structure (crystal, linking), reinforcement structure, surface
  - Processes:
    - Automated fiber placement, spray-and-lay, winding, tailoring
  - Forethought:
    - Physical properties testing, thermal properties testing, FTIR, SEM/EDS
  - Limitation:
    - Sample preparation, constraints of sample preparation given multiple major material assemblages, potential variability of reinforcement structure
  - Elevation:
    - Potential for unique properties, evaluating new composites for intellectual property, dedicating resources to acquire correlated property measurements

Systems engineers developing complex material systems can also combine specified approaches to accommodate advanced composites and complex material assemblages. While beginning with major material constituents, the full system perspective requires the evaluation of all system elements. It is beneficial to apply the CSE method and the implementation guide not only to the system components, but also to the more complex, system-scale integrations in an iterative manner. The composite family CSE method application can be used as a template to evaluate complex materials.

Along with tailoring to major material groups, a tailoring effort for differing business sizes is also of value. Business size and internal vs. external resources dictate a substantial percentage of the risk and opportunity drivers for characterizability and comprehensiveness of datasets.

Kvitka and Kramarenko, 2018 investigate the effects of market saturation on the interactions among small, medium, and large businesses. They find that larger companies suffer from a lack of flexibility that provides a market opportunity for small and medium-sized enterprises to flourish. These smaller organizations adapt quickly to new concepts and can develop quickly in new directions given market needs. Large companies are able to maintain technological niches for long periods of time and are more able to prevent new companies from entering into legacy markets but have difficulty gaining a foothold in new business sectors if these sectors are not quickly identified and incorporated into the business structure of the enterprise. They even relate this dynamic to the “concept of technology” paradigm where naturally cyclic rates of success and failure follow large company developments. New technologies are discovered and developed by smaller companies, which become economically advantaged, until larger companies can adapt to the new technology. This implies that smaller organizations are a particularly fertile development ground for the implementation of CSE.

Businesses of varying sizes have been evaluated financially in a broad number of scenarios to determine capital allocation tendencies and impact factors (Zunckel and Nyide, 2019). Managerial goals, such as individual goals and preferences, combined with firm-level factors, including firm profitability and size, are typically jointly responsible for driving capital structure and asset allocation. If this concept is applied to systems engineering of complex materials, it can be understood that the size of the firm is a contributing factor to attitude regarding characterization, however, managerial perspectives can also contribute to success or failure. It is important for systems engineers to justify not only the technological potential of characterization work, but also the monetary value and projected fiscal upside.

Holmes and Kent, 1991 evaluated the financial structure of small and large manufacturing enterprises. They identified management funding preferences as a significant driving factor with respect to what projects are selected and supported and what strategies are adopted and enforced rather than relying solely on a finance gap as an explanation for different choices. Accounting for this with respect to characterization sciences can certainly provide guidance for systems engineers to dedicate resources to these efforts in the earliest stages of the project planning phase. By calculating for the appropriate allocation of resources, small or large companies alike can determine value added by this function, proactively, rather than assigning cost without benefit. This ideology also provides an opportunity for small businesses with more focused technological strategies to specialize, in terms of equipment and expertise, and elevate characterization functions as high-value assets.

A small business, within the materials development space, can be defined as one that owns fewer than ten pieces of characterization equipment and typically focuses on a particular material property or application focus. Figure 5.1 describes the relationship between a small business and the capability space. The capability space signifies the body of knowledge related to a material as well as the tools, techniques, and equipment needed to adequately innovate, engineer, characterize, and produce within that space. Small businesses tend to own some characterization equipment but need to work with an industry partner or third party laboratory to complete work either due to lack of equipment or lack of expertise. Small businesses can also leverage academic collaborations to raise their industry profile, develop novel materials, and publish studies in academic journals. The small size and simple fiscal overhead structure of small businesses allows them to be nimble and flexible to adapt to new technologies.

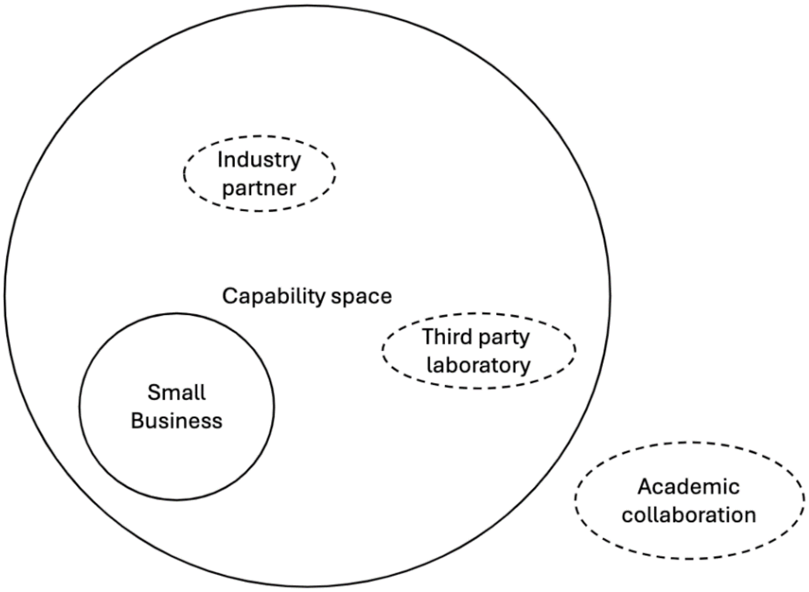


Figure 5.1: Depiction of the position of a small business within the material characterization capability space

A medium business, within the materials development space, can be defined as one that owns between ten and twenty pieces of characterization equipment and typically focuses on (1.) a particular material property with multiple applications or (2.) an application market need and several materials that serve that market sector. Medium businesses can have a sister facility to handle different types of materials development work or analyze sample backlogs. They can work with industry partners for mutual gain, third party laboratories for additional analysis needs, and can collaborate on new capabilities and opportunities alongside academic and interdisciplinary partners.

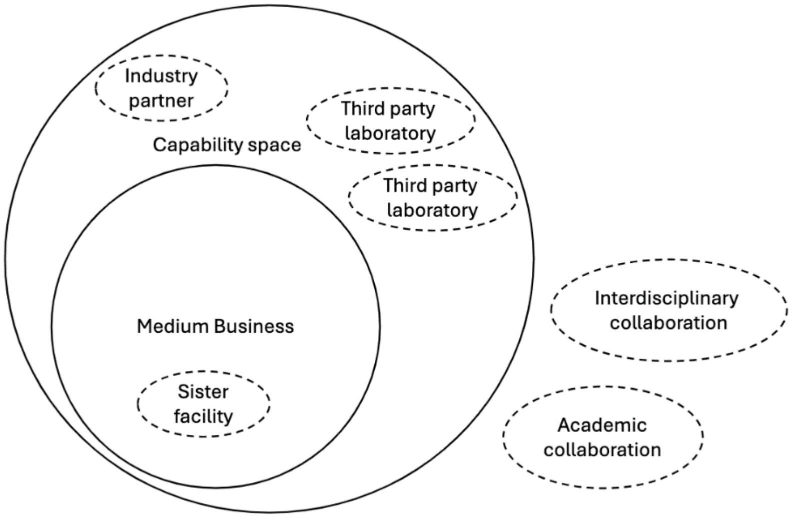


Figure 5.2: Depiction of the position of a medium business within the material characterization capability space

A large business, within the materials development space, can be defined as one that owns more than twenty pieces of characterization equipment and typically focuses on several main legacy material technologies, makes an attempt to develop their market share through multiple applications of these technologies, and invests slowly in materials outside of their main focus. Large businesses tend to have multiple facilities, giving them the ability to absorb workloads or auxiliary projects that smaller businesses cannot. They can also have industry partnerships, third party laboratory contracts, and multiple collaborators in adjacent capability spaces, whether that be in academia, partnering-companies in a joint venture, or complementary technology developers.

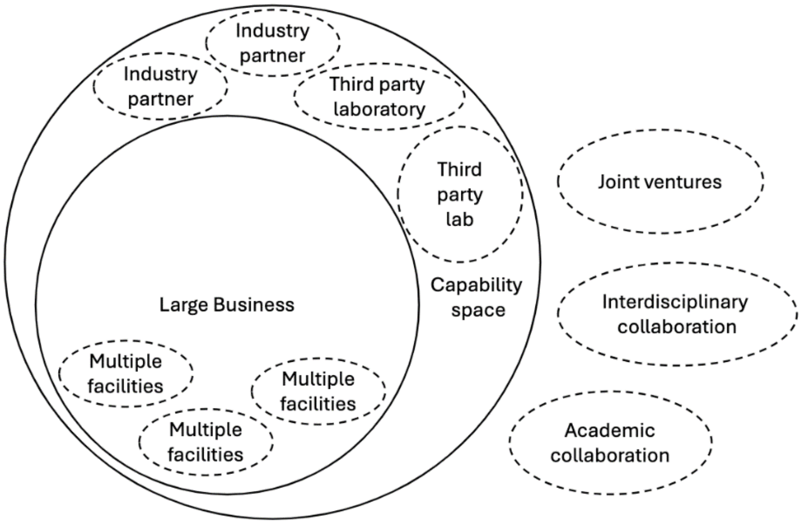


Figure 5.3: Depiction of the position of a large business within the material characterization capability space

As the systems engineer, it is important to understand the position of each organization within the capability space, use the resources available, and adapt to changing circumstances. Large companies tend to have a rigid and inflexible structure but have established processes and substantial resources. Smaller companies tend to be able to adapt more quickly to changing technological paradigms but are limited in experience with the new technology and do not necessarily have the resources to develop multiple products simultaneously.

Life cycle impact assessments have been used to develop impact categories for materials (Jang et al., 2022). While the referenced study is targeted toward environmental impact of construction materials, the concept can be further explored to manage not only risk of damage from various materials but also opportunity provided from the material given its level of novelty and potential positive technological impact. In either case, subdividing material groups into categories of similar properties can provide analytical clarity to systems engineers designing and developing material systems. Subcategories can also, typically, be more closely tied to a metric or some sort of quantitative proxy to allow for in-depth analysis among complex system interactions as well as among similar technology groups historically.

Jonsson and Mattsson, 2006 investigated material purchase planning as a function of resupply efficiency. They found that reviewing planning protocols iteratively serves to enhance the efficiency associated with supply chain functionality as well as material production. This is a useful parallel in that physical materials as well as the data associated with these materials are tracked and managed in a cohesive way. In characterization, the flow of samples, ware, and material systems entirely should be understood over the full lifecycle. Their data should be tracked from concept development to retirement and disposal. By tracking systems individually, systems engineers can develop quality traceability and discover trends in emergent materials behavior leading to more refined products and improved simulations of material behavior and failure modes.

Similar methodologies have been applied to material efficiency measures (MEMs), whereby raw material process inputs are compared to finished good material outputs (Fischer, 2013). In these calculations, the measurements are fairly straightforward and simple to compute. They also help systems engineers and project managers direct process improvement plans and reduce waste system-wide by reducing inputs to achieve the same output product. By subdividing the classifications of manufacturing systems, MEMs can more adequately target improvement initiatives. While the process of measuring material efficiency provides a useful example of process improvement within materials development and manufacturing, it fails to capture the complexity inherent to materials characterization efforts.

It is worth noting that data associated with testing of the CSE method and associated workflows is theoretically generated for the purpose of illustrative example. More complete datasets incorporating material maturity, technique, instrument operator, data gathered, and impact provided from the acquired data would be required to more thoroughly evaluate this technique comprehensively. From a technical standpoint, it is important to be able to track how the data was acquired and what value was provided by that data. This could be tested by monitoring ongoing instrumentation involved in product development to discern analysis time (a.k.a cost) vs. benefit. Benefits could include patents, trade secrets, direct financial gains, or the number of next-generation projects generated. It is quite difficult to quantify the value provided by data, and a good deal of that practical definition may be specific to a company, industry, or stakeholder.

From a project management standpoint, the simplest form of experiment would consist of comparing a control project, using legacy methods to manage materials characterization, against a similar project using the CSE approach and workflows. During this experiment, schedule, budget, and technical performance would be tracked alongside characterization time, personnel specialization, and technical achievements of the project, along with longer standing observations to determine the opportunity for innovation potential provided by CSE methodology.

With characterization tools and techniques rapidly advancing technologically, it is not difficult to image a data-rich environment in the near future with which additional verification, validation, and testing of the CSE concepts can be evaluated. Automated processes inherent to new classes of materials characterization instrumentation can track analysis conditions, data gained, value of the data, time spent on analysis, and resources consumed during experimentation and development. It is entirely possible that instrument manufacturers may be interested in incorporating CSE logic into automated instrumentation and analysis protocols. Furthermore, open-source programming using CSE methodologies could become available and modifiable for smaller organizations, allowing for increased innovation potential within the small business or independent operator space when compared to larger organizations. This would drive a cross-pollination of ideas and intellectual property amongst a variety of businesses that would otherwise not be able to compete with the large budgets and sustainable resource inventories of large entities.

It is important when applying the CSE methodology and workflows to respect the limitations of the technique. Characterization instrumentation inherently has limitations in sensitivity and resolution. Furthermore, equipment necessary for certain datasets may be inaccessible to the organization or prohibitively expensive. This affords systems engineers the opportunity to understand the potential options available, while simultaneously, and realistically, elucidating the pragmatic financial and technological parameters of the product development. Limitations with respect to human factors should also be considered. For extraordinarily specialized techniques, cross-training multiple personnel may be a resource limited proposition. Operators may be unavailable for an analysis physically or otherwise occupied with alternative projects. A good deal of this uncertainty can be calculated, to at least provide an approximation of risk cost, however more resource limited, or specialization dependent, endeavors may suffer from high criticality, low likelihood events.

It is worth mentioning that, as with any system development, the project manager and systems engineers responsible for the system cannot predict the future with absolute certainty. The CSE methodologies provide insight into the risks and opportunities associated with the characterization efforts required for materials development and production, however a completely flawless prediction model for complex system development is not possible. It is the systems engineer's responsibility to understand the uncertainties associated with material systems and proactively address foreseeable challenges while accepting a degree of unknowability. Stakeholders and management oversight can also interfere with CSE implementation. Resources may be limited or reassigned by executives, stakeholder preferences or politics may change, and technological strategies may evolve over time. It is the role of the systems engineer to coordinate resources throughout the system lifecycle and remain flexible under changing conditions.

By using the CSE approach, systems engineers can more capably manage risk and opportunity throughout the system lifecycle thereby enhancing value when compared to traditional materials characterization.

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