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A General Theory of Emergence in Engineered Systems

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ABSTRACT

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Engineered systems are designed to satisfy specific needs and produce explainable/predictable results. But despite this intent, engineered systems don't always do what they are designed to do once they are implemented. Some engineered systems produce properties and behaviors that are not clearly explainable or predictable by the properties of their components. This is a problem recognized in government and private sectors as having broad ranging financial and security consequences. It is also the essence of the emergence phenomena. A review of the literature reveals two significant gaps in the current body of knowledge on emergence as it pertains to engineered systems: 1) no conceptual model that reconciles conflicting aspects of emergence; and 2) no explanation of system factors and their relationships that affect the occurrence of emergence. The gaps are addressed in this dissertation through research using a methodology that incorporates rationalist inductive methods with modeling & simulation frameworks. Where other research and models of emergence focus on entity or agent behavior; the research in this dissertation takes place from a systems perspective. The focus is on system level behaviors and system factors as they pertain to the occurrence of emergent effects. Generally accepted thermodynamic principles and axioms for chemical reactions are used to develop scientific analogies for factors in engineered systems. A theory is derived consisting of six factors that are determinants in a mathematical model of a tipping point at which emergent effects will occur in engineered systems: 1) interoperability; 2) concentration of components; 3) component degrees of freedom; 4) variety of system regulators; 5) rate of information received vs transmitted by the system; and 6) relative amount of information received by the system vs a threshold for change in the system configuration. The theory and its implications are explored in simulation experiments. Other products and contributions of the research include: a) an ontology of emergence concepts; b) a unifying definition of emergence; and c) a system dynamics model of emergence in engineered systems.

This work is dedicated to Karen, John, and Kourtney. Your unselfish willingness to share our precious time and take this journey with me, is an act of love for which I am eternally grateful.

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NOMENCLATURE

iff   If and only if

R   Relationship

Δ   Change

→   If then

w/   With

≈   Approximately equal to

≠   Does not equal to

≥   Greater than or equal to

≤   Less than or equal to

>   Greater than

>>   Much greater than

<   Less than

<<   Much less than

f   Function

X   Trans

{}   Set of

| Such that

∈   Element of

^   Raised to

/   Or

¬   Not

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CHAPTER 1

INTRODUCTION

The term emergence often brings to mind a familiar paradox, "…the whole is greater than the sum of its parts." The actual statement, "…the whole is something beside the parts," is from Aristotle's discussion on the nature of material things and the substances of which they are composed (Aristotle, 350 B.C.). The implication is that material things have something that their parts don't have. But how can this be? After all, some might argue that parts are mere fractions of a whole; and a whole is completely composed of its parts. Systems engineers count on Aristotle's statement being true. Engineered systems (i.e., systems produced by humans) are ensembles that are designed to produce effects (behaviors, properties, qualities, etc.) that fulfill a purpose that cannot be satisfied by individual parts alone (Ackoff, 1971; Checkland, 1999; Blanchard & Fabrycky, 2006). Aristotle might say that engineered systems are wholes that are something beside their parts. The other basic aspect of the emergence concept is the apparent absence of traceability between the nature of parts in a system and the system effects (Lewes, 1875). This is the aspect of the emergence concept that presents a potential problem for engineers and stakeholders in engineered systems.

System effects that are not traceable (i.e., explainable in terms of or derivable from its parts), are not intentional consequences of design. "Classical" engineering design seeks to eliminate unexpected and unintended effects (Mina et al., 2006). While some unintended system effects may indeed be serendipitous, there is also a risk that unintended consequences will negatively impact the intended purpose of the system. The problem of unintentional system effects is recognized in government and private sectors as having broad ranging financial and security consequences:

- **Carnegie Mellon (Schroeder & Gibson, 2010).** A study of high-performance-computing systems at Los Alamos National Labs found that 20-30% of the root causes for failures was unknown and untraceable. Designing highly dependable systems requires a better understanding of system failures.
- **DoD Missile Defense System (Willman, 2014).** Ongoing flight test failures costing 100's of millions of dollars and creating doubts about the $40B system. "…scientists have been hard-pressed to pinpoint the causes of the failures".
- **National Science Foundation (Guckenheimer & Ottino, 2008).** Participants in a workshop on Foundations for Complex Systems Research concludes that there is a need to "…preclude undesirable emergent behavior and to generate or exploit desirable ones". A recommended strategy is to seek a means to anticipate "tipping points" in which abrupt changes in system performance will occur.
- **American Society of Mechanical Engineers (ASME, 2011).** An **i**nitiative to address Complex Systems Failure, points to a need to manage risk and design systems to reduce likelihood of cascading failures without excessively increasing system cost. High priority is placed developing risk analysis methodology, models, and tools.
- **National Institute of Standards and Technology (NIST, 2016)**. A conclusions from the Measurement Science for Complex Information Systems Project is "There is no science today that offers the fundamental knowledge necessary to design large

> complex networks [so] that their behaviors can be predicted prior to building them.“ This situation threatens national security and cost billions of dollars.

The current body of knowledge on emergence abounds with theories about its nature, yet there are persistent gaps that support the need for additional theories. Silberstein and McGeever (1999), Corning (2002), Campbell (2015) and Sartenaer (2016) are among those that discuss persistent gaps, supporting the need for a theory of emergence that: 1) provides a unifying and unambiguous definition of the concept; and 2) explains its causal factors. The need is especially true for engineered systems because they are expected to produce intentional consequences (behaviors, properties, qualities, etc.) of their design. Take a jet or a ship for instance. Despite potentially millions of very complicated and interwoven components, velocity and direction of the jet or the yaw and buoyance of a ship can be explained (i.e., described in detail) in terms of its components and interactions. Even when these systems fail to perform as intended, the failure effect is typically explainable in terms of its components and interactions. This is not the case for all properties and behaviors of all systems. Consider the lateral vibration phenomena in London’s Millennium Footbridge. Unexpected synchronization of pedestrian footsteps and bridge motion accumulated to a point that required the closing of the bridge due to excessive lateral vibration (Dallard et al., 2001). Somehow the interaction between the pedestrians and the bridge created an unexpected and unexplainable effect (lateral vibration). Lateral vibration due to foot traffic is a repeatable phenomenon that occurred on multiple occasions with other bridges for over 30 years. However, it was not explained until years after it was observed in the Millennium Footbridge case (Macdonald, 2008). After the phenomena was explained it was possible to predict it, and solutions to prevent or mitigate future occurrences were implemented.

The apparent unexplainable nature of the lateral vibration phenomena is an example of emergent effects in an engineered system.

These examples raise the questions that are the focus of the dissertation: what are the factors in engineered systems that affect the occurrence of emergents; and what are their causal relationships? The importance of the questions is emphasized in Checkland's (1999) plan for a systems movement:

> "*…to search for conditions governing emergent properties and a spelling out of the relations between such properties and the wholes which exhibit them*"

The movement has the potential to change how systems are designed and managed. If causal factors of systems that contribute to emergent effects are known: 1) the risk that unexplainable effects will occur could be assessed; 2) design alternatives with fewer causal factors could be selected; 3) if the causal factors are actually capable of being adjusted (i.e., they are mechanisms), then the likelihood of unexplainable effects could be controlled; and 4) to the extent emergent effects are positive, their occurrence could be encouraged. These are motivations for developing a general theory of emergence in engineered systems and the inspiration for this dissertation.

One way to answer a question is to look at something we know and use it to explain something we don't (i.e., analogical reasoning). The research in this dissertation takes this approach by using the axioms and generally accepted theories from thermochemistry (a branch of thermodynamics) to build a simulation model to explain causal factors in engineered systems that affect emergence. Thermochemistry was selected as the medium of study for several reasons: As a branch of thermodynamics, thermochemistry is the study of transformations (i.e., changes) in chemical systems. Initial findings show similarities between thermochemical transformations and the transformation from explainable to unexplainable effects in engineered systems. Thermochemistry concepts are very well established and can be found in any high school chemistry textbook. Thermochemistry also happens to be the point of origin for the original concepts of emergence (Mill, 1846; Lewes, 1875). A rational research methodology is applied to take what is already known about thermochemistry and use it to help explain what we don't know about emergence in engineered systems. The methodology includes: 1) a detailed literature review to define the nature of the emergence phenomena and systems where it occurs; 2) steps to ensure correspondence with thermochemistry's generally accepted axioms / laws and the concepts, theories and models; and 3) a structure/framework to ensure the logical coherence of the propositions, models and theories that are developed from the research.

Chapter One of the dissertation defines the problem of emergence; justifies the significance of the research; and formulates a research question and provides an overview of the research that takes place. The research methodology and its supporting methods and frameworks are discussed in Chapter Two, including a formal method for analogical reasoning, a theory building framework, and a modeling and simulation framework to ensure the correspondence and coherence of the theory produced by the dissertation research. A detailed literature review of the emergence phenomena is presented in Chapter Three. Prevailing theories are discussed and synthesized into common themes that characterize the nature of emergence and systems where it occurs. The results from the literature review are used to develop the concept of emergence for the research that will take place. The concept is developed in Chapter Four using thermochemistry as a medium of study. The chemical system concepts are summarized and a conceptual model of endothermic reactions in chemical systems is presented. A theory of emergence in engineered systems is derived in Chapter Five from scientific analogies to the thermochemistry concepts. A simulation model based on the theory is then constructed and studied through experimentation in Chapter Six. The model is used to explore the ideas and concepts of the theory, and test it theoretical propositions. Conclusions and recommendation for potential applications and future research are presented in Chapter Seven.

1.1 Thesis Statement

The potential for emergents in engineered systems makes designing, managing, and operating them less tenable for its stakeholders. To address this risk, a general theory is required that defines emergence and explains its causal factors in engineered systems.

1.2 Research Significance

There is no shortage of theories of emergence. However, it is still not clear what the term [emergence] denotes or, more important, how emergence emerges (Corning, 2002). The significance of this research is a contribution toward answering these persistent questions.

Corning is not alone in pointing out the “multifarious,” “confusing,” and “contradictory” claims about emergence:

- **Silberstein and McGeever (1999)** discusses the confusion of emergence as a concept where system properties are in no way determined by or derivable from their constituents, vs. properties that are actually determined by constituents but are very difficult in reality to derive.
- **Corning (2002)** list examples of “ambiguous” and “contradictory” claims from theorists and the science community, such as: the relevance vs irrelevance of perception by an

observer; whether or not emergents are the irreducible or predicable; the requirement for interactions vs a change in scale of observation.

- **Campbell (2015)** identifies issues in the concepts of emergence that need clarification, including: what it means to emerge; what it is that emerges (entities, properties, behaviors, etc.); what constitutes an emergent property as novel; and are the spacio-temporal aspects of emergence synchronic, diachronic, or both.
- **Sartenaer (2016)** describes the insufficiency or "emptiness" in emergence concepts in three categories: 1) positivity (defining what emergence is *not* rather than what it is); 2) consistency (a system simultaneously determined yet unexplainable by its constituents is contradictory); and 3) triviality (the unqualified definition that emergents are properties of wholes that are not properties of parts can be an obvious observation with insignificant consequences).

An initial review of the literature on emergence supports the assertions that there are gaps in the body of knowledge on emergence. A sample of the prevailing theories that are frequently referenced in the literature are summarized in Table 1.

Source	Theory / Definition	Causal Factors
Lewes, 1875	Emergents are system effects caused by the *coalescence* of dissimilar components, and is not traceable/reducible to the steps of the coalescence process.	*…coalescence of dissimilar components*
Broad, 1925	Emergents are behaviors theoretically unexplainable by their components due to *lack of knowledge* of component microscopic structures and *"mathematical incompetence."*	*… lack of component knowledge; "mathematical incompetence".*
Ashby, 1956	Emergents are properties that are not shared by the system and its components due to *large variations in the size* of the parts relative to the size of the system (i.e., scale).	*…large part to system size variations*
Crutchfield, 1994	Emergence is the *dynamic interaction* of subsystems and components that create new patterns that produce new system capabilities / functions.	*… dynamic interaction of subsystems*
Bedau, 1997	Emergents are properties possessed by macro objects that are caused by *interwoven non-linear relationships* between their micro constitutes, but cannot be posed by them and are only derivable by simulation (i.e., apparently underivable).	*… interwoven non-linear relationships*
Holland, J.H., 1998	Emergents are recognizable, persistent, and reoccurring patterns that are not predicated due to the *inherent difficulty* of calculation and the size of potential state space.	*… inherent difficulty*

Table 1. Prevailing Theories of Emergence

Table 1 (continued)

Bar-Yam, 2004	Emergents are properties of the system that cannot be inferred from observations of components and are the result of *system level constraints* (Bar-Yam, 2004).	… *system level constraints*
Maier, 2015	Emergents are properties possessed by an assemblage of things that are not possessed by its members; that vary in degree of derivability in models; and is the result of *interactions between components* and time scales.	… *interactions between components*

The initial survey in Table 1 highlights the variety of definitions and contributing factors that are found in the literature. On the surface, several conflicts seem apparent and raise questions as to what emergents are: 1) properties, patterns, or behaviors; 2) new or reoccurring/persistent; 3) originates from the bottom up or the top down; 4) provisional or permanent; 5) observer dependent or independent. An equally wide range of assertions about the factors that cause emergence is also observed, including: coalescence of components; lack of knowledge; evolution; "mathematical incompetence;" interactions; variations in the size; and inherent difficulty, just to name a few. While these and other available definitions of emergents provide some insight into the concept, ambiguity persists and causal factors that affect the occurrence of emergents are not clearly identified and explained.

The need for a theory to address the identified gaps is further amplified by proposed research agendas from commercial industries, defense companies and academia:

- **Mogul (2006)** focuses on problems created by emergent behavior ("misbehavior") in complex software systems. His objective is to gain a better understanding of emergent misbehavior in complex software systems. He posits that this understanding is a prerequisite for improved design strategies and system management. He proposes several research agenda to support his objective including the development of … "a taxonomy of frequent causes of emergent misbehavior."

- **Valerdi et al. (2008)** discuss the risks to the resilience of System of Systems (SoS) that is posed by emergent behavior. They recommend research that will help determine the architectural factors of products that will make them less likely to demonstrate emergence due to the interactions among elements of individual systems in the SoS. They also identify the potential benefits and need to develop "Guided Emergence" architecture strategies. These are strategies "to steer emergent behavior" in desired directions to achieve mission objectives and goals.
- **Bloebaum and McGowan (2012)** discuss the challenges of unintended consequences (i.e., emergents) in Large-Scale Complex Engineered Systems (LSCES) such as aircraft carriers, nuclear power plants, spacecraft, submarines' water supply systems, electric power grids, offshore oilrigs, and air and ground transportation systems. They identify as a research opportunity the need to "…fully understand, manage, and exploit the inherent interactions in the system (from people, organizations and the physics), in a rigorous manner grounded in theory, so as to avoid unanticipated consequences during the design and development process."
- **Rainey and Tolk (2015)** question the acceptance of positive emergence as "…a welcomed coincident." Alternatively, they challenge the engineering community to conduct research that leads to emergence as the intentional "…product of engineering efforts." Rather than steering inherent emergence toward some benefit as in "guided

emergence" strategies; engineering emergence involves designing systems to actually produce beneficial emergent behaviors and properties.

The common thread in these agenda items is their call for research that leads to "… [gaining] a deeper understanding…" of emergence and particularly how it occurs in engineered systems.

Developing formal models of emergence can help us understand emergence in engineered systems and move toward closing the identified gaps. Conceptual models provide a coherent set of claims, assumptions, and constraints to reduce (if not eliminate) the concept's ambiguity. A simulation model would enable the study of causal factors in engineered systems that affect the occurrence of emergents. Developing such an understanding would open the door to changing how systems are designed and managed. If causal factors that contribute to the occurrence of emergent effects in engineered systems are identified: 1) the risk that emergent effects will occur could be assessed; 2) design alternatives with fewer causal factors could be selected; 3) if the causal factors are actually capable of being adjusted (i.e., they are mechanisms), then the likelihood of emergent effects could be controlled; and 4) to the extent emergent effects are positive, their occurrence could be encouraged. For these reasons, understanding the mechanisms of emergence in engineered systems is an important and worthy effort for research.

1.3 Research Question

The research in this dissertation addresses the emergence problem in the context of engineered systems. Emergence is essentially a phenomenon in systems that brings about unintended system effects; specifically effects that are not apparently explained by the system parts and their relationships. In order to defend against or exploit the emergence phenomenon, it would be beneficial to have a general theory for engineered systems that unambiguously defines emergence and explains causal factors in engineered systems that affect the occurrence of emergent effects. The author posits that the theory resulting from the research will have implications on the operation and design of engineered systems. The research in this dissertation intends to develop such a theory for engineered systems by answering the following research question:

What are the factors in engineered systems that affect the occurrence of emergence, and how are the factors related?

The research will provide:

- A conceptual model of emergence in engineered systems that resolves conflicting claims and assumptions.
- A simulation model that enables the study of causal factors in engineered system that affect the occurrence of emergents.
- Definitions and propositions for emergents in engineered systems.

Delimitation:

The research is a study of system level behaviors and characteristics rather than those of entities or agents. The focus of the research is limited to epistemological explanations of causal factors in engineered systems: identification, definition, and relationships. It does not include the ontological explanations of the emergents themselves: truth of their existence, particular qualities they display. The research is further limited to systems produced by humans; those that include people, processes, materials, and equipment. Systems that naturally occur in the environment are not addressed by this research.

1.4 Medium of Study

Research in this dissertation is conducted to address the problem of emergence in engineered systems. Given the gaps in the current body of knowledge, an alternative body of knowledge was identified that can serve as a medium of study to further investigate the problem. The research uses a rationalist inductive approach according to Sousa-Poza, et al. (2008). In applying this approach, the accepted theories for phenomenon in the medium of study are used to inform the development of a new theory for the problem phenomenon or phenomena of interest. The research in this dissertation follows this approach by using the axioms and generally accepted theories from thermodynamics; more specifically thermochemistry. Initial reasons for selecting thermochemistry as a medium include a broad applicability as a source of analogies to explain concepts; a well-established precedence in explanations of emergence; and general coherence with characteristics of engineered systems.

Klein and Nellis (1991) posit that the simplicity of its basic postulates makes thermodynamics applicable to "…any discipline technology, application, or process." Ott and Boerio-Goates (2000) expresses the same sentiment and reference Albert Einstein's impression of thermodynamics: *"A theory is the more impressive the greater is the simplicity of its premises, the more different are the kinds of things it relates and the more extended the range of its applicability. Therefore [is] the impression which classical thermodynamics [has] made upon me."* The simplicity and applicability of thermodynamics makes it a rich source for analogies that are used for their explanatory power in a variety of ways. Table 2 lists a sample of analogies based on thermodynamic concepts.

Reference	**Application**	**Thermodynamic Concept**
Sawada & Caley, 1985	Education systems and the process of learning.	Entropy and thermodynamic equilibrium.
Dyer, 1996	Effective scholarly conversations.	Exothermic / endothermic reactions.
Kotov, 2002	Dynamics of human culture.	Biogeochemistry and dissipative structures.
Chassin et al., 2004	Control of complex adaptive systems.	Carnot cycle.
Sergeev, 2006	Economic equilibrium in financial markets.	Entropy and thermodynamic equilibrium.
Kauffman & Clayton (2006)	Emergence of order in biological systems	Chemical reactions
Dyer, 2007	Emergence of individual learning.	Change in enthalpy.
Bratianu & Andriessen, 2008	Knowledge as energy.	Mechanical and thermal energy.
Chew & Choo, 2008	Resistance to changing a banking system.	Changing states of matter.
Pati, 2009	Stress management and innovation in business systems.	Enthalpy and the conservation of energy.
Ortega & Braun, 2013	Rational decision making and maximum utility.	Free energy and entropy.
Kovacic (2013)	Effect of shared awareness within multiple Cognitive Representations of Reality.	Percolation theory (i.e., statistical mechanics).

Table 2. Thermodynamic Analogies

In each of the examples in Table 2 the analogy relies on the consistency of the thermodynamic behavior and the broad acceptance of its governing principals to explain non-thermodynamic phenomena.

In addition to its broad variety of applications, there is a well-established precedence (over 150 years) for using principles of thermodynamics and specifically thermochemistry, to explain the concepts of emergence in systems. Thermochemistry is the point of origin for the original concepts of emergence (Mill, 1846; Lewes, 1875). Mill (1846) uses the thermochemical combination substances (i.e., chemical reactions) as a contrast to his Composition of Cause principle. Composition of Cause states that the joint effect of several causes is the same and the sum of their separate effects. Chemical reactions produce “special and exceptional” cases where Composition of Cause does not apply because the joint effect of the combination is not the same as the sum of the separate effects of the substances. Though not specifically called emergence, this is considered one of the early expressions of the emergence concept. Lewes (1875) uses many examples of chemical reactions to explain the nature of emergent effects where some combinations produce properties that are different from the properties of their parts. One example he cites is the orange color produced from the combination of colorless oxygen and colorless nitrogen. The orange color is novel (i.e., new) and not traceable to the properties of its oxygen and nitrogen components or the process of combining them.

A review of the literature also reveals that thermochemical systems and engineered systems share several common characteristics (see Table 3).

Characteristic	Engineered Systems	Chemical Systems
Type of system (naturally occurring vs produced by humans)	Produced by humans	Produced by humans
Structure	Engineered systems structures that are composed of lower levels of parts that combine to form a whole (i.e., a system) with novel properties and behaviors that evolve over time (Morgan, 1929).	Chemical species (or systems) are hierarchal structures composed of thermochemical elements arranges in a certain configuration to form the species (Fogler, 2011).
Micro / Macro Relationship	When emergence occurs in an engineered system, components combine in a way to produce new system level properties and behaviors while the properties and behaviors of the components remain the same. (Ablowitz,1939; Lewes, 1875)	Chemical elements combine to produce new chemical identities (i.e., a set of chemical properties) that define new chemical species while the identity of the elements is preserved (Matsoukas, 2013).
Dynamics	Changes in the exchange of information at the micro levels of the systems causes changes in interactions of the components of the system leading to new systems properties and behaviors (Johnson IV et al., 2013).	Changes in the internal energy of the chemical species (i.e., enthalpy) causes changes in molecular order (entropy) resulting in the emergence of a new chemical species with new chemical identities (Dyer, 1996; Gallicchio et al., 1998).

Table 3. Correspondence between Engineered Systems and Chemical Systems

Given the a broad applicability as a source of analogies to explain concepts; a well-established precedence in explanations of emergence; and general coherence with characteristics of engineered systems; it is concluded that thermochemistry is a suitable medium of study to develop theories for emergence in engineered systems.

1.5 Research Approach

Conducting research with engineered systems comes with certain challenges: 1) they are potentially large in scale; 2) the distance between its constituent's members can be significant; 3) their behavior can be episodic; and 4) replication of the systems may be prohibitive. These challenges make it difficult to directly observe and test an engineered system in its environment. The problem is further complicated by the absence of a coherent set of claims and assumptions for emergence in engineered systems. The research in this dissertation attempts to solve a problem that is difficult to define and to formulate, and will require multiple frameworks and methods to successfully develop a solution:

- A rational method is required to conduct research without direct observation of the emergence phenomena in engineered systems.
- A method is required to inductively transfer knowledge from accepted theories into a proposed theory of emergence in engineered systems.
- A framework for developing theory is necessary to guide the research and ensure that a theory is produced that meets generally accepted best practices for theory building.
- Modeling and Simulation (M&S) framework is used to ensure the consistency and completeness of the modeling products.

The frameworks and method are used within a rationalist inductive research methodology which is defined and discussed in Chapter Two.

CHAPTER 2

METHODOLOGY

The research question under study is:

What are the factors in engineered systems that affect the occurrence of emergence, and how are the factors related?

Answering the research question comes with particular challenges. The type of system that the theory will apply to may be complex and may not necessarily lend themselves to study through traditional system engineering methods and direct observation (Keating, 2008): 1) they are potentially large in scale; 2) the distance between its constituent's members can be significant; 3) their behavior can be episodic; and 4) replication of the systems may be prohibitive or not possible. To overcome these challenges it is necessary to choose a research methodology that leads to a theory that is not dependent on direct observations.

2.1 Rationalist Inductive Methodology

The research in this dissertation uses a Methodology for Rationalist Inductive Research (Sousa-Poza, Padilla, Bozkurt, 2008). The methodology has been applied by Brewer (2010), Padilla (2010), and Kovacic (2013) in their respective research for Ph.D. dissertations. The methodology is based on establishing truth in theories through coherence through a rational belief system rather than direct observation (i.e., correspondence).   In other word, a theory is true if it coheres to other theories that are accepted as true. It enables the extrapolation of a new theory from a set of theories that have already been justified and accepted as part of a body of knowledge. The methodology approach has three primary components (see Figure 1): exploration, structuration, and conclusion.

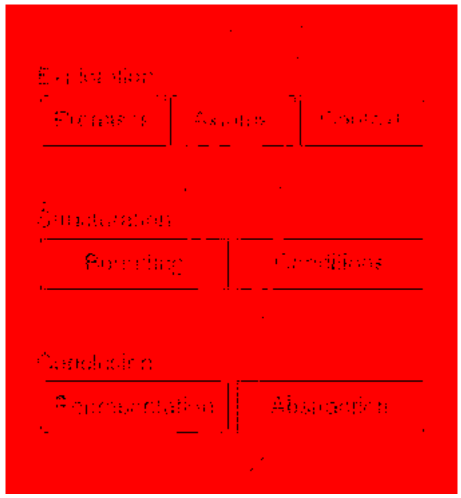


Figure 1. Rationalist Inductive Research Methodology

- ***Exploration*** gathers what is currently known about the research subject and identifies a problem. A thorough literature review, case studies or other methods are used to capture the rules, axioms, definitions, ontologies, and other foundational elements of the problem (i.e., what is known). The scope of the research is narrowed and place in a specific context.
- ***Structuration*** defines the architecture that supports the coherence of the system of beliefs (i.e., theory) produced by the research. The architecture is a system of

logic that all statements produced by the system must conform. It provides the necessary rigor to claim that the outputs of the research are true by coherence.

- ***Conclusion*** is where the result of the research are interpreted and implications are considered. .

In the methodology, new theories are inductively built through coherence with existing theories as depicted in Figure 2.

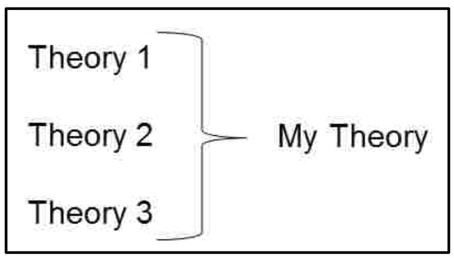


Figure 2. Inductively Building Theory through Coherence

The new theory ("My Theory") is justified if the inductively established structure of the theory is true according to a coherent system of beliefs.

Supporting methods and frameworks are used in this dissertation to provide the rigor required by the structurization component of methodology. The rigor in structurization establishes validity of the new theory through coherence in the inductive process and the structure of a logical belief system.

- *Analogical Reasoning* Method *(ARM)* – Justifies the transfer of knowledge from existing theories in the domain of the research medium of study (thermos chemistry) to the new theory in the domain of engineered systems.
- *Theory Building Framework (TBF)* – Sets a standard for defining the proposed theory of emergence in engineered systems.
- *Modeling & Simulation System Development Framework (MS-SDF)* – Provides a logical structure for developing models and simulations in the dissertation.

The supporting methods and framework are detailed in the followings sections.

2.2 Analogical Reasoning Method

Analogies are basically explanations about entities or phenomena based on knowledge from a different domain (Bartha, 2010; Gentner, 1983). Campbell (1920) argues that theories are distinguished from laws in that they can contain hypothetical ideas that are not measurable and cannot be proved or disproved by experimentation. Conversely, laws only contain measurable concepts that can be proved or disproved by experiential means. The truth and value of theories is established by analogies to other theories or laws and concepts that are already accepted as true. The vital role of analogies in theories is also discussed by Hesse (1966, 2000). He posits that analogies play a vital role in theories by explaining unobservable (or difficult to observe) phenomena in terms of observable phenomena in different domain. Analogies make theories more intelligible and extend their predictions by introducing new descriptive terms and inferences from familiar phenomena.

Analogical reasoning is the process of drawing inferences and transferring knowledge between domains based on analogies. There are many examples of analogical reasoning in scientific research. The variety of applications found in the literature are represented in Table 4 .

Example	Description
Particle Physics (Nambu & Jona-Lasinio, 1961)	A theory is developed to explain how masses of subatomic particles (fermion, mesons, and nucleons) are formed. The theory is based on an analogies to the mechanisms that cause energy gaps in the theory of superconductivity.
Artificial Intelligence (Eremeev & Varshavsky, 2005)	Real Time Intelligent Decision Support Systems (RT IDSS) are investigated. The researchers study how analogical reasoning is used in RT IDSS mechanisms to efficiently make decisions: analysis of the problem situation; search for solutions; learning; modelling, and forecasting
Engineering Design (Kalogerakis et al., 2010)	The researchers explore the effects of analogical reasoning in the engineering design process. They consider application of analogies in accessing knowledge and transferring it to innovative solutions across multiple industries.
Electrical Engineering (Li,2012)	Dissertation research is conducted on methods to identify and visualize electromagnetic coupling paths. Theories in fluid mechanics and electromagnetics are mapped to establish the analogy that energy flow is like fluid flow. Base on the analogy, a method is proposed that uses algorithms from fluid mechanics to identify and visualize electromagnetic coupling paths.

Table 4. Applications of Analogical Reasoning in Scientific Research

Table 4 (continued)

Shared Awareness (Kovacic, 2013)	Research is conducted based on analogies between the Cognitive Representation of Reality (CRR) and statistical mechanics (specifically, percolation theory) The author establishes functional relationships between postulates in CRR and those in percolation theory. The functional similarities are used in the development of a new theory for the emergence of shared awareness within Cognitive Representation of Reality.
Information Systems (Jog, 2015)	A new theory is developed that explains the natural growth in the volume of sequential convex sets in information systems (ex., emergence of constraints in communication channels). The theory is derived from analogies between concepts in geometry and information theory.

In each of the examples in Table 4knowledge from a source domain was transferred to a target domain and used to draw conclusions and make inferences.

The transfer of knowledge from a source domain to a target domain is valid to the extent there is correspondence between the relevant structural elements of the domains (see Figure 3).

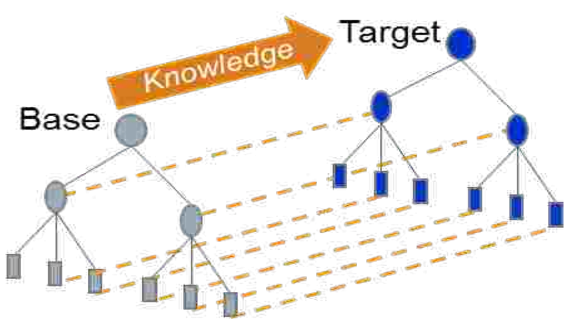


Figure 3. Structural Mapping and Knowledge Transfer

The structure of a domain includes the: properties; relationships; patterns; constraints; roles; and concepts that characterize the objects in the domain. A formal method for structural mapping and analogical reasoning is defined by Gentner (1983) and enhanced by Holyoak and Thagard (1989), Gentner and Markman (2006); and Lee and Holyoak (2008). A summary of basic rules and assumptions for the method are listed in Table 5.

Criteria	Description	Source
Domains	System of objects, attributes of objects, and object relationships.	Gentner (1983)
Domain Knowledge	Represented with predicate logic; a system of clauses that describe objects in the domain. Predicates are: a) attributes when the argument is a single object; b) relationships when the argument is two or more objects.	Gentner (1983)
1 to 1 Mapping	Elements in one domain must correspond to a single element in another domain	Gentner & Markman (2006)
Parallel Connectivity	If two predicates correspond their arguments must also correspond.	Gentner & Markman (2006)
Pragmatic	Only those elements in the domains that are relevant to the purpose of the analogy is considered in the structural mapping.	Gentner (1983)
Semantics	Predicate describing structural element must have similar meaning but do not have to be identical.	Gentner (1983)
Systematicity	Highest preference is given to structural elements that have causal, mathematical, or other functional implications.	Gentner (1983); Lee & Holyoak (2008)

Table 5. Structural Mapping Criteria

Analogies are not absolute; they exist on a continuum from weak to strong. The more an analogy fits the structural mapping criteria the stronger the analogy and the stronger case for applying analogical reasoning. This is especially true for the Systematicity criteria for structural mapping. Correspondence between functional elements of a domain makes the greatest contribution to establishing the relationships as a strong analogy. Formally stated, the proposition for the theory of the scientific analogy is: if the structural components B= {b1, b2, b3,…bn} of system B describe the relationships and attributes of the parts in system B, can be mapped to structural components T= {t1, t2, t3, ….tn} of system T; then knowledge about system B can be used to explain system T. The conclusions holds to the extent that the structural components in the mapping are relevant to the phenomena or entity to which the knowledge is being applied (i.e., they satisfy the pragmatic criteria for structural mapping).

2.3 Theory Building Framework

A standard for good theory based on a survey of best practices is constructed. The standard is used as guidance in defining the proposed theory of emergence in engineered systems.

There are a wide variety of definitions of theory. The research question concerns theory as it relates to observable phenomena. A survey of the various definitions of theory related to observable phenomenon was conducted and is summarized in Table 6.

Definition	Explanation	Prediction
A complete theory contains an element that corresponds to an element in reality such that the element in reality can be predicted with certainty (probability of 1) from theory (Einstein et al., 1935).		X
Theories are logical structures that explain phenomena and determine the rules for deductive inference (Hempel, 1958).	X	X
A set of laws, axioms, or causal processes that provide explanations, predictions, and a "sense of understanding" i.e., why phenomenon occurs (Reynolds, 1971).	X	X
Dubin (1978) defines theory as a closed systems that produces testable predictions about phenomenon.		X
Gioia (1990), a theory is a coherent explanation of experienced or observed phenomenon	X	
Meredith (1993), a theory is a model that explains why and how phenomenon occur in terms of postulates (logical statements) and the primary characteristics of the phenomenon.	X	
Strauss (1998) defines theory as a set of concepts related by statements that can be used to explain or predict phenomenon.	X	X
Theory is a statement of relationships between units observed or approximated in the empirical world. (Wacker, 1998).	X	

Table 6. Definitions of Theory

It can be concluded from Table 6 that the contents of a theory may vary, but it is consistently defined as a means to explain and or predict a phenomena. However, not all theories are created equal; some are considered better than others. There is some question in the literature as to what represents good theory. Some qualities rise to the level of being more than desirable "virtues"; without them theories are merely opinionated statements or collections of ideas. These qualities are the basis for building "good theory" and are summarized in Table 7.

Standard	Description	Reference
Identified Need	Supporting reasons to develop an explanation of a theme within a specified boundary	Dubin (1969)
Definitions	Use generally accepted definitions to unambiguously define the phenomenon, concepts, and variables of the theory.	Reynolds (1971)
Propositions	Testable conclusions and knowledge claims that explain the phenomena and predict future states/ behaviors.	Dubin (1969)
Falsifiability	Propositions and hypothesis have empirical indicators, are testable, and capable of being false.	Popper (1953); Dubin (1969)
Analogies	Analogies lead to the discovery and refine conceptual models by applying knowledge from a source domain to explain phenomena in a target domain.	Hesse (1966;2000)
Cause-effects Statements	Rational statements defining the conditions and interactions between variables that cause changes in system states (i.e., effects).	Dubin (1969); Reynolds (1971)
Rigor	Establish the coherence and internally consistency of relationships in the theory to a system of logic.	Reynolds (1971)

Table 7. Standards for Good Theory

Table 7 (continued)

Parsimony	State a minimum number of internally consistent relationships to support the claims of the theory.	Wacker (1998)
Uniqueness	Concepts, propositions, or “good theory” virtues that are not posed by existing theories.	Wacker (1998)
Generalizable	Integrates multiple concepts creating is broad applicability	Wacker (1998)
Fecundity	Enables the expansion of the research into new areas and leads to additional theories (concepts, models, hypothesis, etc.).	Wacker (1998)

2.4 Modeling and Simulation System Development Framework (MS-SDF)

Modeling & Simulation System Development Framework (MS-SDF), proposed by Tolk et al. (2013), provides guideline when dealing with problems that are difficult to define and formulate. MS-SDF integrates three system engineering concepts with M&S: capturing requirements; defining component relationships; and verification and validation

The MS-SDF captures the problem situation through reference modeling, conceptual modeling, and simulation. Reference models define the set of concepts, requirements, facts, and assumptions about a system phenomenon. The intent is to capture a comprehensive view of the subject from relevant perspectives; including inconsistent or conflicting interpretations. While reference models attempt to comprehensively capture what is known and assumed about the system; the purpose of a conceptual model is to provide a more appropriate level of abstraction and simplification of a real world system (Robinson, 2008). Conceptual models capture a consistent sub-set of the reference model that can be implemented in a simulation. They are the artifacts (tables and diagrams) that describe a system’s objectives, inputs, outputs, and content in a way that address a specific problem or answers question of interest regarding the system (i.e., the modeling questions).

The final phase of the MS-SDF consists of constructing a simulation based on the conceptual model. Simulation modeling produces a finite state machine realization of the conceptual model that answers the modeling questions. Simulations provide the environment to observe the interactions of system components and the dynamics of the system phenomena in order to answers the modeling questions.

The MS-SDF is implementation agnostic. There are no requirements for using any particular tool or modeling language. However, the authors recommend using a formal modeling method to facilitate logical consistency and provide the architecture for building a simulation. It is a rigorous modeling method based on cause-effect relationships that enables formal computer simulations of systems. Given the focus of the dissertation is developing a theory that explains causes; System Dynamics is particularly well suited as a modeling method. The seven major steps of this solution agnostic framework are defined in Table 8.

Step	Description
1) Problem situation.	Capture the subject of the study or the focus of the modeling effort as represented by what stakeholder claim or state to be true or false about the problem.
2) Assumptions & Constraints.	Identify Stakeholder assertions that are necessary but have no specific justification.

Table 8. M&S System Development Framework

Table 8 (continued)

3) Reference model.	Define the set of requirements, facts, and assumptions for the system (or problem). The set is documented in terms of statements, claims, and constraints based on relevant theories, rules, and stakeholder perceptions. Even inconsistent or conflicting interpretations are included.
4) Modeling questions.	Develop questions of interest about the problem, the relationships, and behaviors as documented in the reference model.
5) Conceptual model.	Define a subset from the reference model that has consistent interpretations of the systems (or problem) and can be used to answer the modeling questions. Document the subset using a solution agnostic modeling language to remove ambiguity and insure logical relationships in the model.
6) Simulation.	Create a dynamic representation (i.e., a virtual world) for the problem using the information from the conceptual model and a simulation modeling software package.
7) Verification & Validation	Verify that the model that was built is the model that was designed; and validate that the model meets is intended purpose.

2.5 Research Process

The actions that will be taken to answer the research question are defined in the research process. Each action is justified by mapping it to one of the components of the Rationalist Inductive Research Methodology (RIRM) or one of its supporting methods/frameworks: Analogical Reasoning Method (ARM); Theory Building Framework (TBF); Modeling & Simulation System Development Framework (MS-SDF). The process steps and mapping are detailed in Table 9.

Process Steps	Frameworks/ Methodologies
1) Identify a research opportunity: a problem related to a phenomenon of interest.	RIRM
2) Define the context that the proposed theory will be applicable and that the research will be conducted.	RIRM
3) Conduct a detailed literature review of the current body of knowledge for the problem.	RIRM
4) Develop a reference model based on a broad set of claims and assumptions found in the literature about the problem.	MS-SDF
5) Identify a gap in the body of knowledge for how the problem is currently addressed and develop a research question.	RIRM
6) Identify an alternative body of knowledge (i.e., a suitable medium) to study the problem and inductively develop the theory.	RIRM
7) Justify the use of the selected medium by establishing correspondence between the body of knowledge for the medium of study and the nature of the body of knowledge for the phenomenon. If correspondence is not established, identify a new medium and repeat the step 6.	ARM
8) Develop a conceptual model (i.e., a set of coherent set of claims, assumptions, laws, theories, axioms, conditions, boundaries, etc.) that explain the phenomenon occurring in the medium of study.	MS-SDF
9) Establish correspondence between the nature of the phenomena in the medium of study and its nature according to the problem's current body of knowledge. If correspondence is not established, identify a new medium and repeat the step 6.	ARM

Table 9. Research Process Steps

Table 9 (continued)

10) Develop analogies using the medium's theories and conceptual model that explain the operational nature of the problem phenomenon in terms of the operational nature of the phenomena in the medium of study.	RIRM /ARM
11) Identify a system of logic as a structure for coherence of the new theoretical model to address the problem.	RIRM /TBF
12) Develop a conceptual model of the problem phenomenon using the analogies and the system of logic.	ARM
13) Develop a set of logical propositions based on the analogies and the conceptual model for the problem phenomenon.	TBF
14) Verify that the set of claims, assumptions, laws, conditions, boundaries, propositions, hypotheses (i.e., the theoretical model) are coherent and conform to good theory building practices. If not verified, repeat 10-14.	RIRM /TBF
15) Define a modeling question and create a simulation model based on the theoretical and conceptual models.	MS-SDF
16) Design and conduct simulation experiments to further study of the problem and refine the theory.	MS-SDF
17) Analyze the results of the simulation experiments and determine if: a) there is any failure of the theoretical model to cohere with its body of beliefs (i.e., logical coherence with claims, assumptions, laws, conditions, and boundaries); b) there is correspondence with behavior of the medium's phenomenon. If correspondence or coherence fails, repeat 15-17.	RIRM
18) Analyze the overall results of the research; determine if the research questions has been answered. If not answered, repeat 6-18.	RIRM
19) Document the conclusions, propositions, predictions, and knowledge claims.	RIRM

The steps and decision gates in the process are depicted using Business Process Modeling Notation (BPMN). The BPMN flow chart in Figure 4 shows the research steps in major process groups and decisions gates.

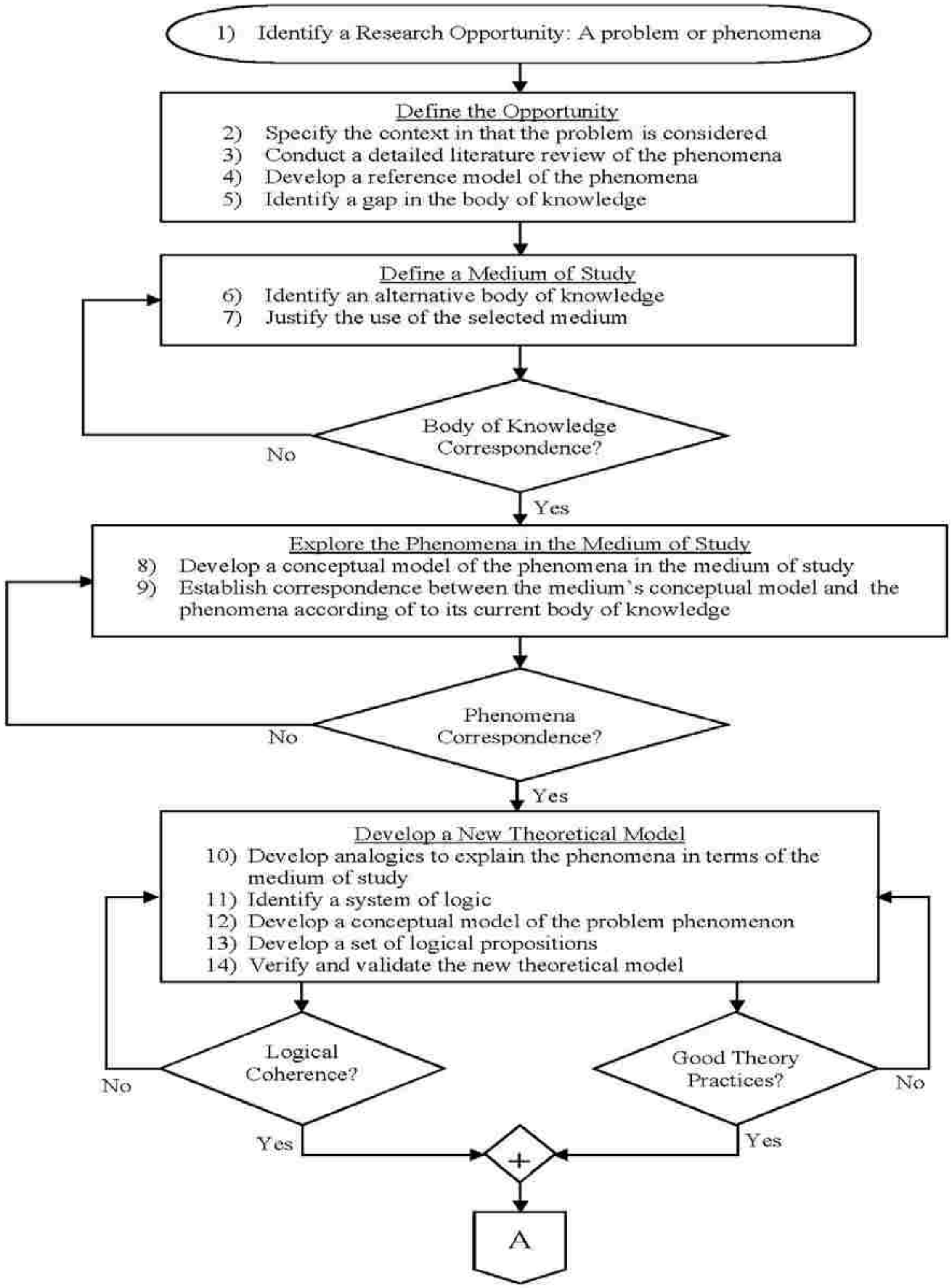
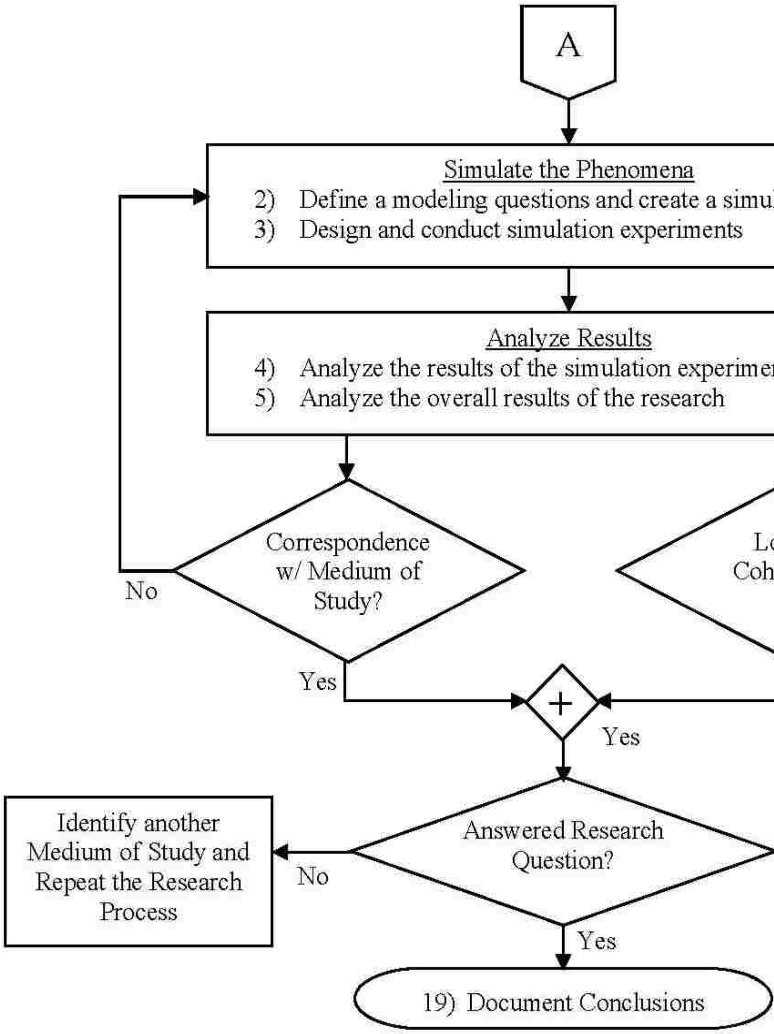


Figure 4. Research Process Flow Chart

Figure 4 (continued)



From the BPMN flow chart, seven decision gates are identified. These gates represent the significant milestones in the research process towards reaching a conclusion for the research question. The process flow chart provides a logical framework for conducting the research.

CHAPTER 3

LITERATURE REVIEW

There is no single generally accepted definition of emergence (the verb) or emergents (the noun) that captures all of their important elements. The history of emergence is ancient and full of ambiguous and sometimes conflicting assertions. Silberstein and McGeever (1999), Corning (2002), Campbell (2015), and Sartenaer (2016) are among those that discuss the "multifarious", "confusing", and "contradictory" claims in the domain of emergence. The first objective of the literature review is to study the domain of knowledge for the concept of emergence and capture its theories, definitions, descriptors, distinctions, and other important elements. The next objective is to use the result of the first objective to unambiguously define what emergents are and how they occur. The artifacts of the review are a reference model that captures what is known and assumed about emergents, and an ontology of the emergent concept. An ontology is a formal representation of the nature of a concept; its terms, properties, relationships, restrictions, and otherwise its essential elements (Gruber, 1993). The reference model informs the ontology by providing a comprehensive view of the domain for concepts including its conflicting and inconsistent aspects. The ontology contributes to answering the research question by providing a congruent and unambiguous representation of the emergence concept.

The study covers a wide variety of historical and contemporary concepts including those in Table 1 as well as others identified during the literature review. There are easily hundreds papers and books on emergence concepts. An attempt was made to capture original concepts and those most frequently referenced in the literature. Each conceptual element captured in the review is assigned a unique identifier consisting of a number preceded by the first two letters of the primary author’s last name (adding a third letter and or first name initials if necessary to distinguish between authors. The inputs from the literature review are used to construct an ontology according to the Web Ontology Language standard (McGuinness et al., 2004) using the Protégé tool for developing and maintaining ontologies (Protégé, 2016). The extended literature review, reference model, and detailed ontology (Figure 21) are presented in Appendix A. The summary of finding is presented in the following section.

3.1 Literature Review Findings

The literature review reveals multiple theories and varied definitions of emergence; some of which contradict one another. Building an ontology of emergence led to the discovery of common classes and properties that can be used to define the concept in an unambiguous way. Figure **5** depicts the hierarchy of classes and subclasses for the emergence ontology.

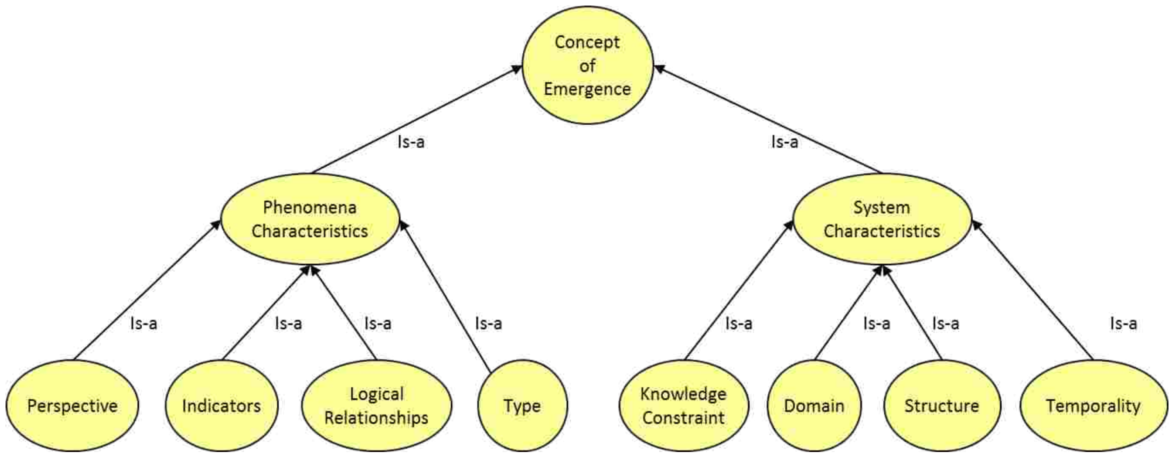


Figure 5. Ontology of Emergence

The author posits that the ontology at the level depicted in Figure 5 represents an unambiguous and unifying general definition of the emergence concept. Emergence is defined by two primary classes: characteristics of the emergent effects, and characteristics of systems where emergent effects take place. The primary classes are broken down into eight subclasses: type; logical relationship; perspective; indicators; temporality; structure; knowledge constraint; and application domain. Conflicts among emergence concepts are reconciled by grouping them into the eight subclasses.   For examples, the conflict between emergence as a diachronic vs synchronic concept is resolved by grouping both concepts in the category of Temporality. Whether emergence is a time dependent (diachronic) or independent (synchronic) or not, in either case there is an aspect of time (temporality) that defines emergence.

The concept is further defined by propositions for each subclass:

Phenomena Characteristics:

- *Perspectives.* The existence of emergents depends on the point of view that the novelty of the effect is determined. If the significance is determined and varies according to the observer, then emergence is extrinsic (i.e., observer dependent). If the significance is inherent to the system and does not vary according to the observer, then emergence is intrinsic (i.e., observer independent).
- *Indicators.* The occurrence of emergent effects is marked by certain measurable facts, i.e., parameters. The parameters are not the causes of emergents; they are the quantitative signs that emergent effects have taken place. Parameters have magnitude (size or amount) and direction (increasing or decreasing). Examples include: non-linear results from components interactions; uncertainty, randomness, or disorder of the future system states (i.e., entropy); variety of potential system states relative to the initial variety; the number of distinguishable states or the number of variables required to define a state (i.e., complexity); data that describe or are actionable by the system (i.e., information).
- *Logical Relationships.* The relationship between system components and emergent effects is characterized by being able to derive or explain an effect from system components and their interactions. Derive is used in the context of being able to start with an initial point of knowledge about the system's parts and interactions, and make logical progressions to arrive at the system level effects. Explain is used in a similar way but in the opposite direction. To explain is to start with the system level effect and logically trace its origin back to knowledge about the parts in the system. Relationships

are either currently derivable / explainable; theoretically derivable/explainable in the future; or completely underivable /explainable.

- *Type.* Emergents are the consequence of the interaction of components in a system. They include behaviors (the particular way in which the system functions); qualities (characteristics of the system); patterns (a reoccurring sequence or identifiable form); and structures (particular configurations of the system parts).

System Characteristics:

- *Domain.* Emergent concepts apply to different type of systems. There are three general domains of systems types to which emergence concept apply: Physical systems that are engineered by humans; physical system that occur naturally in the environment; and metaphysical systems that occur naturally in the environment.
- *Knowledge Constraint.* The ability to derive/explain emergents effects is limited by insufficient knowledge of component properties and their interrelationships in the system. The various type of constraints that inhibit deriving / explaining effects include but are not limited to: experience of the observer; density of information in the system; capability to view the system as a whole; inherent difficulty due to iterative aggregations.
- *Structure.* Nature of the configurations of components that form the system are described by certain characteristics, which include but are not limited to: hierarchal order; assemblage of dissimilar parts; components with non-linear functions; coupled / interconnected components.
- *Temporality.* The state of the system is the configuration if its parts and the values of their variable at a point in time. The state may or may not be time dependent. If the state

that produces emergent effects develops over time, the system temporality diachronic. If then emergent state is constant and always exist, the system temporality is synchronic.

It was determined that each instant of emergence theory studied in the in the literature review contained claims and or assumptions in each of the eight sub-classes. Variation among the theories was found below the level depicted in Figure 5. However, the consistency among theories at the class and sub-class level support the ontology as a unifying definition of emergence.

The ontology covers physical and metaphysical domains. Given the focus of the research is on engineered systems, operational definitions of emergents (the noun) and emergence (the verb) in the physical domain are synthesized from the literature review:

a) Emergents are system effects that are approximately underivable based on system components and their interrelationships.

b) Emergence is the action of producing system effects that are approximately underivable based on system components and their interrelationships.

Definitions for both emergent (the noun) and emergence (the verb) are offered to provide additional clarity given both words are frequently used throughout the body of knowledge as well as the dissertation. The operative words in the definitions are “underivable” and “approximately”. Underivable describes the limitation on logically determining in advance the effects of component interactions based on knowledge of the components and their interrelationships. A corollary for the underivable limitation is unexplainable. It is assumed that a limit on the ability to derive and effect is also a limitation on the ability to explain it. “Approximately” is used to qualify the underivable limitation. It captures the concept that emergents in the physical domain are theoretically derivable, but doing so is inherently difficult and may not have occurred. The qualifier of being "approximately" underivable is necessary to distinguish the concept of emergence in the physical domain from its application in the metaphysical domain. The metaphysical domain refers to that which is unperceivable by the senses (i.e., the mind, consciousness, etc.). In the metaphysical domain, emergents are completely underivable vs. being theoretically derivable in the physical domain. Restricting the operational definition to the physical domain is appropriate as the dissertation is concerned with engineered systems.

The operational definitions and propositions inform the design of the simulation model for emergence in engineered systems. The ontology will be used to guide the development of models and a theory of emergence in engineered systems.

3.2 Context

The emergence phenomena has broad ranging in applications across multiple disciples including but not limited to: cosmology; quantum physics; biophysics; cell biology; primate evolution; neuroscience; consciousness; and religion (Clayton, 2006). The research interest of this dissertation is in the emergence phenomena as it pertains to engineered systems. This is the context in which the products of the dissertation are developed. For this reason, a discussion on systems and the impact of emergence is presented.

3.2.1 Engineered Systems

Systems exist to accomplish tasks, solve problems and meet vital needs in our society by providing capabilities that are not possible by their discrete components (i.e., parts). In the most basic form, a systems is naively accepted to be a set of individual parts that form a whole. By this definition almost everything is a system of some sort: a set of books on a shelf is a library; a group of ants in the same general area might be a colony; a set of instructions can define a process; a group of girls can form a soccer team. But can we really consider a pile of bricks or a room full of people to be a system?

The operative words for defining a systems are connections (i.e., relationships) and functions (i.e., behaviors). Bertalanffy (1956) formally defines a system as a set elements where the behavior of the elements varies based on the nature of their relationship to each other. The parts of a system must be connected in a way that allows them to perform a function that could not be performed by the parts of subsets of parts. Elements in a system have an affect each other as well as the properties and behaviors of the systems as a whole (Blanchard & Fabrycky, 2006). Set theory can be used to formalize Bertalanffy's definitions of a system. Elements Q = {q1, q2,… qn} stand in relation R to each other such that they have system behaviors A= {a1, a2, a3, …an}. In a different relation R′ the system behaviors are A′ = {a′1, a′2, a′3, …a′n}. Elements Q are a system iff $A \neq A'$.

The research for this dissertation is concerned with the class of systems that are created by humans (i.e., engineered) rather than those that occur naturally in the environment. Engineered systems are designed and made to perform intentional functions that accomplish an explicitly defined purpose (Ackoff, 1971; Checkland, 1999; Blanchard & Fabrycky, 2006). In this context the engineered system is the artifact (the "thing") that is produced by the engineering effort. Engineered systems have certain characteristics that distinguish them from natural systems. From Simon (1969), Blanchard and Fabrycky (2006), and Buede (2011) these characteristics can be generalized as:

- Designed by humans.
- A functional purpose, a set of specifically defined objectives, or mission in response to a specified need.
- Defined combinations of resources (people, hardware, software, equipment, processes, rules, etc.).
- Interfaces to connect the resources.
- Interactions among the resources and with the environment that produce system behaviors in desirable and undesirable ways.
- Hierarchical relationships.

Simon (1969) discusses two modes (or propositions) of design that are required to realize an engineered system: 1) there must be a proposition of the desired states (the properties and behaviors that the system should have); and 2) a proposition for how to intentionally achieve the desired states (parts, assemblies, subsystems, structures, processes, etc.). For example, consider the propositions that a system has desired states (behaviors) consisting of set A {a1, a2, a3, …an}, and an intentional means for achieving them that consist of set B {b1, b2, b3, …bn}. To the extent that "A" can be achieved by "B", the application of engineering methods is tenable and produces a successfully engineered system. However, to the extent that "B" produces states that are different from "A" (greater than, less than, or otherwise not equal to), the application of engineering methods is less tenable and the original purpose of the system may not be realized.

Designing engineered systems is an iterative process of defining requirements and identifying solutions (Blanchard & Fabrycky, 2006). Requirements are statements that represent specific ways that the system will be useful to its stakeholders and serve its intended purpose (Buede, 2011). Each requirement can have many potential solutions; i.e., combinations and configurations of components that produce system states to satisfy one or more requirements. The universe of all potential solutions is the available design space. Throughout the design process, the available design space is explored; solution alternatives are evaluated, and decisions are made regarding which configurations of components will be used to satisfy the system requirements. As design decisions are made, the available design space gets smaller until eventually an area is defined that contains the design solution and the set of system states that satisfy the system requirements. The set of system states for the design solution establish the limits of acceptable performance for the system. All system states that fall outside these limits are errors (Blanchard & Fabrycky, 2006). The circles in Figure 6 represent the area of the state space for each type of state related to designing engineered systems: a) designed; b) designable; c) undesignable.

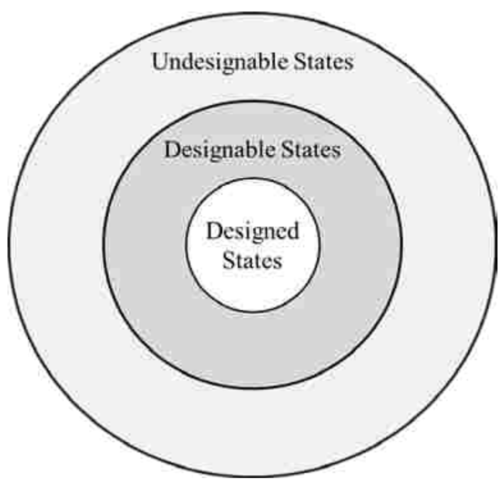


Figure 6. State Space Segmentation

- Designed: The states of a system according to its design will fall in this area. A system is designed to produce certain states that meet stakeholder requirements (functions, capabilities, missions, etc.) and to conform to constraints of cost, schedule, and performance. This represents conformance to Simon's (1969) first design proposition for an engineered system by specifying the properties and behaviors the systems should have as well as the second proposition as to how the properties and behaviors will be achieved with the components of the system. In this space, system states are derivable from and explainable by the system components.
- Designable: There are many ways to meet requirements and conform to constraints. The universe of states for all possible designs for all possible solutions is represented by what is designable (i.e., the available design space domain), where each design option has its own set of system states. While all states in this space are capable of being designed they may not have been selected for inclusion in the particular engineered system. These states also represent the state that are specifically not desired (i.e., errors and failures). State that occur in this space are failures of Simon's (1969) first design proposition for an engineered system by falling outside of the specified properties and behaviors the systems should have. Whether excluded as part of the design process or occurring because of some failure/error event, system states in this space are derivable from and explainable by the system components.
- Undesignable: Some system requirements and constraints are apparently beyond human capabilities to devise a means by which they can be satisfied. The systems states for these requirements and constraints are undesignable. States that occur in this space are

failures of Simon's (1969) first and second propositions. System states in this space are underivable from and unexplainable by the system components.

3.2.2 Definition and Examples of Emergence in Engineered Systems

All systems produced by artificial means do not strictly conform to the propositions of an engineered system. Some engineered systems begin with specifically designed functions and capabilities, and then evolve into new systems characterized by functions and capabilities that are not a result of intentional design effort or explainable by the initial design. Other systems retain their original design characteristics, yet they have apparently unexplainable behaviors or properties. In both exceptions, the engineered systems have states that fall in the undesignable space where system states are apparently unexplainable / underivable.

Based on the ontology developed from the literature review, operational definitions of emergence (the verb) and emergents (the noun) in the physical domain are:

a) Emergents are system effects that are approximately underivable based on system components and their interrelationships.

b) Emergence is the action of producing system effects that are approximately underivable based on system components and their interrelationships.

With the operational definitions in mind, we can conclude that system states in the undesignable state space are emergent effects. Consider the following examples in the literature of systems that display this phenomena:

National Airspace System *(Bonnefoy, 2004/2006).* The original National Airspace System (NAS) was composed of 19 airports and was designed to move large volumes of people over far distances. Each airport was paired with a Terminal Radar Control Facility (TRACON).

The job of the TRACON is to manage local aircraft arriving, departing, or transiting airspace. A decentralized network of airports, local control of air traffic, and large high capacity aircraft were general features of the original system. Demand for air transportation increased and airport capacity grew. At some point, the structure of the system changed. Political, social, and economic forces constrained the growth of the large regional airports and led to: 1) the emergence of smaller secondary airports and accompanying TRACONs; 2) secondary airports spurring growth of smaller airlines, offering more frequent, lower capacity, lower cost, regional flights; 3) declining average passengers per flight with increasing total numbers of travelers; and 4) increased dependency of airports and increased centralization of air traffic control. The changes in the NAS were not a result of design and were not predicable based on the original components of the system.

Stock Market (Aldridge, 2014; Bowley, 2010; CFTC, 2010; Kirilenko et al., 2015 Levine, 2015; Serritella, 2010; Sommerville et al., 2012). The primary purpose of the New York Stock Exchange (NYSE) is to maintain liquidity in the market. Liquidity is defined as the ability to execute contracts in a timely fashion between buyers and sellers without effecting price. In a 20 minute period on May 6, 2010, the market saw a complete evaporation of liquidity and individual stock prices swings from $.01 to $100K. The phenomenon is known as a “flash crash” and is characterized by: 1) the evaporation of liquidity; 2) extreme price swings and a return to normalcy in a relatively short period of time; 3) irrational prices that are not based on economic information. Several causes have been suspected, from malicious acts to electronic trading algorithms, but none have been confirmed as the root cause. When considered separately, the properties and relationships of the system components do not explain or provide a means for predicting the flash crash phenomenon.

Network Routing System (Mogul, 2006). Mogul describes an unexpected global behavior that occurred in the Planetary-Scale Event Propagation and Routing (PsEPR) system. The system attempts to optimize the routing of traffic between clients accessing servers in a network. The routing system design is based on the proposition that optimization is achieved when: 1) clients are allowed to select any server in the network; 2) clients are evenly distributed among servers; and 3) the selection of servers by clients is based on local preference heuristics. For instance, clients would select servers that they were closest to in proximity and for which they historically had the longest connection times. When a client was not able to connect to a server on its preference list, the server would move to the bottoms of the client's local list and the next server would rise to the top. However, as the routing system scales there was a convergence among clients to a global preference for the same servers. With the clients attempting to accesses the same servers, a cycle of overloading and network instability ensued. It is true that this particular convergence effect would not exist in modern routing technology. However, it was not apparent at the time in the local properties of the system components before the global system phenomena of was observed.

London Millennium Footbridge (Bocian, 2013; Dallard et al., 2001, Macdonald, 2008). In June 2000, London's Millennium Footbridge opened with over 80,000 visitors. At some point during the day unexpected excessive lateral vibrations accumulated to a point that required the closing of the bridge. Subsequent analysis eliminated the design or deviations from design standards as the cause. It is suspected that the synchronization of pedestrian footsteps or negative damping from the pedestrian traffic is the likely source. Lateral vibration due to pedestrian-structure interactions is a repeatable phenomenon that had occurred on occasion for

30 years. However, it was not explained and predictable until years after it was observed in the Millennium Footbridge case.

Future Combat System *(Blanchette et al., 2010; Pernin, et al., 2012).* The Future Combat System (FCS) was a modernization effort intended to “revolutionize the way the Army fights” by replacing existing combat units with assets integrated by a central communications network. Entire brigades would outfitted with mobile technologies protected by improved sensors and superior situational awareness. It was a $200B effort that was largely consider a failure and was ultimately canceled.   One of the many challenges was the difficulty in testing the system due to the unforeseen behavior arising from the dynamic interactions of constituent systems. For example, in a “fires scenario”, the sensors in the system detect and report a target, and the software algorithms determine which available shooter is best to engage the target. However, it could not be determined in advance which shooter would be selected or what the contributions would be of component-level design changes. Seemingly small, non-critical changes had unexplainable impacts to the system’s overall performance.

The common thread among these examples is a system state that is not readily explainable by or derivable from the system components and component relationships. The National Airspace system is an example of an evolved structure where environmental constraints developed over time, creating global system behaviors that are not derivable from the system components in isolation. If there is knowledge of the component properties, their relationships, and the system constraints then deriving the global behavior is possible. Stock Market systems is an example of a system where global behavior is a result of the interdependencies (i.e., coupling) between the system components. Because of these interrelationships, system behaviors and properties cannot be derived from information about the components without observing them in relationship to each other. The network routing system, London's Millennium Footbridge, and the Future Combat System demonstrate how some engineered systems produce unintended consequences that are contrary to the intended purpose of the system design. The system behaviors are completely determined by the system components and their relationships. However, deriving the unintended system behaviors or explaining them in terms of the components and their relationships is intrinsically difficult.

All of the examples presented fall under the undesignable state space depicted in Figure 6. They are undesignable in the sense that they were not intended by the design, and they are not explainable by the design or its components. They fail Simon's (1969) propositions for engineered systems. They are engineered only in the sense that they are produced by humans and contain subsystems that are designed.

The examples in this section represent the wide range of types of engineered systems that frame the context in which the research is conducted.

CHAPTER 4

CONCEPT DEVELOPMENT

The research question is:

What are the factors in engineered systems that affect the occurrence of emergence, and how are the factors related?

In Chapter One, thermochemistry was established as a medium to investigate and inform the development of a theory of emergence that will answer the research question. Thermochemistry was initially selected for its broad applicability as a source of analogies to explain concepts; its well-established precedence in explanations of emergence; and its coherence with characteristics of engineered systems. Chapter Four presents reference and conceptual models of endothermic reactions in chemical system based on generally accepted definitions and concepts from Thermochemistry. The background and foundational concepts of thermochemistry that were used in this chapter are available in Appendix B.

4.1 Chemical Reactions

A chemical systems is a hierarchal structure of chemical substances (i.e, components). The structure has macro level properties and characteristics (i.e., macro states) that are determined by combinations individual substances (i.e., microstates) of the system. A chemical reaction is a phenomena characterized by changes in the macro and micro states of a chemical system. The changes are caused by interactions of chemical system components with the environment, and other chemical systems. Like engineered systems, sometimes the effects of the interactions are properties and behaviors that are explainable based on their parts. Other times, the interaction changes the system and the effects are not apparent in its parts (i.e., they are emergents). The chemical reaction phenomena is consistent with the operational definitions of emergents and emergence in the physical domain derived from the ontology in Chapter three and Appendix A:

a) *Emergents are system effects that are approximately underivable based on system components and their interrelationships.*

b) *Emergence is the action of producing system effects that are approximately underivable based on system components and their interrelationships.*

The transition of chemical systems to producing interaction effects that are underivable describes the emergence phenomena we wish to understand in engineered systems. The objective now is to identify causal factors for chemical reactions in chemical systems and used that knowledge to inform the development of a theory of emergence in engineered systems.

4.1.1 Endothermic Reactions

Components in a chemical system are held together in a certain configurations by forces (bonds). Each configuration is a microstate of the chemical system which determine the systems macro states (its properties and behaviors). In order for a chemical reaction to take place, there must be a sufficient change in the systems internal energy (*U*) to break the bonds that are holding the molecules together. Chemical systems interact by exchanging energy with the environment (which can include other chemical systems). Endothermic reactions are an examples of chemical reactions where new microstates produce a new macro state of the chemical system has more energy than its initial state. The properties, behaviors, and the configuration of the molecules in the chemical system are a function of its internal energy. Therefore, a chemical reaction results in a change in the configuration, behavior, and properties. An example of a chemical reaction is depicted by in Figure 7.

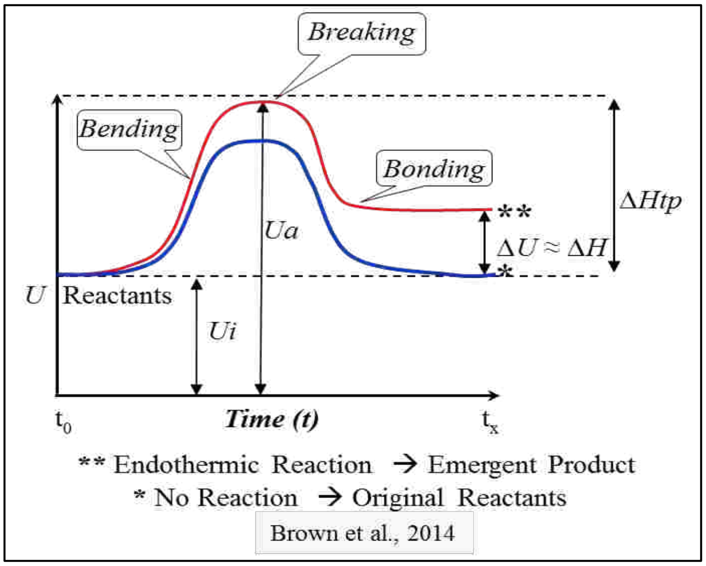


Figure 7. Endothermic Chemical Reaction

Consider the blue line (*) in Figure 7. Chemical systems are initially in a state of equilibrium where its initial internal energy (Ui), the configuration of its components, and the associated properties and behaviors of are constant. While interacting with the environment or other chemical systems, the internal energy increases and causes the bonds that maintain the configuration to bend. If the change in internal energy (U-Ui), also known as change in enthalpy (ΔH), does not exceed the difference between the activation threshold (Ua) and Ui; eventually the additional energy dissipates to the environment or another chemical system; and the system returns to its original state of equilibrium. Ua is the minimum amount of energy required to break the bonds that maintain the configurations of the system. Ua-Ui is the enthalpy tipping point (ΔHtp) that must be exceed before a chemical reaction can occur. In the case for the blue dotted line, the internal energy did not exceed ΔHtp. Because the exchange of energy was insufficient to exceed the required threshold, final ΔH is zero; and the configuration, behavior, and properties of the chemical system return to their original state.

Consider the red (**) line in Figure 7. While interacting with the environment or other chemical systems, the internal energy increases and exceeds the activation threshold (Ua) and the enthalpy tipping point (ΔHtp). The bonds that maintain the configuration break; some of the additional energy is absorbed into the system and some dissipates back to the environment or another chemical systems; new bonds are formed; and the system settles at a new state of equilibrium, and at a higher level of internal energy. In this case, the change in enthalpy (ΔH), is greater than zero and a chemical reaction has occurred. The configuration, behavior, and properties of the chemical system change.

The chemical reaction in Figure 7 depicts a transition that occurs in chemical system; to a new level of equilibrium where the configuration of its parts and the nature of its properties are different (i.e., emergent). This transition is a demonstration of emergence.

4.1.2 Factors that Affect Chemical Reactions

There are generally four factors of chemical systems that are mechanisms (or means) by which the chemical reaction rate and likelihood of occurrence can be changed: 1) the frequency of contacts (i.e., collisions) between molecules; 2) the force at which they collide; 3) orientation of the molecules when they collide; and 4) the activation energy (Ua) of the system. These mechanisms are elements of the rate law where the rate of a chemical reaction is given by [4.1] and the Arrhenius Equation [4.2]

$$\text{Rate} = k^*(\text{substance 1})^{a} \times (\text{substance 2})^{b} \times (\text{substance 2})^{c} \ldots \qquad [4.1]$$

Where:

k= the rate constant and;

The exponents a, b, c,… are the reaction orders for each substance which indicates how much the rate of reaction is affected by the substance. Increasing the amount of substance 1, 2, or 3 will exponentially increase the rate based on the reaction order of the concentration of the substance(s) in the chemical system

$$\textit{Rate constant, } k = A \times e^{(-Ua)/RT} \qquad [4.2]$$

Where:

A = Frequency factor for favorably orientated collisions

R= the gas constant

Ua = Activation Energy

T = Temperature of the system

.

1) **Concentrations**. The energy in a chemical system causes the molecule in its substance to move. In order for a chemical reaction to occur, the molecules in the chemical substances must collide with one another. The greater the number of molecules there are in the chemical system, the higher the probability that there will be a collision. The number of molecules is increased by increasing the volume (i.e., concentration) of one or more substances relative to the total volume. Increasing the concentration, increases the frequency of collisions between molecules of the substances in the chemical system which increases the rate of the reaction according to the rate law [4.1]. The change in rate is exponential if the order of the substance is greater than 1. For example, increasing

the volume of a substance by 50% (or a multiple of 1.5) with a reaction order of 2 would increase the reaction rate by a multiple of 1.5^2 or 2.25.

2) **Molecular Freedom.** There are a certain number particles in each molecule of the substances in a chemical system. Each particle has a certain charge (positive, negative, or neutral). Substances in a chemical system will only react if the number and charges of their particles are in the required alignment (i.e., orientation) when they collide with each other. The freedom of movement among molecules in a substance varies according to the state of the substance: solids have the least freedom while plasma has the most. The variations in states affect the molecular movement and the chances that the particles will collide and be in the correct orientation to cause a chemical reaction. The chemical reaction rate is increased as a linear function of molecular freedom of the substances in the chemical system.

3) **Temperature.** The kinetic energy in a chemical system is determined in part by the speed that the molecular components in the system are moving. The faster the components move; the greater the frequency and intensity (force) of their collisions with each other. Molecules move faster at higher temperatures causing the kinetic energy and consequently the internal energy in the system to increase. The rate of a chemical reaction grows exponentially as a function of temperature (T) where the change in the rate constant = $e^{-1/T}$ according to the Arrhenius equation [4.2].

4) **Catalyst**. Adding substances or energy from an external source causes the internal energy (U) of a chemical system to increase. New chemical products are formed when the change in the system's enthalpy (ΔH) plus its initial internal energy (U) exceed the system's activation energy (Ua). Some substances possess the ability to be added to a

chemical system without changing the chemical products of the reaction. These substances (catalyst) maintain their structure while lowering the activation energy (Ua) and/or improving particle orientation during a collision. The rate of a chemical reaction grows exponentially as a function of reductions in Ua where the change in rate constant= e^{-Ua} according to the Arrhenius equation [4.2]

Figure 8 maps the relationships between the factors that influence a chemical reaction and the mechanism by which they affect change.

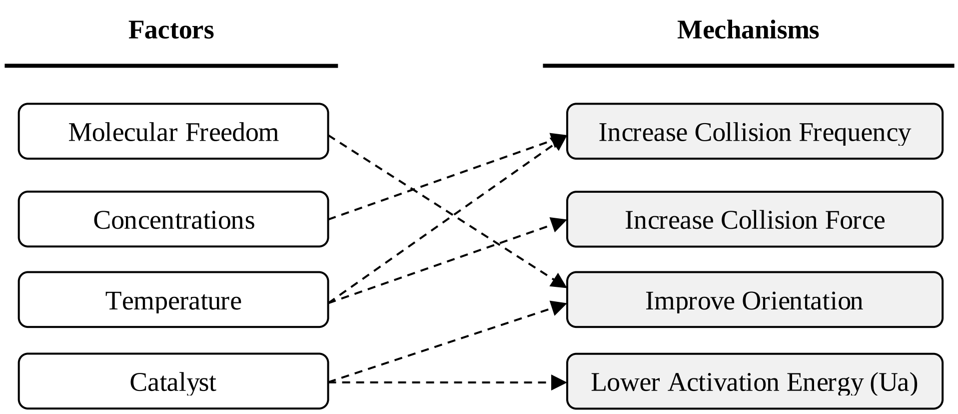


Figure 8. Chemical Reaction Factors

4.2 Chemical System Model

Chemical reactions depicted in Figure 7 provide a foundation for building a conceptual model of emergents. Models are abstractions of reality that can be instrumental in understanding systems and their behavior. The Modeling and Simulation-System Development Framework (MS-SDF), proposed by Tolk et al. (2013) provides a methodology for the design and construction of models to study phenomena. MS-SDF is used to develop models of emergents in chemical systems.

4.2.1 Chemical Reaction Reference Model

A set of claims, assumptions, and constraints are constructed from the definitions and discussion of chemical reaction concepts (see). Claims are statements explicitly stated by the laws and axioms that govern the processes; assumptions are not explicitly stated but a logical conclusions based on combinations of claims; and constraints are statements that define the boundaries of the system being studied.

Characteristics	**Claims, Assumptions, Constraints**
Chemical systems are hierarchal structures	Claim
Chemical system exchange energy with its environment.	Constraint
The net change in them sum of system energy and environment energy is always zero.	Claim
Emergent properties are the macro properties of the system that are different from the properties of its micro components.	Assumptions
Properties of the products produced by chemical reactions are different from the properties of the substances in the chemical system before the chemical reaction.	Claim
Change in internal energy (ΔU) ≈ change in enthalpy (ΔH) under constant pressure.	Claim

Table 10. Chemical Reaction Reference Model

Table 10 (continued)

Chemical systems produce products with emergent properties when the change in enthalpy (ΔH) > the difference between the activation energy (U_a) point and the initial internal energy (Ui) of the system.	Claim
Enthalpy (H) > 0 indicates the environment transferred heat to the chemical system.	Claim
Enthalpy (H) < 0 indicates the chemical system transferred heat to the environment.	Claim
Enthalpy (H) > 0 indicates the entropy (disorder) in the system is increasing.	Claim
Enthalpy (H) < 0 indicates the entropy (disorder) in the system is decreasing.	Claim
Interaction between chemical system components increases as heat is transferred to the system.	Claim
Chemical reactions increase by changes in concentration, temperature, molecular freedom, or catalytic volume.	Claim
Chemical reactions increase as a non-linear function of concentration if the chemical substances reaction order is >1; otherwise reaction increases as a linear function.	Claim
Chemical reactions increase as a non-linear function of temperature.	Claim
Chemical reactions increase as a linear function of molecular freedom.	Claim
Chemical reactions increase as a non-linear function of catalytic volume.	Claim
Chemical systems eventually return to equilibrium when there are no changes in concentration, temperature, molecular freedom, and catalytic volume.	Claim

Table 10 (continued)

Chemical reaction is occurring in an open system under constant pressure with insignificant or no pressure (P) × volume (V) work component in the total energy of the system.	Assumptions
Substances vary in their ability to lower the activation energy of a chemical system without becoming part of the products produces by the chemical reactions.	Assumptions
The more freedom of motion the molecules in the substances of a chemical system have, the more likely they are to be properly aligned and produce a chemical reaction.	Claim
The greater the restriction in movement of the molecules in the substances, the in a chemical system the less likely they are to be properly aligned and produce a chemical reaction.	Assumption
Certain additional substances (catalyst) can reduce the required activation energy of a chemical reaction without changing the end product.	Claim
Rate of reaction tends to decline during the chemical reaction as the concentration of reactants to products declines.	Claim
Rate of enthalpy change = rate of chemical reaction as change in enthalpy depends on the amount of material that under goes change in the chemical reaction.	Assumption

4.2.2 Modeling Question for Chemical System

Thermochemistry is being used a medium of study to address the dissertation research question. As such, the following modeling question is formulated study emergence in a chemical system (i.e., a thermodynamic system):

What are the factors in chemical systems that cause a chemical reaction and affect the occurrence of emergents?

4.2.3 Conceptual Model for Endothermic Reactions in Chemical Systems

Conceptual models capture a consistent sub-set of the reference model that can be implemented in a simulation. A subset from the reference model in form the basis for developing a conceptual model in the form of a causal loop diagram (CLD). CLDs are a System Dynamic modeling concept that represents the causal relationships between system variables, and graphically depicts the behavior of the system (Sterman, 2000). They are especially relevant to the modeling question in this paper given that the essence of the research question concerns causal relationships. The variables for the chemical reaction CLD are defined in Table 11.

Variable Name and Definition	Symbol	Relationship: (+) = Increase; (-) = Decrease
Activation Energy: Minimum energy required to cause a chemical reaction.	Ua	+Ua →+ ΔHtp
Catalytic Volume: Amount of substance in a chemical system that lowers the activation energy but does not react with the other substances.	Vc	+Vc→-Ua

Table 11. CLD Variables and Behaviors for Chemical reactions

Table 11 (continued)

Concentration: Volume of a substance relative to total volume of substances.	C	+C→+Rr
Energy Differential: Available heat to transfer from the environment to the system	Qe	+Qe →+ Rr
Energy Transferred Gap: The remaining heat energy that was available to be received (Ue-Ui) but not absorbed by the system.	Qg	+Qg→-Xr
Energy Transferred: Heat energy transferred from the system to the environment.	Qs	+Qs →-Qg
Enthalpy Change: Change in system total energy.	ΔH	+ΔH→+ER
Enthalpy Ratio: The fraction of the tipping point that the system has reached for chemical reaction to occur	ER	+ER → -Xr
Enthalpy Tipping Point: Difference between the Activation Energy (Ua) and Initial Internal Energy (Ui).	ΔHtp	+ΔHtp→- Hr
Initial Internal Energy: Internal energy of the system at $t=t_0$	Ui	+Ui→ -Qg, -ΔHtp
Internal Energy: Internal energy of the system at $t >t_0$.	U	+U →+Rr, +Xr
Molecular Freedom: Ability to move and change orientation.	F	+F→+Rr
Receptions Rate: Amount of energy flowing into the system from the environment per unit of time.	Rr	$+R_r$→ +ΔH
Receptions Time: The fractional amount of time over which energy is absorbed (received and retained) by the system.	Rt	+Rt→- Rr
Temperature: Average heat energy in the system.	Ts	+ T_S→+ Rr
Xfer (Transfer) Rate: Amount of energy flowing into the system from the environment per unit of time.	Xr	+Xr→-U
Xfer (Transfer) Time: The fractional amount of time over which energy is transferred from the system to the environment.	Xt	Xt→- Xr

The structure of a system determines its behavior (Sterman, 2000). The Vensim modeling & simulation software provided a system of logic to structure CLD (Ventana Systems, 2016). The CLD represent the structure by using (+) signs on arrows to indicate that the originating variable causes a positive change in the variable at the end of the arrow. A negative (-) signs indicates that the originating variable causes a negative change in the variable at the end of the arrow. Based on the variables and causal behaviors in, a CLD for endothermic reactions has been constructed and is depicted in Figure 9.

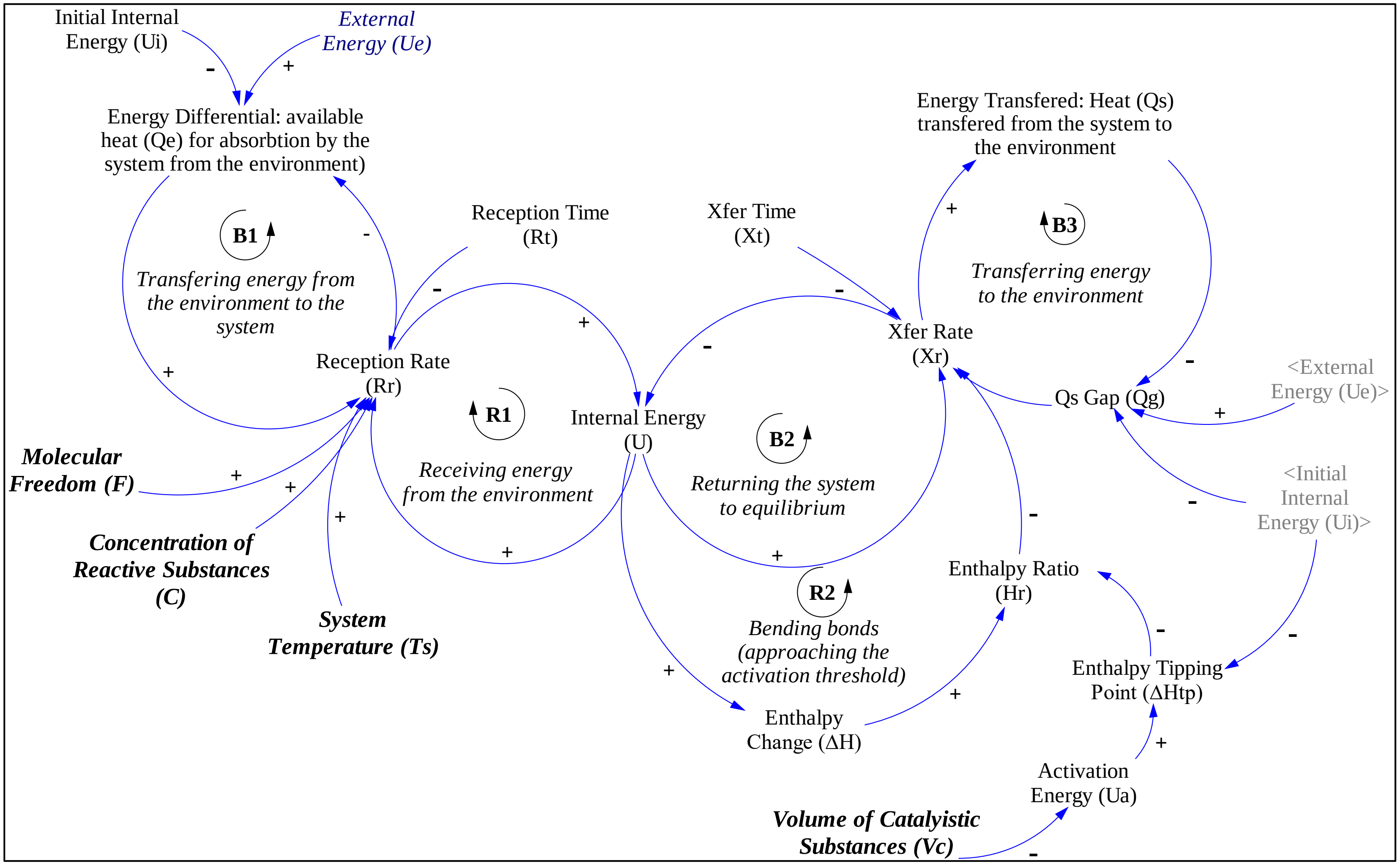


Figure 9. Conceptual Model of Endothermic Chemical Reactions

The CLD is best understood by examining each causal loops in isolation. A causal loop is a continuous sequence of variables connected by arrows. Loops that reinforce behavior are indicated with the letter R in a circular arrow. Loops that provide balance and prevent the continuous growth of a behavior are indicated with the letter B in a circular arrow.

- **B1, Transferring energy from the environment to the system.** The chemical reaction process begins with an input from an external energy source (Ue): a new substance, another chemical system, exposure to a heat source, etc. The energy differential (Qe) between the system's initial internal energy (Ui) and the external energy source (Ue) is the amount of energy that is available to be transferred to the system. The system requires a certain amount of time to receive each fraction of energy (i.e., absorption time). The greater the differential and the shorter the absorption time (At), the faster the rate of absorption (Ra). Ra increases with increases in concentration (C), molecular freedom (F), and system temperature (T). Given enough time and without the continuous addition of more energy from an external source, the system will receive all available energy, and the energy differential will reduced to zero.
- **R1, Receiving energy from the environment.** When the chemical reaction begins at time (t) =0, the energy differential (i.e., the potential energy to be absorbed) is at its maximum; internal energy (U) is not changing, i.e., change in enthalpy (ΔH) is at its minimum; and the system is in an initial state of equilibrium (energy absorbed =energy transferred and $\Delta H = 0$). During the chemical reaction the system receives the energy differential (Qe) causing

increases in the system's internal energy (U) such that the system is no longer in equilibrium (energy absorbed ≠ energy transferred and $\Delta H \neq 0$). The greater the energy differential the greater the internal information growth in magnitude (ΔH) and rate (Ra). The increasing internal information and ΔH continues to grow and grow faster until there is no energy differential to absorb.

- **R2, Bending bonds (approaching the activation threshold)**. As the energy differential continues to be absorbed by the system, the enthalpy change (ΔH) approaches the tipping point required for a chemical reaction to occur. ΔH approaching the tipping point (ΔHtp) indicates that the bonds between the molecules maintaining the current configuration of the chemical system are bending. If $\Delta H > \Delta Htp$, i.e., the enthalpy ratio (ER) >1, the bonds will break, and a chemical reaction will occur. If the internal energy (U) does not reach the activation threshold (Ua), ΔH will be $<\Delta Htp$, Hr will be < 1, and a chemical reaction will not occur.
- **B2, Returning the system to equilibrium**. The chemical system receives and transfers energy. Initially the R1 loop is dominant and the system is receiving more energy than it transfers (i.e., ΔH is increasing). A tipping point will occur where the system will begin to transfer more energy than it absorbs. At that point dominance will shift to the B2 loop where ΔH and the system internal energy will decline until the system returns to equilibrium. For each fraction of energy, a certain amount of time to transfer (Xfer) to the environment is required to complete the chemical reaction and return the system to equilibrium. The rate of

energy that transfers (Xfers) out of the system as it returns to equilibrium is the Xfer rate (Xr).

- **B3, Transferring energy to the environment.** Chemical systems will receive information as they interact with their environment and other chemical systems. Initially the gap between the available energy to be receive and the energy transferred back to the environment is large and the transfer rate (Xr) of energy back to the environment is high. If the enthalpy tipping point (ΔHtp) is not reached, enthalpy ratio (Hr) will be < 1, and the chemical reaction will not occur. The system will continue to transfer energy back to the environment until the gap between energy transferred and available energy to be received is zero (Qg = 0 at t_x) and the interaction ends. However, if the peak of ΔH > ΔHtp, Hr will be > 1 and a chemical reaction will occur. If a chemical reaction occurs some of the available energy will be absorbed by the system and the balanced will be transferred back to the environment, i.e., Qg>0 at $t_{x.}$ The addition of catalytic substances (Vc) can lower the activation threshold (Ua) and increase the likelihood that ER will be > 1 between t_1 and t_x.

The conceptual model for chemical reactions in chemical systems is used in chapter five to develop a theory of emergence in engineered systems.

CHAPTER 5

THEORY DEVELOPMENT

In the chapter Three, a literature review, theories and definitions of emergence are summarized in terms of their common classes and subclasses of an ontology (see Figure **5**) Based on the ontology, operational definitions of emergents (the noun) and emergence (the verb) in the physical domain are proposed:

a) *Emergents are system effects that are approximately underivable based on system components and their interrelationships.*

b) *Emergence is the action of producing system effects that are approximately underivable based on system components and their interrelationships.*

The concept of emergence in the context of engineered systems was also explored. System states in the undesignable state space were shown to be underivable in terms of system components and their relationships, and are therefore emergent. However, there is currently no theory that defines the set of factors in engineered systems that affect the occurrence of emergents. In Chapter Four, a modeling methodology (MS-SDF) was used to: a) construct a reference model of what is known and assumed about chemical reactions; and b) construct a conceptual model that defines the relationships of the system variables leading to endothermic reactions in chemical systems.

An initial theory of emergence in engineered systems is now developed in chapter five. Analogies between endothermic chemical reaction and emergence in engineered systems are used to transferring knowledge about the factors affecting chemical reactions to identify factors in engineered system that affect emergence. Analogical reasoning is used to build a conceptual model for emergence in engineered systems based on the conceptual model of endothermic chemical reactions. A theory of emergence in engineered system is then derived from its conceptual model.

5.1 Analogical Reasoning

Analogies are basically explanations about entities or phenomena based on knowledge from a different domain (Bartha, 2010; Gentner, 1983). Analogical reasoning is the process of drawing inferences using analogies. Analogies are effective mechanisms for advancing knowledge. They are an essential aspect in discovering meaningful scientific theories and have been used in a variety of applications: Particle Physics (Nambu & Jona-Lasinio, 1961); Artificial Intelligence (Eremeev & Varshavsky, 2005); Engineering Design (Kalogerakis et al., 2010); Electrical Engineering (Li, 2012); Telecommunication (Martinez & Carmen, 2012); Biometric Engineering (Cheong, 2013); Shared Awareness (Kovacic, 2013); Information Systems (Jog, 2015). In each of these examples, knowledge from a source domain was transferred to a target domain and used to draw conclusions and make inferences. A detailed discussion on analogical reasoning is provided in the methodology section.

As discussed in Chapter One, thermochemistry has broad applicability as a source of analogies to explain concepts; a well-established precedence in explanations of emergence; and general correspondence between characteristics of engineered systems. However, a valid transfer of knowledge between domains requires more formal justification. The transfer of knowledge between domains is possible when there is correspondence between the relevant structural elements of the domains. The structure of a domain includes the: properties; relationships; patterns; constraints; roles; and concepts that characterize the objects in the domain. Transferring knowledge from a source domain to a target domain is valid to the extent there is correspondence between the relevant domain elements. A summary of basic rules and assumptions for structural mapping are listed in Table 5.

Criteria	Description	Source
Domains	System of objects, attributes of objects, and object relationships.	Gentner (1983)
Domain Knowledge	Represented with predicate logic; a system of clauses that describe objects in the domain. Predicates are: a) attributes when the argument is a single object; b) relationships when the argument is two or more objects.	Gentner (1983)
1 to 1 Mapping	Elements in one domain must correspond to a single element in another domain.	Gentner & Markman (2006)
Parallel Connectivity	If two predicates correspond their arguments must also correspond.	Gentner & Markman (2006)
Pragmatic	Only those elements in the domains that are relevant to the purpose of the analogy is considered in the structural mapping.	Gentner (1983)
Semantics	Predicate describing structural element must have similar meaning but do not have to be identical.	Gentner (1983)
Systematicity	Highest preference is given to structural elements that have causal, mathematical, or other functional implications.	Gentner (1983); Lee & Holyoak (2008)

Table 5. Structural Mapping Criteria

Analogies are not absolute; they exist on a continuum from weak to strong. The more an analogy fits the structural mapping criteria the stronger the analogy and the stronger case for applying analogical reasoning. This is especially true for the Systematicity criteria for structural mapping. Correspondence between functional elements of a domain makes the greatest contribution to establishing the relationships as a strong analogy. Formally stated, the proposition for the theory of the scientific analogy is: if the structural components B= {b1, b2, b3,…bn} of system B describe the relationships and attributes of the parts in system B, can be mapped to structural components T= {t1, t2, t3, ….tn} of system T; then knowledge about system B can be used to explain system T. The conclusions holds to the extent that the structural components in the mapping are relevant to the phenomena or entity to which the knowledge is being applied (i.e., they satisfy the pragmatic criteria for structural mapping).

5.1.1 Structural Mapping

Analogies are used to explain emergence in engineered system. Given this purpose, the ontology of emergence provides a rational framework for identifying the relevant structural elements of the domains for structural mapping. Recall from Section 3.1 that there are two classes and eight subclasses that define emergence: Phenomena Characteristics (Type, Perspectives, Logical Relationships, Indicators); and System Characteristics (Structure, Temporality, Knowledge Constraint, Domain). The source domain for knowledge in the analogy is endothermic reactions in chemical systems. The target domain for applying the knowledge is emergence in engineered systems.

Elements from the source and target domains are defined for each of the seven subclasses of the emergence ontology. Each element is defined with a predicate logic statement:

- Attribute statements (A) define a property or characteristic for a single one element or group of elements.
- Relationship statements (R) defines the cause-effect interaction between two or more elements or groups of elements :

For example, Temporality is a subclass the ontology of emergence. Engineered systems and chemical system both change over time. Therefore the predicate statements would be chemical system =CHANGE (over time [chemical system]) and engineered system =CHANGE (over time [engineered system]). In this case both predicate statements are attributes and there is correspondence between the domains.

The matrix in Figure 10 captures the mapping between the domains for endothermic reactions in a chemical systems and emergence in an engineered systems.

A = Attribute
R = Relationship

Target: Emergence in Engineered Systems

Base: Endothermic Chemical Reaction in Chemical Systems

Ontology of Emergence			Base \ Target	DETERMINED intrinsicly (engineered system, emergence)	RESULTS in (emergence [patterns, structures, qualities, behaviors])	¬ DERIVED from (effects, components)	EXIST in (physical domain [engineered system])	CHANGES (over time [engineered system])	INTERACT with (hierarchal [components], environment)	CAUSED by (insufficient[experience, observation, laws	INCREASING (probility [microstate, other macrostates])	INCREASING in proportion to (Shannon's entropy, emergence)
Ontology of Emergence	*Phenomena Characteristics*	*Perspective*	DETERMINED intrinsicly (chemical system, chemical reaction)	R								
		Type	RESULTS in (chemical rection [patterns, structures, qualities, behaviors])		R							
		Logical Relationships	¬ DERIVED from (effects, chemical substances)			R						
	System Characteristics	*Domain*	EXISTS in (physical domain [chemical system])				A					
		Temporality	CHANGES (over time [chemical system])					A				
		Structure	INTERACT with (hierarchal [components], environment)						R			
		Knowledge Constraint	CAUSED by (insufficient[experience, observation, laws)])							R		
	Quantitative Characteristics	*Indicators*	INCREASING (number of [final microstates, initial microstates)])								R	
			INCREASING in proportion to (Boltzmann's entropy, chemical reaction)									R

Figure 10. Structural Mapping Matrix for Chemical System vs Engineered Systems

One of the semanticity elements belongs to the indicator subclass of the emergence ontology. In addition to mapping the predicate statements for the indicator elements, graphical representations are depicted in Figure 11.

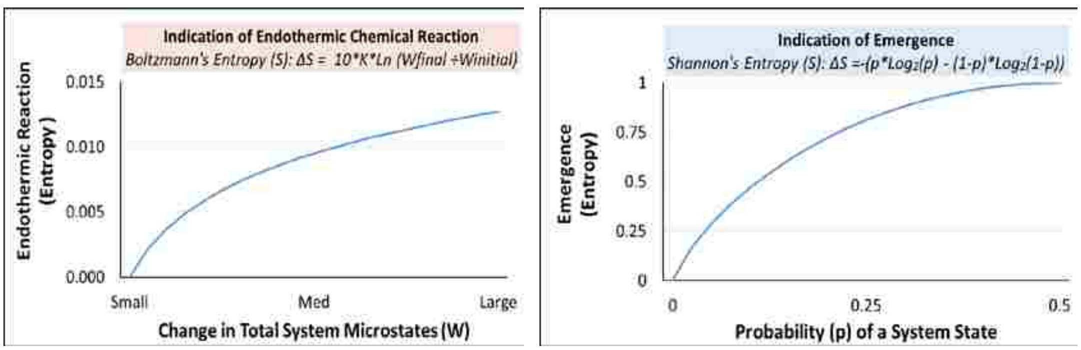


Figure 11. Indicators of Endothermic Reactions and Emergence

Increasing entropy is an indicator of endothermic reactions (Brown et al., 2014), and is also an indicator of emergence (Crutchfield, 1994; Holland, O.T. 2012; Johnson IV, 2013). While the formulas are different, conceptually they represent the same concept of entropy as a measure of disorder and uncertainty.

5.1.2 Valid Basis for Theory Development

Analysis of the structural mapping matrix indicates that: 1) There is correspondence between the domains. Each structural element in the endothermic reaction domain has a predicate and argument that maps directly to a predicate and argument in the emergence in engineered systems domain (i.e., one-to-one relationship). 2) There is coherence with all requirements of the structural mapping criteria in Table 5; 3) The majority (7/9) of the elements have causal, functional or mathematical relationships; which are the most important types of structural elements (i.e., the systematicity mapping criteria in Table 5). It is concluded that analogies from the domain of endothermic reactions in chemical systems would be strong and a valid source for knowledge transfer to then domain for emergence in engineered systems. In the next sections, specific analogies are developed between the causes of endothermic reactions and analogous factors in engineered systems.

5.1.3 Structural Mapping for Causal Factors

Some elements in the system structure have trivial differences between chemical and engineered systems and do not require an extensive mapping and analogical reasoning:

- **Volume** or number of substances in a chemical system is equivalent to the quantity or number of a component(s) in an engineered system.
- **Concentration** is the amount of one or more items relative to the total number of items in the system. Greater concentration results in great number of contacts or interaction. The concentration concept is the same for substances in a chemical system and components in engineered system
- **Time** in chemical systems is exactly the same as time in an engineered system.

There are other structural concepts in chemical systems that are non-trivial and require scientific analogies to transfer knowledge about the behavior of the chemical system to the engineered system. System engineering concepts were identified that have functional similarities to the causal factors in endothermic reactions. The analogical reasoning method was used to establish analogies and make inferences about cause-effect factors in engineered systems. The analogous relationships are: 1) energy vs information; 2) temperature vs. interoperability; 3) molecular freedom vs component degrees of freedom; and 4) volume of catalyst vs variety of regulators. Scientific analogies for these concepts are discussed in the following section. The analogies are defined by functional descriptions of the elements in the source domain (causal factors for endothermic reactions), and target domain (engineered systems).

5.1.4 Energy vs Information

Source Domain: Properties of a chemical systems are a function of the configuration of its molecules (i.e., its parts). Chemical systems exchange energy when they interact with other systems. Energy is the capacity to make a change in an entity's spatial position relative to other entities (i.e., configuration), and to change its capacity to transfer heat.

Predicate statements:

1) CAUSE (molecular configurations, system properties)
2) EXCHANGE energy (molecules, external systems, environment)

Target Domain: Beer (1979) defines information as actionable interpretation of data that causes a change in the systems state; where data is a statement of fact about a person, place or thing. Sunik (2011) defines information as the value of a variable in an algorithm that determines the "changes and movements" (i.e., the configuration) of components. The configuration of components in a system determine it properties. The change determined by the variables in the algorithm are actions that causes a system to have form, content, direction, nature, etc. (i.e., properties) that it would otherwise not have if the object were left undisturbed. Deacon (2007) defines information in context of regularly occurring processes and exchanges between entities as they interact with each other.

Predicate statements:

3) CAUSE (component configurations, system properties)

4) EXCHANGE information (components, external systems, environment)

5.1.5 Temperature vs. Interoperability

Source Domain: Energy in a chemical system is heat. Heat is the energy that causes a change in the temperature (T) of the system. A positive change in temperature increases the rate of the chemical reaction between systems by increasing the frequency and force at which molecules in the chemical system collide; which causes bonds between molecules in the system to break and eventually reconfigure and produce new system properties.

Predicate statements:

5) INCREASE [INTERACTION (molecules, external systems, environment)]

6) CAUSE (new molecule configurations, new system properties)

Target Domain: Interoperability is “the ability of two or more systems or elements to exchange information and to use the information that has been exchanged” (IEEE, 2000, as cited in Morris et al. (2004); Tolk, et al. (2003). Interoperability is accomplished by establishing a common understanding of the information used by the participants in the exchange. Greater interoperability leads to more interactions and information exchange. The consequence of higher levels of interoperability and the successful exchange of information is a change in systems state, and the acquisition of new system functions/ capabilities (i.e., new system properties).

Predicate statements for interoperability in an engineered system:

7) INCREASE [INTERACTION (components, external systems, environment)]

8) CAUSE (system states, new system properties)

5.1.6 Molecular Freedom vs Component Degrees of Freedom

Source Domain: Substances in a chemical system can take on one of four physical states (or types): solid, liquid, gas, or plasma. The physical state of substances influence the freedom of movement among its molecules. The greater the molecular freedom of movement the more likely the molecules will collide in the required orientation to facilitate the exchange of energy, the breaking of bonds, and the forming of new configurations (i.e., a chemical reaction).

Predicate statements:

9) INCREASE [EXCHANGE (molecules, systems, environment)]

10) CAUSE [FORM (new molecule configurations, new system properties)]

Target Domain: There are many types of components in an engineered system, including but are not limited to hardware, software, people, equipment, and processes. The components are differentiated by the number of variables that define them. The degrees of freedom (or distinct number of possible states) for the system is a function of the number of component types, and the number of variables per component (Ashby, 1956). Systems exchange information (i.e., communicate) by sending and receiving messages. Each message has distinct possibilities based on a function of variables that determine its meaning. The successful exchange of information exist to the extent the system or component receiving the message has degrees of freedom that are equal to or greater than the degrees of freedom for the message being sent.

Predicate statements:

11) INCREASE [EXCHANGE (components, external systems, environment)]

12) CAUSE (new system states, new system properties)

5.1.7 Volume of Catalyst vs. Variety of Regulators

Source Domain: Increasing the volume of certain substances (catalyst) lowers the activation energy (Ua) threshold required to cause a chemical reactions. As the threshold is approached, there are more interactions between the molecules in the chemical system and between the system and its environment (or other systems). This increased interaction causes energy to be exchanged and the rate (i.e., speed) of chemical reaction to grow exponentially. As a function of reductions in Ua, Catalyst cause the likelihood of a chemical reaction to increase, and new system configurations and properties to form.

Predicate statements:

13) CAUSE [EXCHANGE (molecules, external systems, environment)]

14) CAUSE (new molecule configurations, new system properties)

Target Domain: Some components in engineered systems act as regulators that limit the results (i.e., states) of system and component interactions by blocking the flow of information. Ashby's (1956) law of Requisite Variety basically states that "… only variety can destroy variety". Variety is the number of distinct possibilities. The variety of outcomes is limited (i.e., regulated) to the extent that the variety of the regulator (Vr) is greater than the variety of the inputs. Requisite variety influences the occurrence of new system states and properties by essentially creating a threshold beyond which the variety of a transmitted information message must exceed in order to have a successful exchange of information and change in system state. In other words the greater (Vr) is relative to the variety of inputs, the lower the variety or number of possible system states; and the lower (Vr) is relative to the variety of inputs the greater the number of possible system states.

Predicate statements:

15) CAUSE [EXCHANGE (components, external systems, environment)]

16) CAUSE (new system states, new system properties)

5.1.8 Analogies for Causal Factors

Analogies of causal factors for endothermic reactions and engineered systems can be formally represented by mapping their structures using the predicates statements from the previous sections. An analogy is stated and a supporting structural map is presented in Table 12 for four structural concepts of chemical and engineered systems: 1) energy vs. information; 2) temperature vs, interoperability; 3) molecular freedom vs. component degrees of freedom; and 4) volume of catalyst vs. variety of regulators.

Analogy	2nd Order Predicate	1st Order Predicate	Chemical System Arguments	Engineered System Arguments
1) Information is like energy.		CAUSE	molecule configurations, system properties	components, system properties
		EXCHANGE	molecules, external systems, environment	components, external systems, environment
2) Interoperability is like temperature.	INCREASE	INTERACTION	molecules, external systems, environment	components, external systems, environment
		CAUSE	new molecule configurations, new system properties	new system states, new system properties
3) Degrees of freedom is like molecular freedom.	INCREASE	EXCHANGE	molecules, external systems, environment	components, external systems, environment
		CAUSE	new molecule configurations, new system properties	new system states, new system properties
4) Variety of regulators is like volume of catalyst.	CAUSE	EXCHANGE	molecules, external systems, environment	components, external systems, environment
		CAUSE	new molecule configurations, new system properties	new system states, new system properties

Table 12. Structural Mapping for Engineered to Chemical System Analogies

An analysis of the mapping in for the Engineered to Chemical system analogies indicates that there is: 1) correspondence between the domains; 2) coherence to the structural mapping criteria in Table 5; and 3) the majority of the mapping elements have causal or mathematical relationships. Based on these observations it is valid to conclude that the analogies are strong. The analogies established between chemical and engineered systems provide the justification for transferring knowledge about behaviors between the two domains. The author posits that an initial theory of emergence in engineered systems can be constructed from the behaviors depicted in the conceptual model for endothermic reactions in chemical systems (Figure 9 causal loop diagram).

5.2 Conceptual Model for Emergence in Engineered Systems

In chapter four, chemical reactions were used to explain endothermic reactions in chemical systems. Analogical reasoning is used to define the chemical reaction CLD variables () in terms of engineered system variables (). The variables are listed in alphabetical order of engineered system variables.

Chemical System Variables	Engineered System Variable	*Variable Type	Relationship: (+) = Increase; (-) = Decrease
Activation Energy (Ua): Minimum energy required to cause a chemical reaction.	**Activation Information Threshold (Ia):** Minimum information required to cause emergence in an engineered system.	Initial Value Constant	+Ia →+ ΔItp
Catalytic Volume (Vc): The amount of substance in a chemical system that lowers the activation energy but does not react with the other substances.	**Variety of Regulators (Vr):** The degrees of freedom for components that regulate outputs / states / behaviors of other components.	State Constant	-Vr→-Ia
Concentration (C): The additional volume of a substance relative to total volume of substances.	**Component Concentration (Cc):** The additional volume of a component relative to total volume of components.	State Constant	+Cc→+Rr
Energy Differential (Qe): Available heat to transfer from the environment to the system	**Information Differential (Id)**: Available information for transfer from the environment to the system.	Stock	+Id →+ Rr
Energy Transferred (Qx): Heat energy transferred from the system to the environment.	**Information Transferred (Ix):** Information transmitted from the system to the environment as the system returns to steady state.	Stock	+Ix →- Xr

Table 13. CLD Variables for Emergence in Engineered Systems

Table 13 (continued)

Energy Transferred Gap (Qg): The remaining heat energy that was available to be received (Ue-Ui) but not absorbed by the system.	**Information Transferred Gap (Ig)**: The remaining information that was available to be received (Ie-Ii) but not absorbed by the system.	Auxiliary	+Ig→-Xr
Enthalpy Change (ΔU): Change in system total energy	**Information Change (ΔI):** Change in system total information.	Auxiliary	+ΔI→+IRE
Enthalpy Ratio (Hr): The fraction of the tipping point that the system has reached for chemical reaction to occur	**Information Ratio of Emergence (IRE):** The fraction of the tipping point that the system has reached for chemical reaction to occur	Auxiliary	+IRE→-Xr
Enthalpy Tipping Point (ΔHtp): The difference between the Activation energy (Ua) and Initial Internal Energy (Ui).	**Information Tipping Point (ΔItp):** The difference between the Activation Information Threshold (Ia) and Initial Internal Information (Ii)	Auxiliary	+ΔItp→- IRE
External Energy (Ue): Energy that exist outside of the system	**External Information (Ie):** Information that exist outside of the system	Initial Value Constant	Ie→+Id
Initial Internal Energy (Ui): Internal energy of the system at $t=t_0$	**Initial Internal Information (Ii):** Internal energy of the system at $t=t_0$	Initial Value Constant	+Ii→ -Ix, -ΔItp

Table 13 (continued)

Internal Energy (U): The system's total energy at t >t_0.	**Internal Information (I):** The system's total energy at t >t_0.	Stock	+I →+Rr, +Xr
Molecular Freedom (F): Ability to move and change orientation.	**Degrees of Freedom (Df)**: Ability of components to move and change orientation.	State Constant	+Df→+Rr
Reception Rate (Rr): The amount of energy flowing into the system from the environment per unit of time.	**Reception Rate (Rr)**: The amount of information flowing into the system from the environment per unit of time.	Flow	+R_r→ +ΔI
Reception Time (Rt): The amount of time over which energy is absorbed (received and retained) by the system.	**Reception Time (Rt)**: The fractional amount of time over which information is absorbed (received and retained) by the system.	Time Constant	+Rt→**-** Rr
Temperature (T): Average heat energy in the system	**Interoperability (Int):** The degree that the system can exchange (absorb /transfer) both quantity and quality of information.	State Constant	+ Int→+ Rr
Xfer (Transfer) Rate (Xr): The amount of energy flowing into the system from the environment per unit of time.	**X-mission Rate (**Xr**):** The amount of information flowing from the system to the environment per unit of time.	Flow	+Xr→**-**ΔI

Table 13 (continued)

Xfer (Transfer) Time (Xt): The amount of time over which energy is transferred from the system to the environment.	**X-mission (Transmission) Time (Xt)**: The fractional amount of time over which information is transferred from the system to the environment.	Time Constant	+Xt→- Rr

* Variable Type is related to the simulation model discussed in Section 6.1.3

The structure of a system determines its behavior (Sterman, 2000). The causal loop diagram (CLD) provides a logical structure for the system by using (+) / (-) signs on arrows to indicate the direction of the causal relationship of the variable joined by the arrows. Based on the variables and causal behaviors in, a CLD for emergence in engineered system has been constructed and is depicted in Figure 12 .

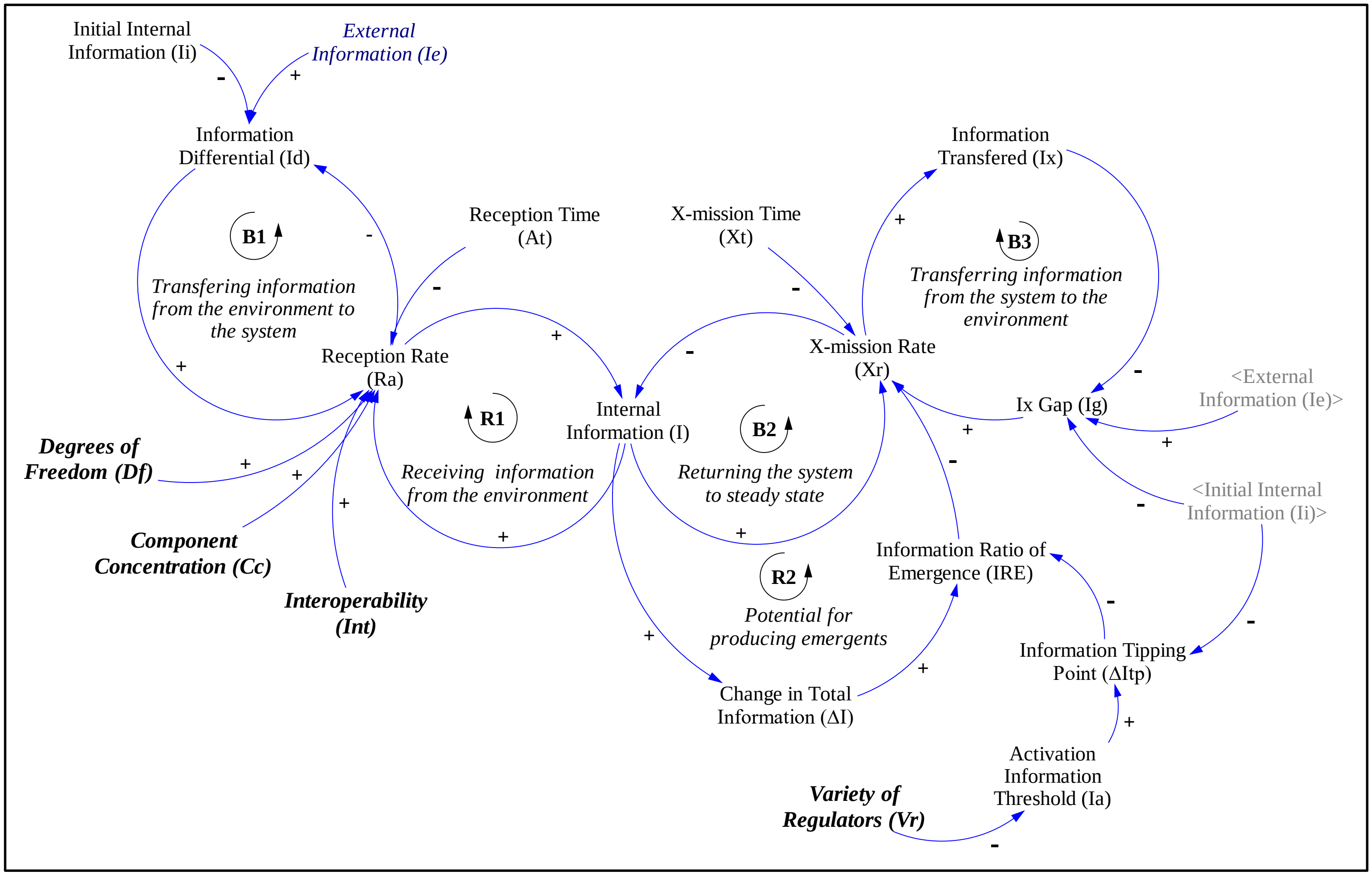


Figure 12. Conceptual Model of Emergence in Engineered Systems

The variable relationships described in and the CLD in in Figure 12 yield several formulas that provided additional insight into concepts of behavior in the engineered system:

- The Activation Information Threshold (Ia) is the amount of information required to cause the interactions in the engineered system to have an emergent effect. The difference between the engineered system's Initial Internal Information (Ii) and the required threshold (Ia) is the Information Tipping Point (ΔItp).

$$\Delta Itp = Ia - Ii \qquad [5.1]$$

- The information Ratio of Emergence (IRE) is an indicator that there has been a sufficient change in the system's Information (ΔI) to cause an emergent effect. A sufficient change would be Maximum ΔI > than the Information Tipping Point (ΔItp).

$$IRE = Max\ \Delta I \div \Delta Itp > 1 \qquad [5.2]$$

- The External Information (Ie) is the information that is available to be received by the engineered system. The maximum change that can occur in the engineered system's total Information (Max ΔI) is limited by the amount of external information that is available in excess of the system's Initial Internal Information (Ii).

$$Max\ \Delta I = Ie - Ii \qquad [5.3]$$

- From Equations [5.1], [5.2], and [5.3] it is determined that emergent effects are dependent on the relationship between the external Information available to be received by the engineered system (Ie) and the threshold requirement to cause an emergent effect (Ia). The relationship between (Ie) and (Ia) is defined by using equations [5.1] and [5.3] to make substitutions in equation [5.2]:

$$IRE = \text{Max } \Delta I \div \Delta Itp \qquad [5.2]$$

$$IRE = \text{Max } \Delta I \div \Delta Itp > 1$$

$$(Ie - Ii) \div (Ia - Ii) > 1$$

$$e - Ii > Ia - Ii$$

$$Ie > Ia$$

The relationship between (Ie) and (Ia) will be referred to as the Activation Ratio for Information (ARI):

$$ARI = Ie \div Ia \qquad [5.4]$$

- As the system is receiving information it is also transferring it. If the system receives information faster than it transfers, the change in information (ΔI) will be positive. ΔI will occur at a faster rate to the extent that the fractional Reception Time (Rt) is greater than the fractional X-mission time (Xt). The Reception to X-mission multiple (RXM) is defined by equation [5.5].

$$RXM = Rt \div Xt \qquad [5.5]$$

In the next section, an initial theory of emergence in engineered systems is derived based on: variable relationships described in; the conceptual model depicted by the CLD in Figure 12; and the conceptual formulas [5.1] - [5.5].

5.3 A Proposed Theory of Emergents in Engineered Systems

Operational definitions of emergents and emergence in the physical domain are derived from the ontology developed in Chapter three and Appendix A are:

a) *Emergents are system effects that are approximately underivable based on system components and their interrelationships.*

b) *Emergence is the action of producing system effects that are approximately underivable based on system components and their interrelationships.*

The casual loop diagram in Figure 12 is a conceptual model and provides a system of logic by which propositions about emergence in engineered systems can be constructed. The propositions in Table 14 are claims about the factors and behaviors of systems where emergent effects are produced. The statements are supported by the logical structure of the conceptual model and associated formulas.

	Propositions for Emergence in Engineered Systems
1)	As the Information Ratio of Emergents (IRE) approaches 1, the probability of emergence increases.
2)	Activation Ratio for Information (ARI) = External Information (Ie) ÷Activation Information Threshold (Ia) >=1 is a necessary condition for IRE>=1 (i.e., emergence to occur).
3)	As the Information Ratio of Emergents (IRE) approaches 1, emergent effects occur faster.

Table 14. Theoretical Propositions for Emergence in Engineered Systems

The main conclusion from the conceptual model and propositions is, emergent effects will occur in engineered systems if there is a sufficient change in the total information in the system (ΔI). A sufficient change would be ΔI > Information Tipping Point (ΔItp). The Activation Ratio for Information (ARI) is a measure of the available information to increase ΔI relative to the information tipping point threshold (ΔItp). Basically, increasing ARI will increase the magnitude of ΔI. Attributes of the system that affect effect how fast ΔI increase are: the Reception to X-mission Multiple (RXM); component degrees of freedom (Df); and component concentration (Cc); and component interoperability (Int). Another system feature affecting the occurrence of emergence is the variety of regulators (Vr) which has a proportional effect on the information activation threshold (Ia). Decreasing Vr will in turn decrease the magnitude of the required information tipping point (ΔItp).

With these relationships in mind a tree diagram is constructed in Figure 13 that captures causal factors of emergent effects in engineered systems.

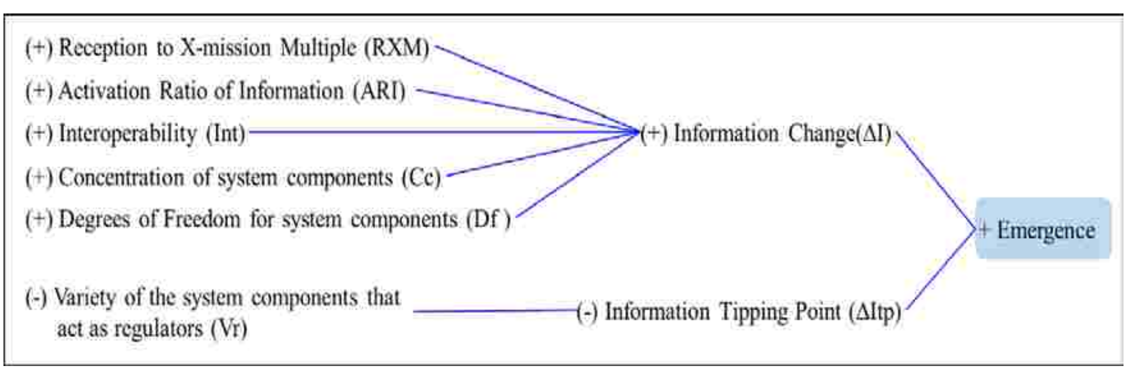


Figure 13. Causal Tree of Factors for Emergent Effects in Engineered System

The transition to emergents in engineered system is defined by the information ratio of emergence (IRE).

$$IRE = \Delta I \div \Delta Itp \qquad [5.2]$$

As ΔI approaches ΔItp, the ratio will approach 1. If IRE ≥ 1 emergent effects will occur. The relationship between the information ratio of emergence (IRE) and the factors that influence whether or not the engineered system becomes emergent can be defined as a tuple of the form [5.6].

$$IRE\ [ARI, RXM, Df, Cc, Int, Vr] \qquad [5.6]$$

Where:

ARI = Activation Ratio of Information

RXM = Reception to X-mission Multiple

Df = Degrees of Freedom for system components

Cc = Concentration of system components

Int = Degree of interoperability

Vr = Variety of the system components that act as regulators

Increases in ARI, RXM, Df, Cc, or Int, will increase ΔI, while decreasing Vr will decreases ΔHtp. As ΔH approaches ΔHtp, IRE approaches 1and engineered systems transitions and produces emergent effects. Therefore, the system factors for emergent effects in engineered systems is defined by the IRE tuple.

The author posits that a valid theory of emergence in engineered systems defined by: the operational definition of emergents and emergence in the physical domain; the Causal Tree in Figure 13; the theoretical propositions in Table 14; and the IRE tuple in equation [5.6]. The validity is supported by the rigor of the methods and framework of the rationalist inductive research methodology used to develop it:

- *Analogical Reasoning* Method *(ARM)* – Justifies the transfer of knowledge from existing theories in the domain of the research medium of study (thermos chemistry) to the new theory in the domain of engineered systems.
- *Theory Building Framework (TBF)* – The proposed theory meets the standards for "Good Theory" defined in (Identified Need; Definitions; Propositions; Falsifiability; Analogies; Cause-effects ;Rigor; Parsimony; Uniqueness; Generalizable; Fecundity).
- *Modeling & Simulation System Development Framework (MS-SDF)* – The models in the theory follow a structured framework and cohere to system of logic.

In Chapter 6, the theory is explored and elaborations are made through simulation experiments.

CHAPTER 6

ELABORATION AND EXPLORATION

An initial theory of emergence in engineered systems was developed in chapter five. The theory is valid based on rigor of the process that was followed. The theory was developed from analogies to then conceptual model of endothermic reactions discussed in Chapter Four. The theory consist of: the operational definition of emergents and emergence in the physical domain; the Causal Tree in Figure 13; the theoretical propositions in Table 14; and the IRE tuple in equation [5.6]. The essence of the theory is that emergence in engineered systems is determined by a tipping point defined by the Information Ratio of Emergence (IRE) tuple.

IRE [ARI, RXM, Df, Cc, Int, Vr] [5.6]

Where:

ARI = Activation Ratio of Information

RXM = Reception to X-mission Multiple

Df = Degrees of Freedom for system components

Cc = Concentration of system components

Int = Degree of interoperability

Vr = Variety of the system components that act as regulators

In the current chapter, a systems dynamics simulation model is constructed and an experiment designed to explore and elaborate on the initial theory.

6.1 Simulation Model of Emergence in Engineered Systems

Qualitative models like the causal loop diagram in Figure 9, are important in the process of understanding and explaining cause and effect relationships. However, these models do not capture the real world effects of feedback, time delays, nonlinearities, and accumulations over time (Sterman, 2000). Simulation models overcome these limitations by creating virtual worlds with dynamic representations of systems, processes, and phenomena over time. Simulation model is constructed using the logic defined by the chemical system conceptual model depicted by the causal loop structure in Figure 9.

6.1.1 The Modeling Questions for Engineered Systems

The previously presented research question is:

> *What are the factors in engineered systems that affect the occurrence of emergence, and how are the factors related?*

The modeling questions are derived from the modeling q and the initial theory of emergence in engineered systems. The modeling questions are:

(a) What is the behavior of IRE over the range of values for its variables?

(b) Are the variables in the IRE tuple significant explanatory factors of emergence in the engineered system model?

(c) How are the variables related to each other and to the occurrence of emergent effects in the engineered system model?

The simulation model is built to answer the modeling questions and study the propositions for the initial theory of emergence in engineered systems.

6.1.2 System Dynamics Model

CLDs provide insight into the cause-effect relationships between variables. They offer a logical structure to build and study conceptual models of a system. However, they are qualitative in nature and do not capture quantitative accumulations, rates of change, and feedback responses. Simulations models capture these quantitative aspects of the system over time.

There are essentially three major paradigms for simulation modeling (Borshchev, 2013; Dooley, 2002): Discrete Event; Agent Based; and System Dynamics. Diallo and Tolk compare the simulation paradigm in Table 15 (as cited by Padilla, 2010).

Characteristic	System Dynamics	Agent Based	Discrete Event
Basic building Block	Feedback Loop	Agent	Process
Unit of Analysis	Structure	Rules	Structure/Queue
Level of Modeling	Macro	Micro	Meso (mid-level)
Perspective	Top-Down	Bottom-Up	Top-Down
Adaption	Change of Dominant structure	Change of Structure	Change of Dominant structure
Mathematical Formulation	Integral Equations	Logic	Distributions
Origin of Dynamics	Levels	Events	Time and Events
Handling of Time	Continuous	Discrete	Discrete

Table 15. Comparison among Modeling Paradigms

A Systems Dynamics approach was selected for the research in this dissertation given the modeling questions are more focused on the system than is constituent entities and processes. To construct a System Dynamic simulation, the CLD must be converted into a stock & flow structure (Sterman, 2000). Stock and flow model structures captures the state of the variable and rates of change over time. Boxed variable (i.e., stocks) indicate that value of the variable accumulates and diminishes as a function of its inflow and outflow rates. The state (or level) of a stock is changed by the rate of inflows and outflows. The inflows are indicated by arrows with valve icons that are pointing toward the stocks which are the boxed variable. Outflows are those arrows with valve icons pointing away from the boxed variable. A variable can be an outflow for one stock and an inflow for another. Other variables include: auxiliary variables that change as a function of other variables but do not accumulate or lose value; attribute or state constants whose values are fixed over time and capture the state of a system attribute; and time constants that define the time over which inflows / outflows occur.

The simulation model of emergence in engineered systems is depicted in Figure 14. See Appendix C for model documentation including formulas, initial conditions, units, and values ranges for constants. The attributes of the model that distinguish it as an engineered system are the engineering decisions associated with the six IRE factors:

ARI = Activation Ratio of Information

RXM = Reception to X-mission Multiple

Df = Degrees of Freedom for system components

Cc = Concentration of system components

Int = Degree of interoperability

Vr = Variety of the system components that act as regulators

The engineering decisions are represented in the simulation model as independent variables.

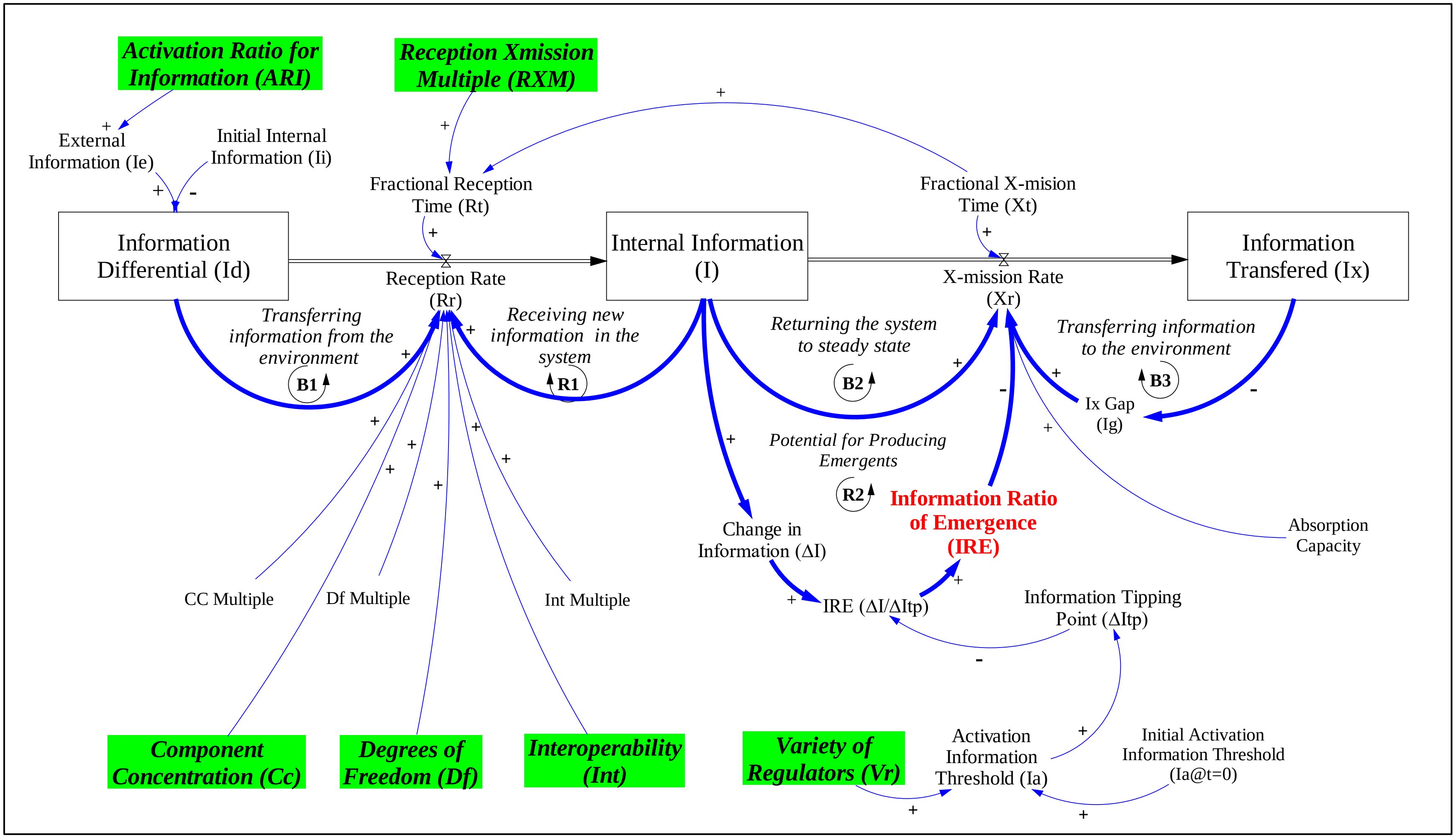


Figure 14. Simulation Model for Emergence in Engineered Systems

The simulation model for emergence in engineered systems has four dynamic loops:

- **B1, Transferring Information from the Environment.** The interaction of the engineered system with its environment begins with an input from an external information source (Ie). The information differential (Id) between the system's initial internal energy (Ii) and the external energy source (Ie) is the amount of energy that is available to be transferred to the system. The system requires a certain amount of time to receive each fraction of information (i.e., reception time). The greater the differential and the shorter the reception time (Rt), the faster the rate of reception (Rr). Rate of reception (Rr) can be increased by increasing component concentration (Cc), degrees of freedom (Df), and system interoperability (Int). Given enough time and without the continuous addition of more information from an external source, the system will receive all available energy, and the information differential will reduced to zero.
- **R1, Receiving New Information in the System.** When the information exchange begins at time (t) =0, the information differential (i.e., the potential new information that can be received) is at its maximum; change in the system's information (ΔI) is at its minimum; and the system is in an initial steady state (information received =information transferred, and $\Delta I = 0$). Over the course of the interaction, the system receives external information (Ie) causing increases in the system's internal information (I) such that the system is no longer in steady state (information received $\neq$information transferred from the system to the environment (Ix) , and $\Delta I \neq 0$). The greater the relative amount of external information (Ie) to the required activation threshold for emergence (Ia) the greater the internal information growth in magnitude (ΔI). As the system is receiving information it is also transmitting information. ΔI will occur at a faster rate to the extent that the

Reception to X-mission Multiple (RXM) is >1. Internal information continues to grow and grow faster until all of the available information (Id) has been received.

- **R2, Potential for Producing Emergents**. As the information differential continues to be received by the system, the change in the total information (ΔI) approaches the tipping point required for emergent effects to occur. ΔI approaching the information tipping point (ΔItp) indicates that the current configuration of the system is changing. If ΔI > ΔItp, i.e., the information ratio of emergence (IRE) >1, emergent effects will occur. If the internal information (I) does not reach the information activation threshold (Ia); ΔI will be <ΔItp, IRE will be < 1, and emergent effects will not occur. The
- **B2, Returning the System to Steady State**. Engineered systems receive and transfer energy. Initially the R1 loop is dominant and the system is receiving more information than it transfers (i.e., ΔI is increasing). A tipping point will occur where the system will begin to transfer more information than it receives. At that point dominance will shift to the B2 loop where ΔI and the system internal information will decline until the system returns to steady state. For each fraction of information, a certain amount of time to transfer (Xfer) to the environment is required to complete the interaction, and return the system to steady state. The rate of information that transfers (Xfers) out of the system as it returns to steady state is the Xfer rate (Xr).
- **B3, Transferring Information Back to the Environment.** Engineered systems receive information as they interact with their environment and other systems. Initially the gap between the available information to be receive and the information transferred back to the environment is large and the transfer rate (Xr) of information back to the environment is high. If the information tipping point (ΔItp) is not reached, information ratio of

emergence (IRE) will be < 1, and emergent effects will not occur. The system will continue to transfer energy back to the environment until the gap between energy transferred and available energy to be received is zero (Ig = 0 at t_x) and the interaction ends. However, if the peak of ΔI is > ΔItp, IRE will be > 1, and emergent effects will occur. If an emergent effects occurs some of the available information will be absorbed by the system and the balanced will be transferred back to the environment, i.e., Ig>0 at $t_{x.}$ Exactly how much of the information will be absorbed is not known. For the purpose of the simulation, a capacity limit is assumed. The limit varies according to a random distribution. A "seed" value selected at the beginning of the simulation determines the distribution. It is assumed that the Internal Information (I) will be = > the Initial Internal Information (Ii). This assumption requires that the time to transmit information back to the environment (Xt) is greater than the time to receive information (Rt). Lowering the variety of regulators (Vr) can lower the information activation threshold (Ia) and increase the likelihood that IRE will be > 1 between t_1 and t_x.

To conduct a quantitative study of these relationships, a measurement framework must be defined for each variable.

6.1.3 Simulation Variable Measurements

The logical relationships between the variables that define emergence in engineered systems are defined in and by the system dynamic model depicted in Figure 14. There are four types of variables are in the model and identified in: stocks; auxiliaries; initial value constants; time constants; flows; and state constants. A measurement framework is defined and applied to each type of variable.

<u>The measurement framework has three elements:</u>

- **Measurement scales**. There are generally three scales of measurements that are suitable for simulation models: 1) Interval measures are integers preserving relative distance and size between measurements but does not have an absolute zero value(Stevens, 1946;); 2) Ratio measures are continuous and include fractional values preserving relative distance and size as well as an absolute zero value (Stevens, 1946;) ; 3) Fuzzy measures use approximate reasoning and compatibility functions to translate linguistic expressions into quantitative values where interval or ratio measures are not directly available (Klir & Yuan, 1995; Zadeh,1975).
- **Units of measure**. Variables in the simulation model represent real world components and attributes of the system being modeled. Units define what a variable represents (i.e., its dimensions), and how they can interact. For example, the addition of a time variable and a volume variable is not a valid function. However, the multiplication of a time variable and a rate variable (i.e., volume per unit of time) is a valid function. In this sense units provide logical constraints in a simulation model.
- **Range of values.** One of the values of computer simulation is the automation of functions and calculations. This allows for large volumes and ranges of data to be considered in simulation studies. Models by definition are abstractions or approximations of real world systems. As an abstraction, limits are placed on how much of the real world will be simulated. The objective in determining the range of values for variables is to ensure that a sufficient amount of data is produced such that the phenomena can be observed. The values are assumed for simulation purposes only. The actual values are based on specific systems.

<u>A measurement for each variable type for the simulation model is defined:</u>

Stocks (dependent variable): Stocks are accumulations of changes in the amount of something being measured over time. Integrating the function that defines the measurement is the mathematical process for determining the total accumulation. The stock variables in the simulation model are: Information Differential (Id); Change in information Enthalpy (ΔH); and Information Transferred (Ix). Information is measured in magnitudes of bits (Megabytes, Gigabytes, Terabytes, etc.). Consistency of units is more important than the actual units used in the mode. For simulation purposes, a generic term, information units ("I-Units"), is used to represent information. The range of possible values for I-Units is all positive real numbers. The range of possible values are any positive real numbers. The relative values of the stocks to each other is more important than their actual values.

Initial value constants (independent variable): Constants are essentially very slow moving stocks. They are accumulations that change at a rate outside of the observable time frame of the simulation. They are used to establish the initial values for the information stocks and auxiliary variables in the simulation. There are three initial value constants: External Information (Ie), Initial Internal Information (Ii); and Initial Activation Information Threshold (Ia@t=0). The relationship between (Ie) and (Ia@t=0) is defined by equation [5.4], the Activation Ratio of Information (ARI) and has dimensionless units. Information is measured in magnitudes of bits (Megabytes, Gigabytes, Terabytes, etc.). Consistency of units is more important than the actual units used in the mode. For simulation purposes, a generic term information units ("I-Units"), is used to represent information measurements for (Ii), (Ie), and (Ia@t=0). The range of possible values for I-Units is all positive real numbers.

Auxiliaries (dependent variable): The auxiliary variables are functions of the stocks and initial value constants. These variables are used to provide additional insight into behaviors that influence or occur as a result of accumulations of stock values. There are six auxiliary information variables: External Information (Ie); Information Tipping Point (ΔItp); Change in Information (ΔI); the Information Activation Threshold (Ia); Maximum Absorption; and Ix Gap (Ig). The auxiliaries are measures of information in I-Units with a range of possible values including all positive real numbers. There is also an auxiliaries that is a dimensionless ratios: Information Ratio of Emergence (IRE) is also an auxiliary variable. It is dimensionless with possible values including all positive real numbers.

Time constants (independent variable): Systems require a certain amount of time to change states. Information delays are an especially important concept in modeling dynamics of systems. It takes time for the components in the system to receive, process and react to information. Time constants capture this concept. Any time units (minutes, seconds, hours, days, etc.) are acceptable in the simulation. The exact units are not important in the model, however, minutes are used to execute the simulation. There are two time constants: Reception Time (Rt); and X-mission (Transmission) Time (Xt). The relationship between Reception and X-mission time is defined by Equation [5.5], Reception to X-mission Multiple (RXM), and has dimensionless units. All Time constants can be any positive real number.

Flows (dependent variable): Flows are changes or derivatives per units of time in the level of the stock variables. Units of time are defined by the time constants. The units of measure for the flow variables are then I-Units per minute. The simulation model has two flow variables: Reception Rate (Rr); and X-mission Rate (Rx). The range of possible values are any positive real numbers.

State constants (independent variable): Concepts that effect changes in state variables and auxiliary variables but do not have clearly defined mathematical relationships are represented by state constants. Even though a precise mathematical function may not be known, the general relationships between the concept and the variables it affects (i.e., positive / negative causation and magnitude) can be defined. State constants are linguistic variables where words are used to express how much the constant is consist with the concept or a requirement. For example, someone who is very tall is more consistent with the concept of begin tall than someone who is moderately tall. The boundaries for consistency with a concept are fuzzy and are determined by a compatibility function. Compatibility functions determine the degree that the constant's value indicates membership in a conceptual category base on being consistent with the category's requirements. For example, someone whose height is greater than six feet may be linguistically "moderately tall" and assigned a compatibility value of .7 indicating its degree of membership in the category of being "tall". Compatibility values for each state constant are real numbers from 0-1 on a ratio scale with a corresponding linguistic value indicating it compatibility with its conceptual category. The quantitative and linguistic values for the state constants have dimensionless (Dmls) units are defined in Table 16 : Degrees of Freedom; Component Concentration; Interoperability; and Variety of Regulators.

State Constant	Compatibility Value	Linguistic Value
Component Concentration (Cc)	$0 < X \leq .1$	Low Compatibility
	$.1 < X \leq .5$	Moderate Compatibility
	$.5 < X \leq 1$	High Compatibility
Degrees of Freedom (Df)	$0 < X \leq .1$	Low Compatibility
	$.1 < X \leq .5$	Moderate Compatibility
	$.5 < X \leq 1$	High Compatibility
Interoperability (Int)	$0 < X \leq .1$	Low Compatibility
	$.1 < X \leq .5$	Moderate Compatibility
	$.5 < X \leq 1$	High Compatibility
Variety of Regulators (Vr)	$0 < X \leq .1$	Low Compatibility
	$.1 < X \leq .5$	Moderate Compatibility
	$.5 < X \leq 1$	High Compatibility

Table 16. State Constant Values

The impact of each state constant is defined by a function. However, the exact functions are not known. To execute the simulation model, assumptions are made for each constant based on its analogy to the four factors in chemical systems that affect the occurrence of chemical reactions (see Section 4.1.2):

- **Component concentration (Cc).** Component concentration (Cc) is analogous Component concentration (Cc) in chemical systems which has a non-linear impact on chemical reactions if the order of the substance >1.

$$\text{Rate} = k^{*}(\text{substance 1})^{a} \times (\text{substance 2})^{b} \times (\text{substance 2})^{c} \ldots \qquad [4.1]$$

It is assumed that the order of the components in the engineered system is >1 and that the impact of (Cc) in engineered systems is also a nonlinear function. The impact (y) of (Cc) on Reception (Rr) is represented by an exponential function where (m) is the impact multiple and (Rr) is increased by a factor of $e^{(m)}$ when (Cc) =1 and a factor of 1 when (Cc) =0.

$$y = e^{(m)*(Cc)} \qquad [6.1]$$

- **Degrees of Freedom (Df).** Degrees of Freedom (Df) is analogous to Molecular Freedom (F) in chemical systems. (F) Increases chemical reactions as a linear function by increasing the frequency factor (A) in the rate constant equation.

$$\text{Rate constant, } k = A \times e^{(-Ua)/RT} \qquad [4.2]$$

It is assumed that the impact of (Df) is also a linear function. The impact (y) of (Df) on Reception (Rr) is defined by a function where (Rr) is increased by a multiple of (m) +1 when (Df) =1 and a factor of 1 when (Df) = 0.

$$y = (m) \times (Df) + 1 \qquad [6.2]$$

- **Interoperability (Int)**. Interoperability (Int) is analogous Temperature (T) in chemical systems which has a non-linear impact on chemical reactions according to the rate constant equation.

$$\text{Rate constant, } k = A \times e^{(-Ua)/RT} \qquad [4.2]$$

$$\text{Rate} = k \times (\text{substance 1})^{a} \times (\text{substance 2})^{b} \times (\text{substance 2})^{c} \qquad [4.1]$$

It is assumed that the impact of (Int) in engineered systems is also a nonlinear function. The impact (y) of (Int) on Reception (Rr) is represented by an exponential function where (m) is the impact multiple and (Rr) is increased by a factor $e^{(m)}$ when (Int) =1, and a factor of 1 when (Int) = 0.

$$y = e^{m*(Int)} \qquad [6.3]$$

- **Variety of Regulators (Vr).** Variety of regulators (Vr) is analogous to catalytic volume (Vc) in chemical systems. (Vc) increases reactions in a nonlinear function by reducing activation threshold (Ua) in the rate constant equation.

  $$\textit{Rate constant, } k = \mathrm{A} \times e^{(-Ua)/RT} \qquad [4.2]$$

  It is assumed that the impact of (Vr) is also a nonlinear function. Activation information threshold (Ia) starts at 100% of its initial value when (Vr) =1 and declines to a lower level as (Vr) decreases from 1 and approaches 0. The impact (y) of (Vr) on information threshold (Ia) is represented by an exponential function with an intercept at some percentage (z) reduction in (Ia) when Vr =0.

  $$y = (1\text{-}z\,\%) \times (Vr)^2 + z\% \qquad [6.4]$$

6.1.4 Verification and Validation

Prior to conducting experiments, the model was tested to confirm that the model that was built is the model that was designed (i.e., verification) and that it meets its intended purpose (i.e., validation). The V&V (verification & validation) is most of all a process of comparing things (Sokolowski & Banks, 2010): the model vs its specifications, and the model vs its purpose. The CLD and simulation models are developed using Vensim modeling & simulation software (Ventana Systems, 2016). Vensim has several functions that support the verification and validation process. The V&V test plan and results are documented in Table 17.

Type	Requirement	Test	Results
Verification	Model consistency: variable relationships and formulas are consistent with the logic of stock & flow model structures	Run Vensim Check Model function. (Appendix D Figure 23)	Pass
	Unit consistency: units are consistent in formulas and variable relationships.	1) Run Vensim Units Check function. (Appendix D Figure 24)	Pass
	Causal Relationships: The relationships defined in the CLD are reflected in the simulation model	2) Visually inspect the Vensim Causal Trees and Use Trees for each variable. (Appendix D Figure 25- Figure 30)	Pass
Validation	The model represents engineered systems	Identify aspects of the model that are associated with being an engineered system	Pass
	Behavior in the engineered system is comparable to the behavior in the chemical system	Compare graphs of total energy in chemical systems to total information in the engineered system model. (Figure 7 and Figure 15)	Pass

Table 17. Verification and Validation Test Plan

Verification: The goal of verification testing is to confirm that the design for the conceptual model has been correctly implemented and that structure of the model follows governing rules. The simulation model is a system dynamic model and is governed by the rules for stock & flow structures. The design for the model is defined by the conceptual model in Figure 12, and the variable relationships defined in Table 13. The Vensim functions used for verification testing are: “Check Model” compares the model to principles for system dynamic modeling structures; “Units Check” performs a dimensional analysis on formulas in the model to identify unit inconsistencies; and Causal Trees / Use Trees provide a mapping of variable relationships. Both Model Check and Units Check passed. Visual inspection of the Causal Trees / Use Trees confirmed that the variables relationships in the conceptual model and variable definitions are accurately represented in the simulation model. Screen shots of the Vensim verification test results can be views in Appendix D, Figure 23 - Figure 30. Based on the results from the Vensim checks and an inspection of the Vensim graphs, it is concluded that the simulation model is correctly built and meets its intended purpose. With the V&V complete, experiments are conducted to answer the modeling questions and study the propositions for the initial theory of emergence in engineered systems.

Validation: The goal for validation testing is to confirm that the model realizes its purpose by representing the behavior it was intended to model. The purpose of the simulation is to study emergence in engineered systems. The engineered system aspect of the model is represented by the decisions associated with the values for the independent variables. The independent variables in the model are: Activation Ratio of Information (ARI); Reception to X-mission Multiple (RXM); Degrees of Freedom for system components (Df); Concentration of system components (Cc); Degree of interoperability (Int); Variety of the system components (Vr). As system design decisions are made, the values of each variable are determined. The consequence of those decisions affects the occurrence of emergence in the engineered system.

The emergence aspect of the model are the analogies that enable emergence in to be studied based on the behavior of endothermic chemical reactions. The behavior of endothermic chemical reactions is depicted in Figure 7, and compared to the general behavior of engineered system with and without emergence (see Figure 15).

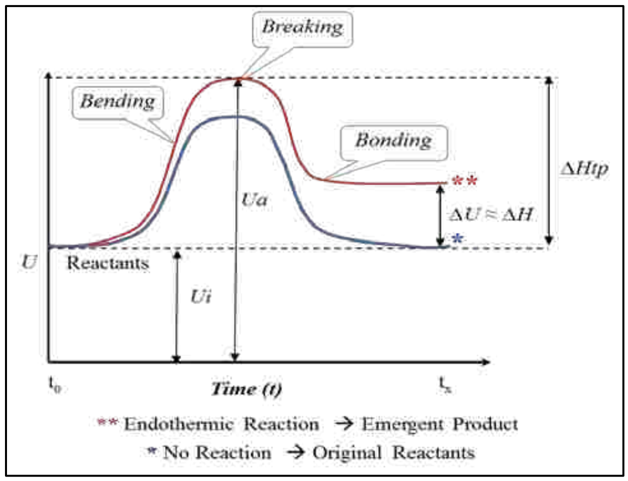


Figure 7. Endothermic Chemical Reaction

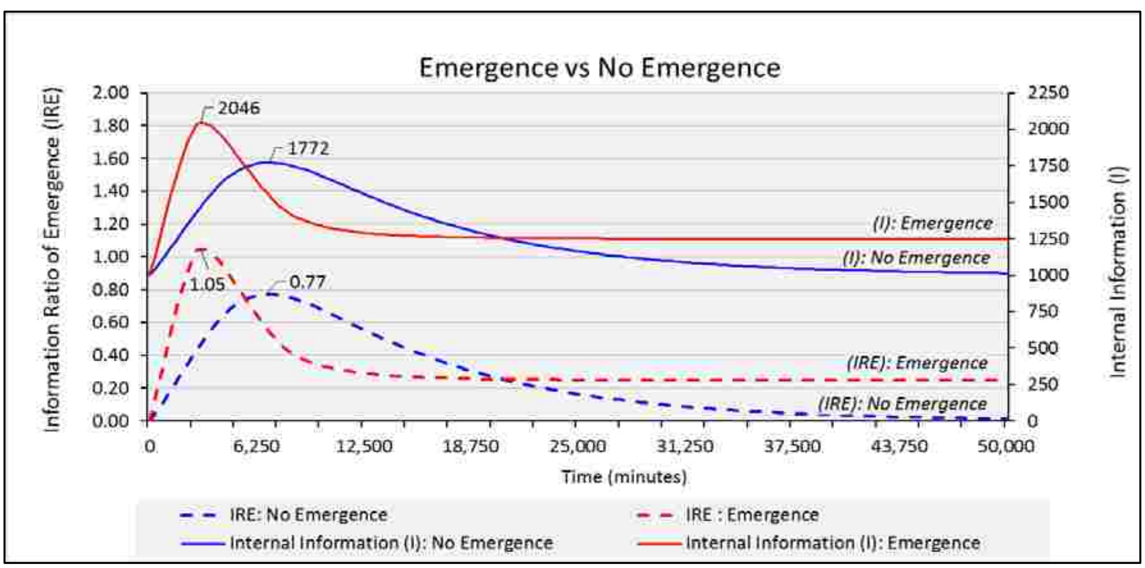


Figure 15. Emergence in Engineered Systems

The Activation Information Threshold (Ia) = 2000 I-Units for the example presented in Figure 15. If the internal information of the engineered system must reach or exceed 2000 I-Units, the information ratios of emergence (IRE) will be >=1 and emergent effects will occur.

The dotted lines in Figure 15 are the trends for the information ratio of emergence (IRE). The max IRE is less than one (value =.77<1) in the trend for the IRE blue dotted line. This indicates that the change in the internal information was not sufficient to cause emergence. The solid blue line shows the progression of internal information as the engineered system receives information, increases to 1772 and returns to its original level of 1000. The change in internal information at the end of the interaction is zero. This behavior is similar to the chemical system behavior when a chemical reaction does not occur (i.e., blue line (*) in Figure 7). The internal energy (U) in the chemical system increases then returns to its original level. The change in internal energy at the end of the chemical interaction is zero.

The max IRE in the dotted red line is greater than one (value =1.05 >1). This indicates that the change in the internal information was sufficient to cause emergence. The solid red line shows the progression of internal information as the engineered system receives information, increases to over 2046 and eventually settles at 1250. The change in internal information at the end of the interaction is 250. This behavior is similar to the chemical system behavior when a chemical reaction occurs (i.e., solid red line (**) in Figure 7). The internal energy (U) in the chemical system increases then settles at a level greater than its initial value. The change in internal energy at the end of the chemical reaction is greater than zero.

6.2 Experimentation

Conducting simulation experiments supports theory development by providing an environment for “theoretical elaboration and exploration” (Davis et al., 2007). Davis goes on to say “... effective experimentation builds new theory by revealing fresh theoretical relationships and novel theoretical logic.” The foundation of experimentation on which Davis makes his claims is being forward looking attempt at answering “what if” scenario questions. “What if “scenarios looks at the status quo and considers what might happen if things were different. Analyzing experimental results can potentially: a) extend what is already known or initially theorized about a system; and b) uncover system behaviors that were previously unknown.

The simulation model represent emergence in engineered systems based on values for the six IRE variables. But “what if” the actual values are not known? This uncertainty can be modeled in Monte Carlo simulation experiments. Real systems generally have a degree of uncertainty and randomness. Even in deterministic systems where the outputs can be predicted with certainty, the exact value of the inputs at a future point in time may not be known. Monte Carlo simulation (or sensitivity analysis) experiments mimic this aspect of real systems by randomly varying independent variables within their distributions and observing the average impact on dependent variable behavior. For these reasons, Monte Carlo experiments are particularly well suited to answer the modeling questions:

a) Are there emergent effects (IRE >=1) over the range of values for the IRE variables?
b) Are the variables in the IRE tuple significant explanatory factors of emergence (IRE >=1) in the engineered system model?

c) How are the variables related to each other and to the occurrence of emergent effects (IRE>=1) in the engineered system model?

Mote Carlo simulations for emergence in engineered systems are further defined in Appendix E. The results are presented as follows:

Monte Carlo Experiment

The distribution for the dependent variable Information Ratio of Emergence (IRE), is defined by a response functions (*f*) whose arguments are the independent variables in the IRE tuple:

IRE =*f* (ARI, RXM, Df, Cc, Int, Vr)

The impact of each IRE variable is explored by setting it to a fixed values (high, nominal, low according to) and allowing the other variables to randomly vary over their distributions. The results are compared to the simulation when all variable randomly vary. The results are presented in Figure 16 and Table 18.

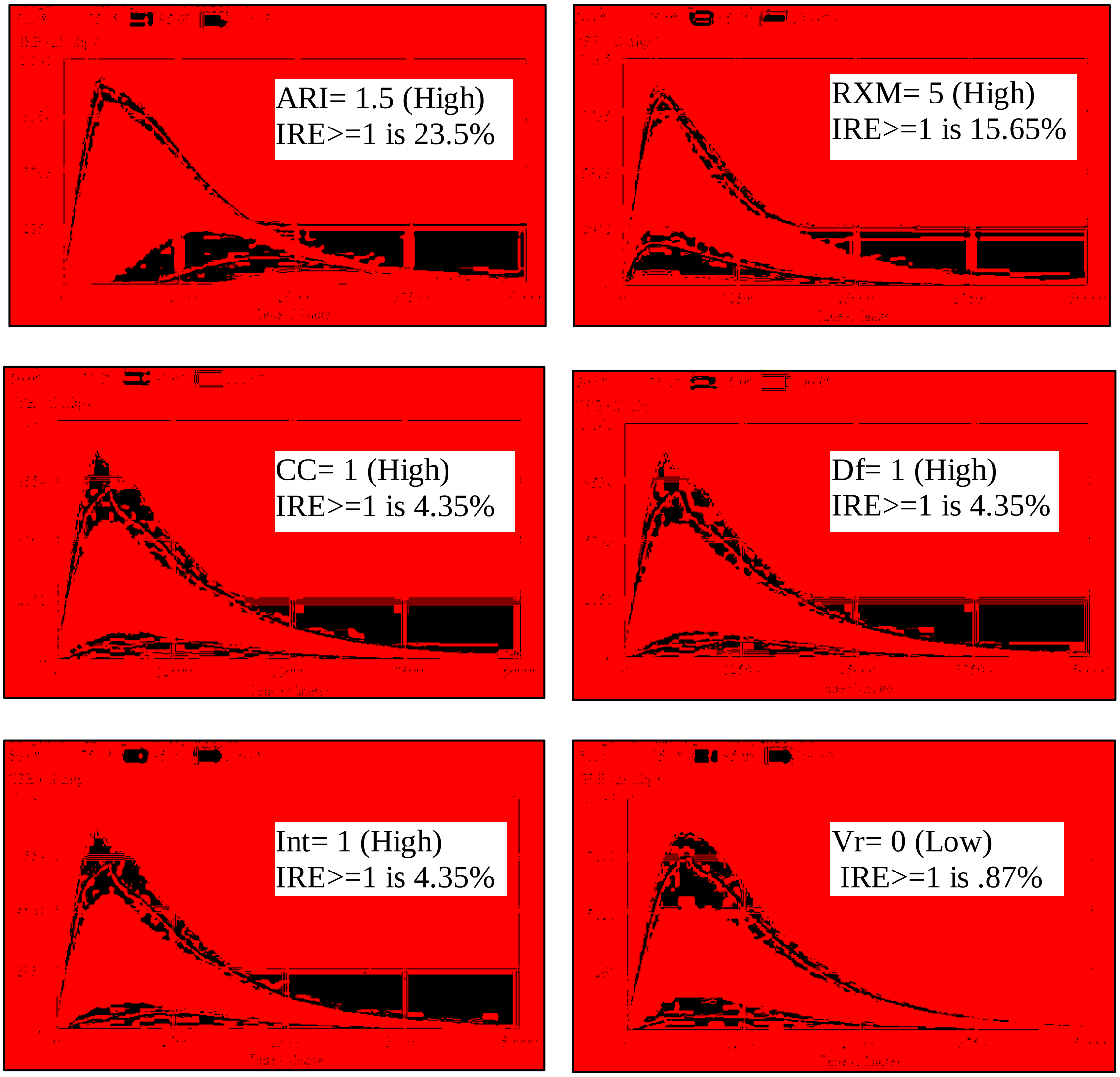


Figure 16. Monte Carlo Simulation Results

IRE Factor	Value	IRE >=1 (% of Runs)
ARI (Activation Ratio of Information)	High = 1.5	23.5
	Nominal =1	0.00
	Low =.5	0.00
RXM (Reception to X-mission Multiple)	High = 5	15.65
	Nominal =3	0.00
	Low =1	0.00
Cc (Concentration of components)	High = 1	4.35
	Nominal =.5	2.61
	Low =0	1.74
Df (Degrees of Freedom for components)	High = 1	4.35
	Nominal =.5	2.61
	Low =0	1.74
Int (Degree of interoperability)	High = 1	4.35
	Nominal =.5	2.61
	Low =0	1.74
Vr (Variety of regulators)	High = 1	0.00
	Nominal =.5	.87
	Low =0	.87
Random Variation for All Factors		**.87**

Table 18. Monte Carlo Simulation Results

Observing the Monte Carlo Simulation results in Figure 16 and Table 18, it is determined that ARI has the greatest impact; increasing the % of emergence runs from .87% to 23.5%. The rank order for all factors in terms of impact on IRE is: ARI, RXM, Cc/Df/Int, and Vr. Based on these results the modeling questions can be answered:

a) Are there emergent effects (IRE >=1) over the range of values for the IRE variables?

   Answer: Yes, there are emergent effects (IRE >=1) over the range of values for the IRE factors values. The % of runs where ITE >=1 ranges from .87% to 23.5%.

b) Are the variables in the IRE tuple significant explanatory factors of emergence (IRE >=1) in the engineered system model?

   Answer: Yes, the variables in the IRE tuple significant explanatory factors of emergence (IRE >=1) in the engineered system model. While no statistical causal significance is determined, it is observed that changes in the IRE variables results in changes in the % of emergence (IRE >=1) in the simulation runs.

c) How are the variables related to each other and to the occurrence of emergent effects (IRE>=1) in the engineered system model?

   Answer: The Monte Carlo simulations show that ARI and RXM are necessary conditions for emergence. Emergence only occurs when one of these variable in high. No emergence occurs when either variable in nominal of low. It is also observed that Vr is sufficient to prevent emergence from occurring (IRE<1). When Vr is zero, emergence does not occur.

6.3 Testing the Theoretical Propositions

The propositions for the theory of emergence in engineered systems are listed in in Table 19. Each proposition is a claim about the information ratio of emergence (IRE) and conditions for when emergent effects will occur. The propositions are tested in the simulation model to determine if it is true. The 2^{nd} order model is used to test the propositions. It is assumed that a proposition test that passes with the 2^{nd} order model would also pass using the 3^{rd} order model given the higher explanatory power and precision of the 3^{rd} order model.

	Propositions for Emergence in Engineered Systems
1)	As the Information Ratio of Emergents (IRE) approaches 1, the probability of emergence increases.
2)	Activation Ratio for Information (ARI) = External Information (Ie) ÷Activation Information Threshold (Ia) >=1 is a necessary condition for IRE>=1 (i.e., emergence to occur).
3)	As the Information Ratio of Emergents (IRE) approaches 1, emergent effects occur faster.

Table 19. Theoretical Propositions for Emergence in Engineered Systems

Proposition #1. As the Information Ratio of Emergents (IRE) approaches 1, the probability of emergence increases.

Test: Probability of emergence is the percentage of time periods where IRE>=1. If the trend in average IRE has a positive correlation with the percentage of total time periods where IRE>=1, then the proposition is true.

Results: Proposition #1 is true. Correlation Coefficient (r_{xy}) = .954585 for Average IRE vs Probability of Emergents (see Figure 17).

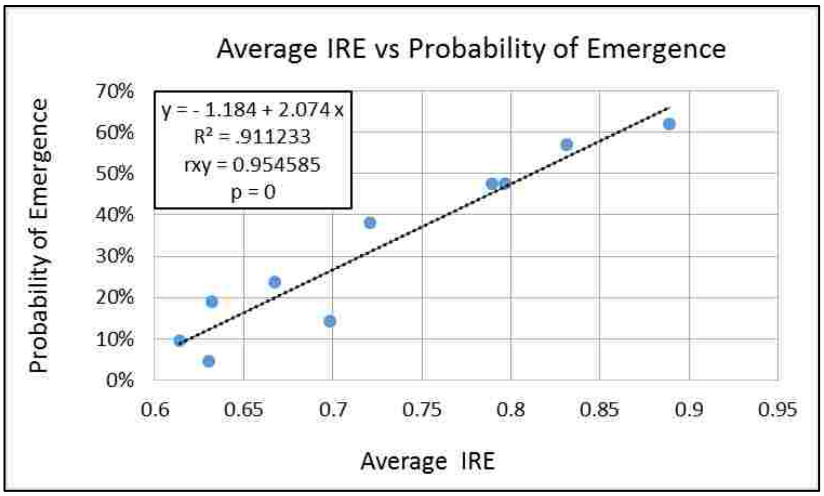


Figure 17. Average IRE vs Probability of Emergence

Proposition #2. Activation Ratio for Information (ARI) = External Information (Ie) ÷Activation Information Threshold (Ia) >=1 is a necessary condition for IRE>=1 (i.e., emergence to occur).

Test: The proposition is true if there are no instances where IRE >=1 when ARI <1 and the other five IRE factors vary.

Results: Proposition #2 is true. 100% of the IRE instances are less than 1 when ARI is less than 1. A sensitivity analysis is performed with five IRE factors (Cc, Df, Int, RXM, and Vr) randomly varying between their min and max values while allowing ARI to vary from it minimum to a maximum value less than 1 (.5<=ARI<1). (See Figure 18).

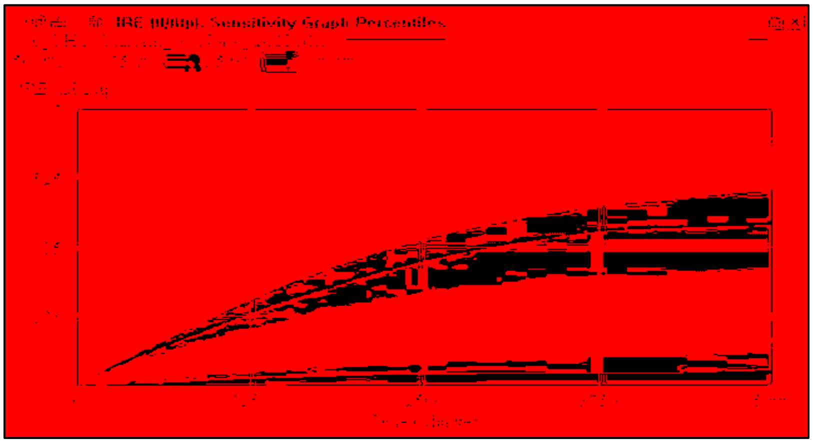


Figure 18. IRE Sensitivity Analysis

Proposition #3. As the Information Ratio of Emergents (IRE) approaches 1, emergent effects occur faster.

Test: The lower the time period for the first occurrence of IRE>=1, the faster the emergent effect bas occurred. If the trend in average IRE has a negative correlation with the first time period where IRE >=1 (i.e., where emergent effects occur), then the proposition is true.

Results: Proposition #3 is true. Correlation Coefficient (r_{xy}) = -.9196 for Average IRE vs 1st Time Period for IRE>1 (see Figure 19).

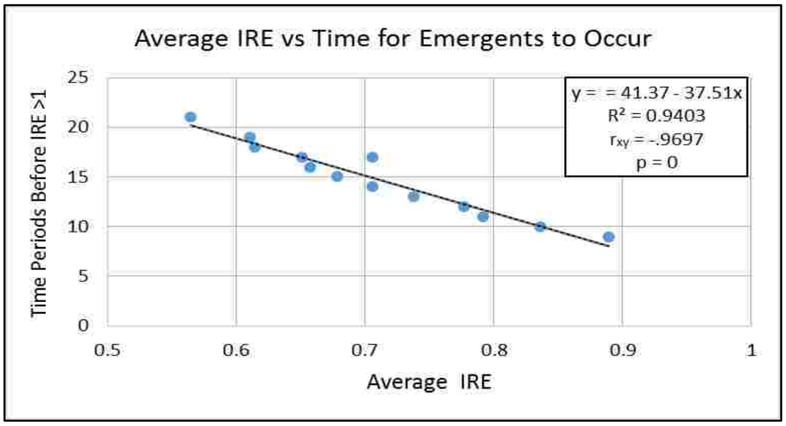


Figure 19. Average IRE vs Time for Emergents to Occur

6.4 Interpretation of Results

The initial theory of emergence in engineered systems proposes six factors that affect the occurrence of emergents. A simulation model was constructed to study and elaborate on the initial theory. The modeling questions are:

(a) What is the behavior of IRE over the range of values for its variables?

(b) Are the variables in the IRE tuple significant explanatory factors of emergence in the engineered system model?

(c) How are the variables related to each other and to the occurrence of emergent effects in the engineered system model?

The experiment results are interpreted in the context of the modeling questions.

CHAPTER 8

CONCLUSIONS, RECOMMENDATIONS, AND FUTURE WORK

Emergence in engineered systems is essentially a phenomenon that brings about unintended system effects; specifically effects that have no apparent explanation in terms of the system's parts and their relationships. It was established that the body of knowledge on emergence and engineered systems would be advanced by the addition of a general theory that unambiguously defines emergence and explains causal factors that affect the occurrence of emergent effects in engineered systems. A research question was derived to address the need for such a theory:

What are the factors in engineered systems that affect the occurrence of emergence, and how are the factors related?

Well established concepts and principles from thermochemistry were used to derive a theory, construct a system dynamics simulation model, conduct experiments, and ultimately answer the research questions.

7.1 Answering the Research Question

The outcome of the research is a proposal for a general theory of emergence in engineered systems. The theory includes: an unambiguous definition; a set of analogies; theoretical propositions; qualitative and quantitative models.

Unambiguous and Unifying Definitions. Definitions are derived from the ontology of emergence summarized in section 3.1, and detailed in of Appendix A:

a) *Emergents are system effects that are approximately underivable based on system components and their interrelationships.*

b) *Emergence is the action of producing system effects that are approximately underivable based on system components and their interrelationships.*

The ontology includes concepts applicable to physical and metaphysical domains. The operational definitions used in the research are specific to the physical domain.

*A Set of Analogies***.** Structural mapping was used to establish the scientific analogies in Table 12 between factors for endothermic reactions and factors in engineered systems. The analogies provide explanation and credibility for the concepts in the proposed theory by using established theories and concepts from thermochemistry.

Theoretical Propositions. The theoretical propositions in Table 14 are claims about the occurrence of emergent effects and the presence of a tipping point in engineered systems. If sufficient information is received, a tipping point will be reached and emergent effects will occur. The tipping point variable is Information Ratio of Emergence (IRE) and is determined by a tuple of six factors that affect the occurrence of emergence in engineered systems:

IRE [ARI, RXM, Df, Cc, Int, Vr] [5.6]

Where:

ARI = Activation Ratio of Information

RXM = Reception to X-mission Multiple

Df = Degrees of Freedom for system components

Cc = Concentration of system components

Int = Degree of interoperability

Vr = Variety of the system components that act as regulators

Qualitative and Quantitative Models. Three models were produced that help explain the emergence phenomena in engineered systems. Each model uses a different method to explain the factors that cause emergent effects: the conceptual model in Figure 12 uses Causal Loop Diagrams to depict balancing and reinforcing behaviors in engineered systems; and the System Dynamics model in Figure 14 uses simulation methods to show behaviors and interactions over time.

Collectively the four components of the proposed theory answer the research question by providing a conceptual and quantifiable explanation of the factors in engineered systems that affect the occurrence of emergents, and how those factors are related.

7.2 Research Contributions

In addition to answering the research question, several other important contributions are made: an ontology of emergence concepts; an unambiguous and unifying definition of emergence; and a systems dynamic model of emergence in engineered systems.

Ontology for Emergence Concepts. The ontology of emergence is database of concepts mapped to a common set of categories (i.e, classes). The concepts are deconstructed into essential attributes, categorized, and logically linked. Queries of the database can be performed and graphs of the relationships between concepts can be constructed.

Unifying Definition of Emergence. Based on the ontology that is developed from the research, a general and unifying concept of emergence is defined. Emergence is defined by two primary classes: characteristics of the emergent effects, and characteristics of systems where emergent effects take place. The primary classes are broken down into eight subclasses: type; logical relationship; perspective; indicators; temporality; structure; knowledge constraint; and application domain. Conflicts among emergence concepts are reconciled by grouping them into the eight subclasses.

System Dynamics Model of Emergence. The literature has many examples of emergence modeled from a bottom up perspective with emphasis on the nature of the interaction between entities or agents in the system (Crutchfield, 1994; Gilbert & Terna, 2000; Holland, O.T., 2012; Kovacic, 2013; Padilla, 2010). While there is a risk of over simplification in not considering variations at the entity level; system dynamics methods enable insights to be gained about the role of the system's features in generating emergent effects. The model provides an environment to further study the emergence problem and factors in engineered systems that affect it occurrence.

The three additional contributions in conjunction with answering the research question, support the significance of the research in advancing the body of knowledge on emergence in engineered systems.

7.3 Potential Implications

The implications of the research are potential advances in the ability of engineers and managers to defend against or exploit the occurrence of emergence in engineered systems. The potential implications are theoretical concepts and require additional research to develop them into operational concepts. The design and management implication can be grouped into four categories: risk assessment; analysis of alternatives (AoA); "designability" assessment; and system control.

Analysis of Alternatives (AoA). AoA is a required process in the acquisition of engineered systems for the department of Defense (DOD, 2015). AoA is an assessment of the various materiel solution alternatives that are being considered to satisfy the need for an engineered system. Recall the discussion on engineered systems in Section 3.2.1, where the concept of an "undesignable state space" was introduced.

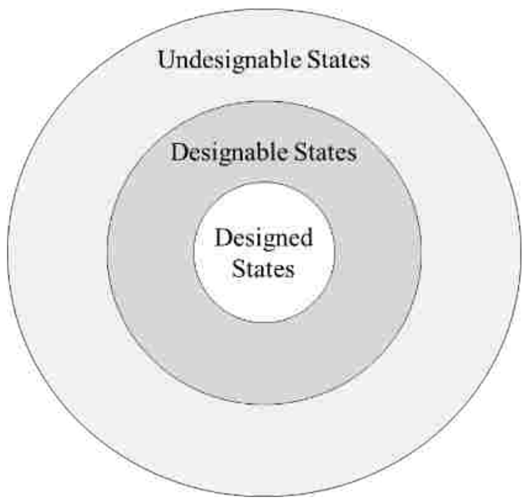


Figure 5. State Space Segmentation

- Undesignable: Some system requirements and constraints are apparently beyond human capabilities to devise a means by which they can be satisfied. The systems states for these requirements and constraints are undesignable. States that occur in this space are failures of Simon's (1969) first and second propositions. System states in this space are underivable from and unexplainable by the system components.

Applying the previously described approach for risk assessment, engineers and stakeholders can include the risk of emergent effects as a design consideration. Sensitivity analysis for each alternative can be performed by varying the assumptions used to determine the values for the IRE factors. As the value for IRE approaches 1, the potential design solution approaches the undesignable state space (where emergent effects will occur). Design solution alternatives can be considered on the basis of likely hood for emergent effects to occur and their sensitivity to the IRE assumptions.

Designability. Systems are designed to solve problems and satisfy capability needs. Based on the purpose of the system (life support vs video game for example), it may be more critical that the designed solution only produce effects according to its design; that is does not produce emergent effects. In the same sense that IRE could be used to assess alternative designs, it could be used to assess a system requirements. Criticality is a relative measure of impact on the mission of a system (Standard, 1980). When the system requirements have high criticality placed on performance according to its design specifications, then IRE must be low (i.e., a low likelihood of emergents). When the system requirements have low criticality placed on performance according to its design specifications, then IRE can be high (i.e., greater likelihood of emergents is tolerated). It is assumed that as criticality increases it becomes more difficult to identify solutions and the available design space gets smaller as. The relationship between the max IRE given a level of criticality, and available design space can be represented by IRE as a function of criticality and design space as the area under the curve generated by the function. To illustrate the concept it is assumed that max IRE is a reciprocal function of criticality, IRE = 1/ (system criticality), and that available design space = all designs such that max IRE<= 1/ (system criticality). Criticality is measured on a scale from 1 to 10 (1<=low<4; 4<= med <7; 7<= high <=10). This concept is depicted in Figure 20.

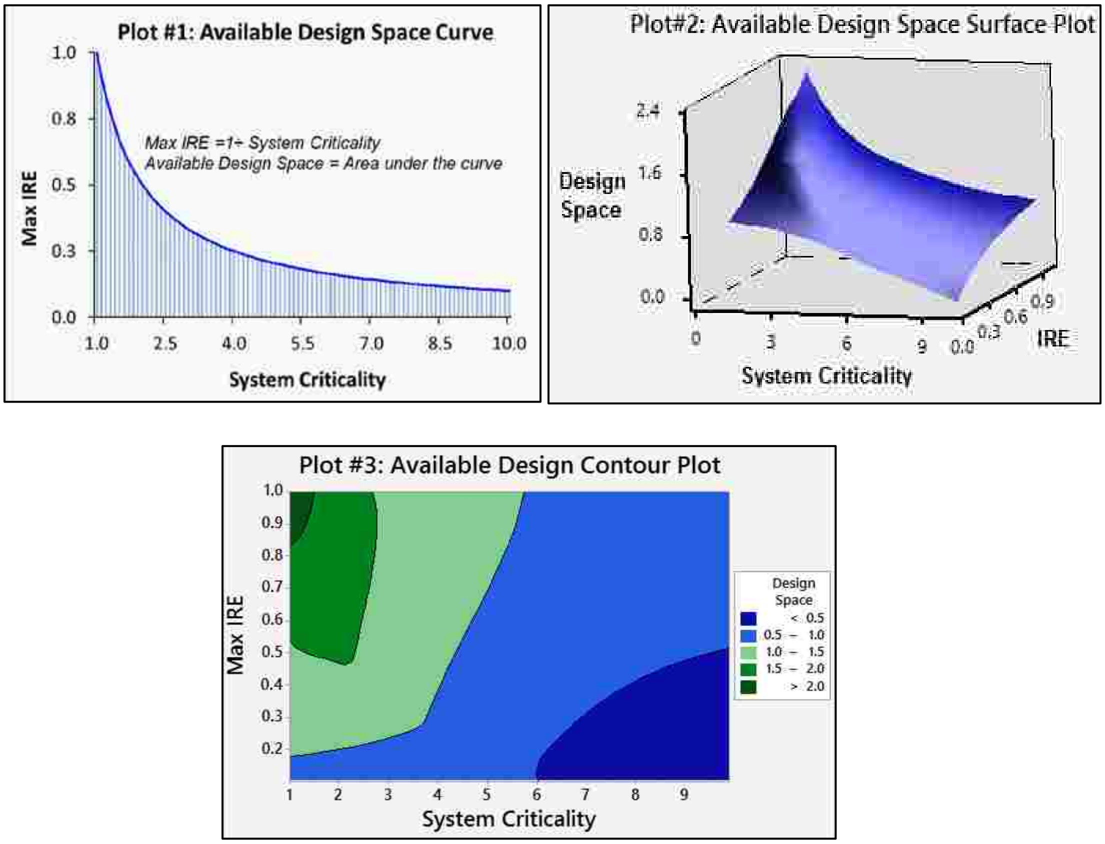


Figure 20. Designability: Available Design Space, IRE, and System Criticality

Plot#1 in Figure 20 illustrates a design space curve. The curve is a function of Max IRE vs System Criticality. The area under the curve is the available design space based on the require system criticality for the design and the maximum acceptable IRE. Plot #2 is a surface area depiction of available design space as a function of max IRE and system criticality. The shaded areas in Plot #3 represent the domains of max IRE and system criticality for five levels of available design space. In all three plots, the available design space peaks at regions where IRE and system criticality approach one, and declines to a minimum level in regions where system criticality maximizes and IRE approaches zero.

System Control. The results of the design of experiment showed that the IRE factors go beyond correlation and actually have a causal relationship with the occurrence of emergents as defined by IRE >=1. The challenge with using the IRE factors to control whether or not emergents will occur is in knowing how to control each of the IRE factors. Assuming this knowledge exist, making adjustments to the design to increase or decrease the factors opens the door for controlling (or at least influencing) the occurrence of emergent effect. Note that the factors are not determinants of the nature of the actual emergent effect. The IRE factors only impact how fast and whether or not emergents effects will occur.

7.4 Recommendations and Future Work

A general theory of emergence in engineered systems has been proposed and the intended research question has been answered. However, the research has its limitations and opportunities for improvement: 1) a set of factors has been proposed that affect the occurrence of emergence , but the research does not address how to measure the factors, how they are determined or how to control them; 3) the actual functions for some of the factors (component concentration, degrees of freedom, interoperability, and variety of regulators) are not known and were assumed in the simulation model; 4) interactions between the factors were identified and prioritized but the exact nature of how the factors interact was not addressed; 5) the theory has not been applied to a real systems and its practical implications have not been tested; 6) the ontology database developed in this research maps historical and contemporary concepts of emergence but could be improved by continuing to add new concepts as they are published.

The six limitations and opportunities identified form the basis of a research agenda for future work. This agenda has the potential to further advance the body of knowledge and improve the proposed theory of emergence in engineered systems.

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APPENDICES

A: LITERATURE REVIEW DETAIL

A.1 Theories and Definitions of Emergence /Emergents

"The whole is greater than the sum of its parts". This familiar expression paraphrases Aristotle's and is considered the earliest expression of the notion of emergence (Aristotle, 350 B.C.). Aristotle's actual statement was "…the whole is something beside the parts", which suggest that the whole is not necessarily "greater" than its parts but rather it is somehow otherwise different. Aristotle was discussing the nature of material things; specifically the relationship between things and the substances of which they are composed. Things can either be a collection of unrelated parts (i.e., "heaps") or they can be related in some way to form a unified whole. As a unified whole, things are indivisible in terms of quantity or quality. He uses as an example the unity of a set of words that forms a definition. The set of words has the "differentia" (distinguishing characteristic) of definition which does not belong to and is indivisible in terms of the individual words in the set. When things have several parts that are related by a "communion or connexion or composition", the whole which they form becomes something indivisible and different from their parts; it becomes emergent.

The actual term "emergent" was coined by G. H. Lewes (1875) in his discussion on the nature of cause and effect. The premise of Lewes' theory is that all effects are completely caused by the interactions of the constituent parts in a whole. Some effects have mathematical expressions and are completely traceable to the steps in the process that brought them about. However, emergents are the properties of the whole that are not identifiable in its parts; their mathematical expressions are nonlinear but unknown; the properties are not logically traceable to interaction "procession" (i.e., orderly process steps over a time frame) of the parts in the whole. While the name emergent is attributed to Lewes, the concept is generally attributed to Mill (1846). Mill's composition of cause principle explains that the total effects (i.e., the consequence) produced by a group of entities (or physical facts) is the same whether acting separately or in combination. The exception is when combinations are governed by laws (heteropathic laws) that are different from the laws that govern individuals. The so called heteropathic laws are only known after the consequence of the combination has occurred. This is another way of stating that the combination (i.e., the cause) has an unknown nonlinear effect. Lewes provides a detailed discussion on cause and effect relationships with examples from a variety of domains (physics, physiology, chemistry, etc.). Rather than a distinction based on differences in governing laws as is the case with Mill, Lewes centers his argument on the proposition that there is less knowledge about the interaction process for emergents because they are the result of interactions between unlike components. The components are incommensurable with each other (of different measurement standards) and produce emergent effects that are incommensurable with the components. Lewes implies that there tends to be less knowledge and greater uncertainty in the relationships between things of "unlike kinds" (i.e., those that are incommensurable), than those of the same kind (i.e., those that are commensurable). After the emergent effect has been experienced, it is possible that "someday" there will be sufficient knowledge of their interaction process steps to mathematically express the effect in terms of its constituent parts. Lewes is indicating in his concept that emergents have the theoretical potential for some form of reduction or explanation as knowledge of the effect and its constituents improves. From Lewes, we can say the limitation on the ability to "trace", reduce, or explain emergents in terms of their constituents is a temporary condition based on currently available knowledge.

Conceptual elements identified from Mill (1846); Lewes (1875):

Le1, Mi1. Emergents are system effects that are not presently traceable to deducible from the properties and interaction process steps of its components, but may become as so in the future as knowledge improves.

Le2, Mi2. Emergents are indicated by non-linear interactions and increase uncertainty about the effects produced by the interactions.

Mi3. Emergents exist when laws that govern combinations of physical facts are different from the laws that govern them separately.

Le3. Emergents are caused by the interaction between unlike (incommensurable) component properties and are incommensurable with the properties of their components.

Le4. Applied concept to: Physics (inanimate objects and events, i.e., phenomena), Physiology (feelings, sensations, consciousness, mind/body relationships), Biology (living bodies); Chemistry (chemical reactions); Philosophy (certitude, truth).

Mi4. Applied concept to physical phenomena: Physics (inanimate objects and events, i.e., phenomena), Biology (living bodies); Chemistry (chemical reactions).

In their concepts of emergents, Alexander (1920), Morgan (1925, 1929) and Broad (1925) emphasize the structure of wholes and changes in their properties relative to time. What Alexander calls “existents” are hierarchical structures of empirical things that occur over time.

He includes the human mind in his concept of empirical/material things. Basically, things that we can observe or experience are composed of multiple levels of other things that we can observer or experience. If at some point in time a grouping of things at one level is formed, then a new level of empirical things will come into existence with its own unique qualities that are not expressible in terms of the qualities of previous levels. These unique qualities at each level are emergents. They are different in nature and not merely degrees of the same quality. Morgan (1929) labels this progression as emergent evolution. He does not distinguish his concept from the general (i.e., Darwin's) concept of evolution. Morgan considers evolution as simply an orderly advance of natural (as opposed to artificial) things from natural events. This is an over simplification of the evolution concept but it serves Morgan's purpose of explaining the time element of emergence. Morgan disagrees with Alexander that minds and consciousness are emergents, but otherwise, he and Alexander seem to be in virtual lock-step in their concepts. In each case there are new groupings or things at one level that cause new properties at another level. They do not posit why new groupings might form other than pointing to the passage of time. The occurrence of the new groupings may be predicable with sufficient empirical data about preceding events and knowledge of laws governing the spatial-temporal change of the events. But as for the unique qualities or behaviors of the new grouping; they can only be deduced/predicted based on experimentation or after observation of the actual new grouping. Emergents are only the "so far unknowns"; with observation / experimentation they are determinable/predictable.

Broad (1925) makes a different structural argument. He explains the difference in behavior between things as a matter of the configurations of their parts (i.e., a particular way in which a group of parts are arranged). Things may have multiple layers of configurations where one configuration is a composition of other configurations which are themselves composed of individual parts or configurations of parts. Broad posits that the behavior of all things can be determined by knowing the: a) individual behaviors of their parts in isolation; and b) the laws that govern the integration of their individual behaviors when the parts are configured together. If both pieces of information about the configuration can be known a priori without observation, then the behaviors are mechanistic (i.e., they are resultants according to Lewes' (1875) concept). However, if the only way to know the individual part behaviors and governing laws for their integration is to observe them, then the behaviors are emergent. Broad posits that emergents exists in a configuration of components for one of two reason: 1) the components have latent properties that do not manifest in isolation and only manifest in the particular configuration; or 2) there are unique laws that govern the integration of components into the particular configuration. Discovery of the latent properties or governing laws can only be accomplished by observing the actual configuration in question. He adds that while observation is possible in the physical world it is not necessarily so in the "trans-physical" (i.e., metaphysical) realm because it is not possible to observe the "brain and its mind". In the physical world, once the governing laws or latent properties are observed, theoretically the emergent property can be logically deduced. "Theoretically" is used in the sense that it is possible if difficulties associated with mathematical computation and access to information are not considered. Other configuration behaviors are completely deducible from knowledge of their components in isolation without ever observing the actual configuration in question (i.e., they are mechanistic). Broad distinguishes the behaviors of things in chemistry (chemical reactions), biology (living beings), physiology (mind / body concepts); physics (mechanical object, spacio-temporal relations) based on whether they have emergent or mechanistic properties.

Conceptual elements identified from Alexander (1920), Morgan (1929), and Broad (1925):

Al1, Mo1. New hierarchical configurations of a system form over time.

Al2, Mo2. The uncertainty of the system properties increases with the addition of new configuration.

Al3, Mo3. Emergents are qualities or properties of material existents (i.e., wholes) that are unique to each hierarchical level that form a structure over time and are only predicable/deducible with observation/experimentation.

Br1. Physical emergents are latent qualities unique to component configurations and are only theoretically deducible after observation.

Br2. New configurations indicates a potential for emergent properties.

Br3. Things are composed of multiple layers of part configurations.

Br4. Mental Emergents are qualities or properties of the mind that are not observable or deducible in terms of its constituents parts (the body).

Al4, Mo4. Applied concept to material things: Chemistry, biology, physics,

Where some emergent theorist are concerned with traceability to efficient causes, Ashby's (1956) concept of emergents is based on Black Box theory and is only concerned with knowledge of behaviors. Cause is not a concern. A "Black Box" is essentially a system (parts and their relationships) whose internal mechanisms are not accessible to direct observation. Only the state of inputs, out puts, and feedbacks at a point in time are directly observable. Black Box theory provides the principles/methods that are appropriate when attempting to answer questions about systems where observation is limited. Knowledge of the contents and laws governing

Black Box behavior are acquired by deduction from historical observation or experimentation. If a number of Black Boxes are coupled (inputs /outputs connected) to form a system, and the acquired knowledge of their behaviors in isolation and their coupling relationships is complete; then all properties of the whole will be predicable. However, the number of black boxes and coupling relationships can grow to such an extent that parts of the system are unobservable and some of its properties are apparently unpredictable (i.e., emergent). Ashby's concept of emergents attributes the phenomena to relative complexity of the system to its parts. Complexity in Ashby's concept is the number of system states or the number of variables required to define system states. Emergents exist when: 1) the complexity of the system relative to the complexity of its parts is great, and 2) the false expectations that wholes will reproduce the properties of their parts and vice versa. As more Black Boxes are coupled together the complexity of the system increases: the number of variables and possible states of the "Black Box" system becomes greater than the number of variables and possible states of each individual Black Box. Bar-Yam (2004) describes the difference in size of the systems vs its parts as a difference in scale (i.e., detail of the system). The system properties are completely contained within its various scales. However, the amount of information is so great in the fine levels of details at the lower scales that system level properties are not readily recognizable. As the gap between scales or the size of the system vs its parts increases, extracting system properties remains possible but becomes virtually impossible. These difficult but possible to derive properties are weak emergents and typically associated with systems that are constructed by humans (i.e., engineered) vs those that naturally occur.

Another aspect of emergence discussed by Ashby is the concept that what is applicable to a group /whole, may or may not be applicable to its members, and vice versa. Ashby cites the example of rubber molecules. A single rubber molecule does not possess the property of elasticity. As the number of rubber molecules in a group increases, they interact with each other and produces the property of elasticity. The property of elasticity in a system of rubber molecules is not deducible from the properties of the rubber molecules in isolation. Bar-Yam (2004) defines this as a type of emergence as strong and the result of the interdependencies/ couplings of the parts into an ensemble or collective. These are emergents in the same sense that Broad (1925) discusses unique properties as a function of the uniqueness of component configurations. The states of interdependent / coupled parts are dependent on the inputs, outputs, and feedback from other parts. When components are studied in isolation the states (and their properties) that are dependent on other parts are not observed. When the components are assembled the dependent states are produced and emergent effects are observed. Bar-Yam refers to the difference between interdependencies at various scales in the system as multiscale variety (or complexity). The other properties lost when observing parts in isolation (i.e., at lower scales) are the effects of constraints on the systems and its components. A constraint puts limits on the system or certain configurations or “collectives” of parts within the system. When observation scales are in context with the entire systems, behaviors are observed that are not observable when the scale is at the subsystem level. This is the essence of what Bar-Yam refers to as multi-scale complexity. Strong emergents that appear not to be logically deducible, are actually deducible from observations of the system from a large scale perspective as a whole rather than observations at lower level scales (subsystem). The stronger variety of emergence is typically found in systems (natural or constructed) that have feedback structures and goal seeking behavior. These systems may evolve over time but not necessarily in the case of constructed systems.

Conceptual elements identified from Ashby (1956) and Bar-Yam (2004):

As1, Emergents are actually predictable behaviors of the system but are *apparently unpredictable due to limited visibility of system parts and their coupling relationships.*

As2. Visibility of the parts and relationships in a system diminishes as the complexity of the system becomes greater than the complexity of its parts.

As3. Complexity of a system increases as a function of the number of system variables and the number of possible states that can be produced from the same set of variables.

Ba1. Weaker emergents are properties/behaviors of groups of components (i.e., subsystems) that are difficult to deduce because the density of information at lower scales obscures the view of properties at higher scales

Ba2. Stronger emergents are properties of the system or subsystems (i.e., scales within a system) that are not applicable to its members and vice versa and are only derivable by observing the system at large rather than scales at the subsystem or component level.

Ba3. Stronger emergents are produced when constraints exist (or evolve) that are applicable to the system or a scale but not to individual parts; and when there are properties associated with the interdependence of parts in a system (i.e, complexity).

As4, Ba4. Applied concept to naturally occurring and human constructed things: Chemistry, biology, physics, phycology

Throughout the literature on emergents the term novelty (i.e., new) is often encountered. In the sense that novelty is new property it is an observation or experience by an observer; it is extrinsic. Crutchfield (1994) considers phenomena found in nature (flocking birds; ant societies, optimal pricing in economies, etc.) and concludes that there is another type of novelty; one that is based on new functionality within the system rather than spatial-temporal or logical novelty as encountered by an outside observer. In this case intrinsic emergents, new patterns appear overtime from the non-linear interactions of subsystems and lower level components but are not directly defined by the constraints and forces in the system. This definition is similar to others where "new" or novelty is associated with properties of the system that are not readily explainable in terms of it components. The critical difference being properties referenced in other emergent definitions are observer dependent, while Crutchfield's offers a definition that is intrinsic to the system and observer independent. The qualification that the "new patterns" are intrinsic emergents, is that the consequence of their existence the system (and the user within the system) gains new capabilities and is able to perform new functions. The phase transition where new patterns become intrinsically important is dues to an increase in the system's information processing which is indicated by an increase in Shannon entropy. He proposes that behavioral models (i.e., computer simulations) representing the system, its constituents and its environment can be used to explain intrinsic emergents and represent the emergence transition phase. Models eliminate the subjectivity and computational limitations of observers by identifying new patterns that form over time, and allow agents in the system to perform new functions and capabilities.

Another functional concept of emergents is that certain properties have the ability/"causal power" to bring about other properties within or between levels in the system. System properties are emergent if they have causal powers that are not explainable in terms of or predicable from system constituents (Kim, 1999). Emergent properties manifest causal powers by bringing about other properties at the same level; at a higher level (upward); or at a lower level (downward causation). Upward and same level causation have general acceptance. However, one of the controversies in emergence literature is the concept of downward causation because it seems to suggest that something can cause changes in the very constituents from which it is composed. Kim is referring to downward causation as defined by Campbell (1974) where the causal powers exist at different times for different levels (diachronic) rather existing simultaneously at the same time (synchronic). The time delay allows the causal roles to switch between levels and within levels. Initially one effect produces properties that causes a subsequent effect with properties at the same or a different level. Time elapses and eventually what were the subsequent effects and properties cause changes in the properties of their constituents. The cycle repeats with the causal roles switching over time. In Kim's functional concept of emergents, only consciousness and mental phenomena (i.e., the metaphysical domain) meet the criteria for emergents in the strictest sense of being unexplainable and unpredictable. Otherwise, it is theoretically possible for the causal powers of the non-metaphysical to be predicted and explained with knowledge of the physical roles of their constituent parts and the laws that govern their relationships.

Conceptual elements identified from Crutchfield (1994), and Kim (1999):

Cr1, Ki1. Novelty of emergents is intrinsic and observer independent because they provide new internal capabilities.

Cr2, Ki2 Emergents develop over time at various levels in the system.

Cr3. Emergents patterns/structures are explainable in terms of the non-linear interactions of their system constituents by using behavioral models.

Cr4. An increase in information processing (Shannon entropy) is an indication of emergence.

Ki3. Emergents properties are not even theoretically explainable or predicable by any means based on system constitutes.

Cr5. Applies the concept to naturally occurring and human constructed things.

Ki4. Limits emergents to consciousness and mental phenomena of mind /body relationships (metaphysical concepts).

Bedau's (1997) introduces a concept where emergents exist in varying degrees based on derivability. In all degrees of emergents share the characteristic of not being properties at higher levels of structures that do not exit at lower levels. The variation occurs in terms of being logically derivable/ logically predictable base on lower level constituents. In the nominal case, the derivability/logical predictability exist due to limited knowledge of the observer. Weak emergents are derivable (i.e., logically predictable) but doing so is very difficult. Strong emergence entails properties that are reductively unexplainable by their micro processes even with perfect information about governing laws and component interactions. Nominal emergents are trivial in Bedau's concept given that they can be resolved with variable information. Strong emergence has the suggestion of an outside force/power beyond the components in the systems. Bedau is among those that are skeptical that strong emergence exist, and consider it scientifically irrelevant beyond questions related to consciousness and mind/body relationships. With these extremes in mind, the most relevant case of emergence is "weak". The difficulty that defines weak emergents in Bedau's (1997) concept has to do with aggregating "non-linear and context-dependent" interactions of lower level constituents into the higher level properties. The non-linear reference suggest that small changes result in large effects and context-dependence indicates that the effects vary over space and time. To capture this dynamic, Bedau defines weak emergents as underivable without simulation where simulation represents the iterative aggregation that must take place to yield the emergent property. The explanation / prediction difficulty as described by Bedau is intrinsic to the system and is not due to any limitation on human capability or computational power.

Maier (2015) presents a concept of emergence that is similar to Bedau (1997). Both authors fundamentally define emergents as properties of the system that are not possessed by its components; and both includes degrees of emergence based on derivability. Bedau attributes emergents to the aggregation of microstate into higher level macro sates, and Maier to information and material exchanges between systems of systems (independent systems and system components). Where Bedau distinguishes degrees of emergence based on derivability and available information; Maier (2015) distinctions are based on derivability and the complexity of models that represent the system: 1) emergents are simple when they can be readily derived without observation from low complexity mathematical models that represent system behaviors but not the interactions of the system components; 2) emergents are weak when the properties can be readily derived after observation but only by high complexity simulation models that represent the interactions of the system components: 3) emergents are strong when they are inconsistently derivable high complexity simulation models even after observation; and 4) emergent are spooky when they are completely underivable even after observation and with the most complex simulation model that fully represents all details of the system.

By describing emergent in terms of their derivability, Bedau (1997) and Maier (2015) are in essence capturing a reductionist type perspective of emergence. A very simplified reductionist perspective would be that all systems are completely generated by their components and rules governing their interactions. Some system properties are apparently irreducible (i.e., novel relative to the properties of the components), but actually all system properties are explainable and derivable from system components and sufficient knowledge of the rules governing their interactions (Broad, 1925; Bertalanffy, 1956). Bedau's Strong emergents and Maier's Spooky emergents are inconsistent with this type of reductionist perspective. While it may be philosophically interesting, there are no examples or evidence where strong/spooky emergence in a physical context has or will exist outside the realm of human consciousness and mental phenomena.

Conceptual elements identified from Bedau (1997) and Maier (2015):

Be1, Ma1. Though emergents are properties of systems that cannot be possessed by their constituents, they can be reductively explained through an iterative aggregation process but it is inherently difficult to do so (i.e., they are intrinsic).

Be2, Ma2. Emergents vary in their degree of difficulty to explain, reduce / reproduce. Its strongest form is limited to consciousness and mental phenomena of mind /body relationships and are not explainable/ predictable even in theory.

Be3. Interactions that produce emergents are nonlinear and vary over space and time.

Ma3. Emergents are produced by information as well as material exchanges between independent systems and system components.

Be4, Ma4. Only reductively explainable emergents are scientifically relevant and applicable to natural and human constructed things, except in its strongest form which is limited to consciousness and mental phenomena of mind /body relationships.

J.H. Holland (1998) studies games and human neurons to identify mechanisms and conditions that foster emergents. His concept of emergents is intrinsic and "weak" in the same sense described by Bedau (1997): properties of higher levels are not present at lower levels and predicting them is inherently difficult but possible. He disagrees that emergents are necessarily a "novel" phenomenon in the sense of be something new. He posits that emergents are recognizable, persistent, and reoccurring patterns (or behaviors) in systems whose logical explanation or reduction in terms system components is difficult. J.H. Holland (1998) makes the point that such an explanation or reduction is only possible when component interactions are taken into account. However, even with the availability of perfect laws that govern the system's interactions, prediction and explanation of patterns are so inherently difficult that when they occur, these patterns (or behaviors) are apparently novel and therefore emergent. The difficulty referenced in Holland's concept is due to the size of system's state space (i.e., all possible arrangements and values of system components) that produce the patterns. The state space for certain systems can increase to such a size that there is perpetual discovery of what appears to be novel outcomes, i.e., emergents. Certain system characteristics contribute to or cause the state space to increase:

- *Multiple component types and instances*. The more components there are the greater the number of possible combinations.

- *Coupled components*. The inputs and outputs of components are connected via to each other making each one dependent on the other (i.e., interdependent).
- *Component interactions are non-linear*. The input and output component functions are exponential.
- *Governing Rules.* Rules determine the ways and conditions for interactions of each type of component can interact and provide constraints for the possible system states.
- *Variable Strategies to accomplish goals.* States vary in priority according to their ability to accomplish goals within the rules and change based on learning from feedback.
- *Multiple paths to the same state*. Aggregating inputs and outputs of different component configurations can produce the same system level state. Numbers of paths per system state is in essence complexity as defined by Ashby (1956).

The characteristics are not intended to be essential elements or required criterion for emergence. J.H. Holland presents them as some of the identifying characteristics of systems that produce emergents. Each characteristics has a causal influence on increasing the system state space. The more systems possess these characteristics the more likely emergents will be encountered.

Conceptual elements identified from J.H. Holland (1998):

J.H. Hol1. Emergents are reoccurring system patterns/behaviors that are apparently unexplainable in terms of system components.

J.H. Hol2. The number of system states is so great that it is inherently difficult (yet possible) to explain, reduce, or predict emergents based on their constituents and governing rules.

J.H. Hol3. The likelihood of encountering emergents increases as the number and type of system components increases.

J.H. Hol4. The likelihood of encountering emergents increases with greater coupling between components.

J.H. Hol5. System inputs are aggregates with exponential functions (i.e., non-linear).

J.H. Hol6. The likelihood of encountering emergents increases as the number of governing rules decreases relative to the number of component types.

J.H. Hol7. The likelihood of encountering emergents increases as learning (i.e., changes based on feedback relative to goals) increases.

J.H. Hol8. The likelihood of encountering emergents increases as number of paths per system state increases (i.e., increase in complexity).

J.H. Hol9. Applied concept to naturally occurring and human constructed things: Chemistry, biology, physics.

B.2 Reference Model and Ontology of Emergence

Reference models are sets of unstructured statements representing what is known and assumed about a subject (Tolk et al., 2013). The intent is to capture a comprehensive view of the subject from relevant perspectives; including inconsistent or conflicting interpretations. The collection of conceptual elements captured in the literature review can be considered a reference model of the emergence concept. Using the reference model to build an ontology further explains the concept by providing a structured representation of its essential elements.

The essential elements formally represented by the ontology are the main ideas that are used to explain what emergence is and how it occurs. Each idea has its own set of defining characteristics and relationships that provide the structure for the concept. In the ontology the main ideas are called “classes” and their structural characteristics are “properties” (Noy & McGuinness, 2001). The ontology is built through an iterative process of searching the reference model for its main ideas (classes) and defining characteristics (properties), then mapping their relationships. In this dissertation mapping was performed in the Protégé ontology tool.

The characteristics of emergents and the systems that exhibit them are captured in a reference model (see below) and used to build an ontology of the concept. The ontology of emergence including a mapping of theories to classes, subclasses and properties is presented in detail in Figure 21 of this appendix and at a summary level in Figure **5** of Chapter Three.

Source Identifier	Conceptual Element	Class	Sub-Class
Le1, Mi1	Emergents are system effects that are not presently traceable to deducible from the properties and interaction process steps of its components, but may become as so in the future as knowledge improves.	Phenomena	Type = Qualities/Properties
			Logical Relationships= Theoretically Explainable/ Derivable
			Perspective = Extrinsic
		Systems	Structure = Coupled / Interconnected
			Temporality = Synchronic
			Knowledge Constraint = Experience/Observations
Le2, Mi2.	Emergents are indicated by non-linear interactions and increase uncertainty about the effects produced by the interactions.	Phenomena	Indicator = Nonlinearity; Uncertainty;
Mi3	Emergents exist when laws that govern combinations of physical facts are different from the laws that govern them separately.	Systems	Structure = Dissimilar Laws
			Temporality = Synchronic
Le3	Emergents are caused by the interaction between unlike (incommensurable) component properties and are incommensurable with the properties of their components.	System	Structure = Dissimilar Parts
			Temporality = Synchronic
Le4	Applied concept to naturally occurring and human constructed things: Chemistry, biology, physics, phycology, philosophy	Systems	Domain =Natural (physical) ; Engineered (physical); Natural (metaphysical)
Mi4	Applied concept to physical phenomena: Physics (inanimate objects and events, i.e., phenomena), Biology (living bodies); Chemistry (chemical reactions).	Systems	Domain =Natural (physical) ; Engineered (physical)
Al1, Mo1	New hierarchical configurations of a system form over time.	Systems	Structure = Hierarchical
			Temporality = Diachronic

Table 20. Reference Model for Emergence

Table 20 (continued)

Al2, Mo2.	The uncertainty of the system properties increases with the addition of new configurations.	Phenomena	Indicator = New configurations; Uncertainty
Al3, Mo3	Emergents are qualities or properties of material existents (i.e., wholes) that are unique to each hierarchical level that form a structure over time and are only predicable/deducible with observation/experimentation.	Phenomena	Type = Qualities/Properties
			Logical Relationships = Theoretically Explainable/ Predictable
			Perspective = Extrinsic
		Systems	Structure = Hierarchical
			Temporality = Diachronic
			Knowledge Constraint = Experience/Observations
Br1	Physical emergents are latent qualities unique to component configurations and are only theoretically deducible after observation.	Phenomena	Type = Qualities/Properties
			Logical Relationships = Theoretically Explainable/ Derivable
			Perspective = Extrinsic
		Systems	Structure = Hierarchical
			Temporality = Diachronic
			Knowledge Constraint = Experience/Observations
Br2	New configurations indicates a potential for emergent properties.	Phenomena	Indicator = New configurations; Uncertainty
Br3	Things are composed of multiple layers of part configurations.	Systems	Structure = Hierarchical
			Temporality = Synchronic
Br4	Mental Emergents are qualities or properties of the mind that are not observable or deducible in terms of its constituents parts (the body).	Phenomena	Logical Relationships = Not Explainable/ Predictable
		System	Domain = Natural (metaphysical)

Table 20 (continued)

Al4, Mo4	Applied concept to material things: Chemistry, biology, physics,	System	Domain =Natural (physical) ; Engineered (physical)
As1	Emergents are actually predicable behaviors of the system but are apparently unpredictable due to limited visibility of system components and coupling/interdependent relationships.	Phenomena	Type of Effect = Behaviors
			Logical Relationships = Theoretically Explainable/ Derivable
			Perspective = Extrinsic
		Systems	Structure = Coupled / Interconnected
			Temporality = Synchronic
			Knowledge Constraint = Observation Inaccessibility
As2	Visibility of the parts and relationships in a system diminishes as the complexity of the system becomes greater than the complexity of its parts.	System	Structure = Dissimilar size/complexity of parts vs system
As3	Complexity of a system increases as a function of the number of system variables and the number of possible states that can be produced from the same set of variables	Phenomena	Indicator = Complexity
Ba1	Weaker emergents are properties or behaviors of groups of components (i.e., subsystems) that are difficult to deduce because the density of information (i.e., complexity) at lower scales obscures the view of properties at higher scales	Phenomena	Effect = System Behaviors; System Properties
			Logical Relationships = Theoretically Explainable/ Derivable
			Perspective = Extrinsic
			Indicator = Information
			Type =Properties or behaviors
		System	Structure = Hierarchical
			Temporality = Synchronic
			Knowledge Constraint = Information Density

Table 20 (continued)

Ba2	Stronger emergents are properties of the system or subsystems (i.e., scales within a system) that are not applicable to its members and vice versa and are only derivable by observing the system at large rather than at subsystem or components.	Phenomena	Logical Relationships = Theoretically Explainable/ Derivable
			Perspective = Extrinsic
Ba3	Stronger emergents are produced when constraints exist (or evolve) that are applicable to the system or a scale but not to individual parts; and when there are properties associated with the interdependence of parts in a system (i.e, complexity).	System	Structure = Hierarchical
			Temporality = Synchronic ; Diachronic
			Knowledge Constraint = Visibility of Whole System; Visibility of Coupling Relationships
		Phenomena	Indicator = Complexity
As4, Ba4	Applied concept to naturally occurring and human constructed things: Chemistry, biology, physics, phycology	System	Domain =Natural (physical) ; Engineered (physical)
Cr1, Ki1	Novelty of emergents is intrinsic and observer independent because they provide new internal capabilities.	Phenomena	Perspective = Intrinsic
Cr2, Ki2	Emergents develop over time at various levels in the system.	System	Structure = Hierarchical
			Temporality = Diachronic
Cr3	Emergents patterns/structures are explainable in terms of the non-linear interactions of their system constituents by using behavioral models	Phenomena	Logical Relationships = Explainable/ Derivable
			Type of Effect = Patterns/Structures
			Indicator = Nonlinearity
		System	Knowledge Constraint = Modeling Capability
Ki3	Emergents properties are not even theoretically explainable or predicable by any means based on system constitutes.	Phenomena	Logical Relationships = Not Explainable/ Derivable
			Type of Effect = Properties/Qualities
			Indicator = Uncertainty
		System	Knowledge Constraint = Human Comprehension

Table 20 (continued)

Cr4	An increase in information processing (Shannon entropy) is an indication of emergence.	Phenomena	Indicator = Information; Shannon Entropy
Cr5	Applies the concept to naturally occurring and human constructed things.	System	Domain =Natural (physical) ; Engineered (physical)
Ki4	Limits emergents to consciousness and mental phenomena of mind /body relationships.	System	Domain = Natural (metaphysical)
Be1, Ma1	Though emergents are properties of systems that cannot be possessed by their constituents and are apparently reductively unexplainable, they can be reductively explained through an iterative aggregation process but it is inherently difficult to do so (i.e., they are intrinsic).	Phenomena	Logical Relationships = Explainable/ Derivable
			Type of Effect = Qualities/Properties
			Perspective = Intrinsic
		System	Knowledge Constraint = Inherent Difficulty (iterative aggregations)
Be2, Ma2,	Emergents vary in their degree of difficulty to explain, reduce / reproduce. Its strongest form is limited to consciousness and mental phenomena of mind /body relationships and are not explainable/ predictable even in theory.	Phenomena	Logical Relationships = Not Explainable/ Derivable
		System	Domain = Natural (metaphysical)
Be3	Interactions that produce emergents are nonlinear and vary over space and time.	System	Temporality = Diachronic
		Phenomena	Indicator = Nonlinearity
Ma3	Emergents are produced by information as well as material exchanges between independent systems and system components.	System	Structure = Coupled/Interconnected
			Temporality = Synchronic
		Phenomena	Indicator = Information
Be4, Ma4	Only reductively explainable emergents are scientifically relevant and applicable to natural and human constructed things.	System	Domain =Natural (physical) ; Engineered (physical)

Table 20 (continued)

J.H. Hol1	Emergents are reoccurring system patterns/behaviors that are apparently unexplainable in terms of system components.	Phenomena	Type of Effect = Behaviors
		System	Temporality = Diachronic
J.H. Hol2	The number of system states is so great that it is inherently difficult (yet possible) to explain, reduce, or predict emergents based on their constituents and governing rules.	Phenomena	Perspective = Intrinsic
			Logical Relationships = Explainable/ Derivable
			Indicator = Number of system states (complexity)
		System	Knowledge Constraint = Inherent Difficulty (size of system state space)
J.H. Hol3	The likelihood of encountering emergents increases as the number and type of system components increases.	System	Structure = Multiple Component Types and Instances
		Phenomena	Indicator = Variety of components (complexity)
J.H. Hol4	The likelihood of encountering emergents increases with greater coupling between components.	System	Structure = Coupled/Interconnected
J.H. Hol5	System inputs are aggregates with exponential functions (i.e., non-linear).	Phenomena	Indicator = Nonlinearity
J.H. Hol6	The likelihood of encountering emergents increases as the number of governing rules decreases relative to the number of component types.	System	Structure = Governing Rules << Component Types
		Phenomena	Indicator = Number of rules vs number components (complexity)
J.H. Hol7	The likelihood of encountering emergents increases as learning (i.e., changes based on feedback relative to goals) increases.	System	Structure = Learning (Δ based on feedback vs goals)
J.H. Hol8	The likelihood of encountering emergents increases as number of paths per system state increases (i.e., complexity).	System	Structure = Multiple Paths Per System State
		Phenomena	Indicator = Complexity
J.H. Hol9	Applied concept to naturally occurring and human constructed things.	System	Domain =Natural (physical) ; Engineered (physical)

Source Identifier	Reference	Abstract
Al1- Al4	Alexander (1920)	New qualities unique to a group of things that does not belong to the things individually.
As1 – As6	Ashby (1956)	System properties are not readily derivable/ explainable in terms of its parts.
Ba1- Ba5.	Bar-Yam (2004)	A system property not captured by its parts
Be1 – Be6	Bedau (1997)	Phenomena that is constituted by, yet autonomous from its underlying processes.
Br1- Br3.	Broad (1925)	A quality belonging to the whole and not to its parts.
Cr1 – Cr3.	Crutchfield (1994)	A property creating new functionality within the system
J.H. Hol1 - J.H. Hol9	Holland, J.H. (1998)	Reoccurring patterns that are intrinsically difficult to explain
Ki1 – Ki3.	Kim (1999)	Novel properties that seems to transcend their constituent parts
Le1- Le5	Lewes (1875)	Properties of wholes not traceable to interactions of dissimilar components.
Ma1 - Ma5	Maier (2015)	System functions that do not reside in any component.
Mi1- Mi4	Mill (1846)	Separate effects ≠ combined effects.
Mo1- Mo3	Morgan (1929)	Evolution of higher level configurations “so far” not deducible from the lower level parts.

Table 21. Source Identifier Definition

		Lewes (1875)	Mill (1846)	Alexander (1920)	Morgan (1929)	Broad (1925)-physical	Broad (1925) - mental	Ashby (1956)	Bar-Yam (2004)-weak	Bar-Yam (2004)-strong	Crutchfield (1994)	Kim (1999)	Bedau (1997) - weak	Bedau (1997) - strong	Maier (2015) -weak/strong	Maier (2015) -spooky	Holland, J.H. (1998)
mona Characterisitics																	
Type																	
	Qualities/Properties	X	X	X	X	X	X		X	X		X	X	X	X	X	
	Behaviors							X	X								X
	Patterns										X						X
	Structures										X						
Logical Reltionships																	
	Explainable/Derivable										X		X		X		X
	Not Explainable/Derivable						X					X		X		X	
	Theoretically Explainable/Derivable	X	X	X	X	X		X	X	X							
Perspective																	
	Intrinsic					X	X		X	X	X	X	X	X	X	X	X
	Extrinsic	X	X	X	X			X									
Indicator																	
	New configurations			X	X												
	Complexity							X						X			X
	Nonlinearity	X	X								X						X
	Uncertainty	X	X	X	X							X					
	Information										X		X		X	X	
	Shannon Entropy										X						
Characteristics																	
Application Domain																	
	Engineered (physical)	X	X	X	X	X		X	X	X	X		X		X		X
	Natural (physical)	X	X	X	X	X		X	X	X	X		X		X		X
	Natutal (metaphysical)	X					X					X		X		X	
Structure																	
	Coupled / Interconnected	X	X					X							X	X	X
	Dissimilar size/complexity of parts vs system							X									
	Dissimular Laws		X														
	Dissimular Parts	X															
	Governing Rules << Component Types																X
	Hierarchical			X	X	X	X		X	X	X	X					
	Learning/Adapability (Δ based on feedback vs goals)																X
	Multiple Component Types and Instances																X
	Multiple Paths Per System State																X
	Non-linear Interactions										X		X	X			X
Temporality																	
	Synchronic	X	X			X	X	X	X	X				X	X		
	Diachronic			X	X					X	X	X	X				X
Knowledge Constraint																	
	Experience/Observations	X		X	X	X											
	Observation Inaccessibility							X									
	Information Density								X								
	Visibility of Whole System									X							
	Visibility of Coupling Relationships									X							
	Modeling Capability										X						
	Human Comprehension						X					X		X		X	
	Inherent Difficulty (iterative aggregations)												X		X		
	Inherent Difficulty (size of system state space)																X

Figure 21. Detailed Ontology of Emergence

B: THERMOCHEMISTRY CONCEPTS

Thermochemistry is a branch of Thermodynamics, a science concerned with the transformation and transfer of heat and other types of energy during a change in the state of a system (Brown et al., 2014; Daintith, 2008; Linder, 2011). It consists of axiomatic laws that govern the dynamics of changes in system components that are brought about by changes in system energy (Haddad et al., 2005). Thermochemistry is the portion of thermodynamics that is concerned with the relationship between energy changes and chemical reactions. Chemical reactions are an example of a thermodynamic process and offers a point from which thermochemical concepts can explored.

By convention and supported by a variety of sources, the following summary of introductory definitions and concepts serve as a prerequisite for a more detailed discussion on the process of chemical reactions (Balmer, 2010; Brown et al., 2014; Harris et al., 2008; Ekambaram, 2013; Linder, 2011; Kumar, 2013; Rajaram, 2013)

Chemical substance: A Chemical substance (or species) is composed of submicroscopic parts (molecules) that are connected in a specific configuration. The ensemble of parts possesses distinct properties and characteristics: color, odor melting point, boiling point, flammability, etc. The structure and properties of a substance do not vary regardless of the quantity (volume); state (solid, liquid, gas, and plasma); or shape (physical dimensions) that it is observed.

Chemical system: When one chemical substance is combined with another or with multiple substances, a chemical system is formed. The new structure has macro level properties and characteristics that are not present in the properties of the chemical substances from which it is composed. The tangible component (i.e., matter) in chemical system are the molecules that compose each substance. They also possess the intangible component of energy. Systems can be classified based on how they interact with their environment in terms of sharing matter and energy: open systems exchange matter and energy with the environment; closed systems exchange energy but not matter; and isolated systems do not interact with their environment.

Energy: Energy is the capacity to make a change in an entity's spatial position (the capacity to do work) or to change its temperature (the capacity to transfer heat). A chemical substance gets its energy from its molecules which derived their energy from the behaviors of their atom and subatomic particles. Some of the particles in the molecules have electrical charges (positive, and negative) where opposite charged particles are attracted and same charged particles are repelled. The repulsion / attraction forces from the electrical charges cause the particles to move and collide with each other (i.e., that have kinetic energy). The closer the particles are to each other the greater the repulsion / attraction forces and the greater their potential energies. The internal energy (U) of a system is to sum of the kinetic and potential energies of its particles and molecules. It is the energy required to form the system.

1st Law of Thermodynamics: The axiomatic law states that energy cannot be created or destroyed. Also known as the conservation of energy, the 1st law of thermodynamics governs the energy change in a system. A change in the system's internal energy requires it to transfer energy to its environment or vice versa (see Figure 22.).

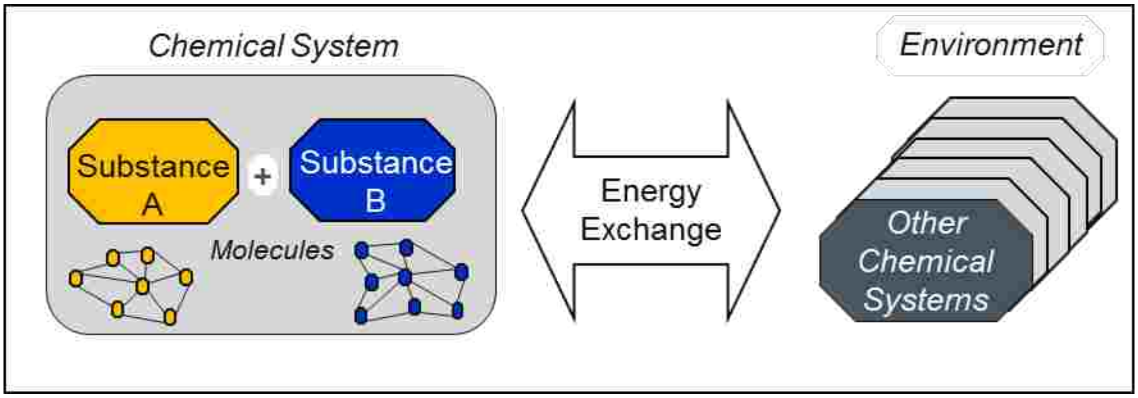

Figure 22. Conservation of Energy

Measuring internal energy is difficult. However, the evidence of a change in internal energy is more readily available. Internal energy (U) of the system is evidenced by the work (W) done on / by the system and /or the heat (Q) transferred to / from the system. The energy in the environment and the internal energy of a chemical system can increase or decrease, but the total energy of the chemical system plus the environment remains unchanged. For chemical systems that exchange energy with their environments, the change in the system's internal energy is sum of heat (Q) transferred to/from that system and work (W) done on/by the system. The change in internal energy (U) is then given by equation [4.1].

$$\Delta U = Q + W \qquad \text{[C.1]}$$

Chemical reaction: A chemical reaction is a process where the parts of chemical systems (the reactants) are separated by heat energy and then reassembled into a different configuration (the product). The product of the reaction is a new chemical system with new properties that are different from the properties of the reactants (i.e., they are emergents). The parts (molecules) in a chemical system are held together by forces (bonds). Energy is required to break the bonds between the parts of the reactants and to make new bonds between the reconfigured parts in the product. The stronger the bonds are in the reactants, the greater the amount of energy that will be required to break them and form the product. In order for the reaction to take place, there must be a sufficient change in the systems internal energy (*U*) to break the bonds that are holding the molecules of the reactant together.

Enthalpy: Heat is a transfer of energy that causes a change in temperature. Heat is not contained in a system; it is a condition of energy exchange between systems and or their environment. Enthalpy (i.e., “to warm”) is known by several names including heat content; heat function, and the total heat, where heat is a transfer of *energy*. Enthalpy (*H*) is also the total energy of the system. It is similar to internal energy (*U*) in that both U and H include the energy to form the system. They differ in that H include additional work energy required to displace or change its environment and U does not. The additional work energy is the pressure (*P*) in the system that is applied to the change in the system’s volume (*V*).

$$H = U + PV \qquad [C.2]$$

Many chemical systems occur under constant pressure and have negligible changes in volume. When this is the case, the change in enthalpy (U) reduces to then heat transfer component of internal energy (*U*).

$$\Delta H = \Delta U = Q \qquad [C.3]$$

The change in enthalpy (H) is the heat energy (Q) transferred between a system and its environment at constant pressure.

Entropy: Entropy (S) is the amount of disorder or randomness in a system. Order in a system is defined as predictability of system macro states of based on the configurations of system components (i.e., its microstates). A change in the number of system macro states results in a change in the number of possible microstates. If each microstate has an equal probability of occurrence, then system disorder (i.e., lack of predictability) is proportional to the number of microstates (W). Disorder can be measured using Boltzmann's equation for entropy [C.4].

$$S = k \times ln\,(W) \qquad [C.4]$$

$$\Delta S = k \times ln\,(W_{final} \div W_{initial})$$

Where, k (Boltzmann's constant) $=1.38 \times 10^{-23}$ J/K

Equilibrium: The state of the system when there are no changes in its properties over time is the state of thermodynamic equilibrium where there is: no change in its internal energy (thermal equilibrium); no change in its chemical composition or concentration (chemical equilibrium); and no work performed on or by the system (mechanical equilibrium). Equilibrium is a special case of system steady state (sometimes known as dynamic equilibrium) where the properties of the system are changing but they are balanced with changes in opposite directions: transfer of energy in = transfer of energy out; forward reaction = reverse reaction; work done on the system = work done by the system. Steady state condition is where the net change in the system's properties over time is zero. In both equilibrium and steady state, the systems is considered to be at rest.

Spontaneity: Given a set of conditions, some chemical reactions are favored to occur or naturally evolve over time (i.e., they are spontaneous). While the conditions can be artificially created, the actual exchange of energy will naturally occur in one direction, if given enough time and no other interventions are made. For example, ice will spontaneously absorb energy from the environment if the environment's temperature is greater than that of the ice. Unless there is some sort of interventions the ice will eventually melt and its state will change from solid to liquid and eventually to vapor. The same is true in the opposite direction for a hot cup of chocolate. The heat from the liquid will transfer to its environment if the environment's temperature is less than that of the liquid. Three important characteristics of spontaneous reactions are: 1) they only occur in one direction; 2) they are irreversible without the addition of more energy to force them in the opposite direction; 3) they tend toward a point of thermodynamic equilibrium.

2nd Law of Thermodynamics: While the First Law of Thermodynamics requires that energy is conserved, it does not specify how energy flows such that conservation is maintained. The Second Law of Thermodynamics complements the First Law by addressing the nature of the flow of energy in a system. The axiomatic law states that energy spontaneously flows from the highest source of energy to the lowest: high heat to low heat; high pressure to low pressure; high potential to low potential. The flow of energy in spontaneous processes can result in either a positive or negative change in the entropy (disorder) for the system ($\Delta S_{)}$. However, the change in total entropy for the universe ($\Delta S_{univ)}$ is always positive. The change in total entropy (ΔS_{univ}) is the sum of the changes in entropy for the system ($\Delta S_{)}$ and the changes in entropy for the environment ($\Delta S_{environment}$).

$$\Delta S_{univ} = \Delta S + \Delta S_{environment} > 0 \qquad [C.5]$$

Changing the number of possible microstates and consequently the entropy in a chemical systems occurs when there is a sufficient change in the system's internal energy. Chemical reactions change the internal energy of a chemical system. If the internal energy increases (increasing microstates, increasing entropy), the chemical reaction is endothermic. If the internal energy decreases (decreasing microstates, decreasing entropy), the chemical reaction is exothermic.

C: MODEL DOCUMENTATION

(01) Absorption Capacity= RANDOM UNIFORM (0.25, 0.5, Seed)
Units: Dmnl [0.01,1,0.001]

(02) "Activation Information Threshold (Ia)"= (0.1*"Variety of Regulators (Vr)"^2+0.9)*"Initial Activation Information Threshold (Ia@t=0)"
Units: I Units

(03) "Activation Ratio for Information (ARI)"=0.5
Units: Dmnl [0.5,1.5,0.01]

(04) CC Multiple=0.2
Units: Dmnl [0.01,10,0.01]

(05) "Change in Information (ΔI)"=IF THEN ELSE(("Internal Information (I)"-"Initial Internal Information (Ii)")<0,0,"Internal Information (I)"-"Initial Internal Information (Ii)")
Units: I Units

(06) "Component Concentration (Cc)"=0
Units: Dmnl [0,1,0.01]

(07) "Degrees of Freedom (Df)"=0
Units: Dmnl [0,1,0.01]

(08) Df Multiple=0.2
Units: Dmnl [0.01,20,0.01]

(09) "External Information (Ie)"= "Activation Ratio for Information (ARI)"*"Initial Activation Information Threshold (Ia@t=0)"

Units: I Units

(10) FINAL TIME = 5000

Units: Minute

The final time for the simulation.

(11) "Fractional Reception Time (Rt)"= "Reception Xmission Multiple (RXM)"*"Fractional X-mision Time (Xt)"

Units: 1/Minute [0.01,10,0.001]

(12) "Fractional X-mision Time (Xt)"=0.1

Units: 1/Minute [0.01,1,0.01]

(13) "Information Differential (Id)"= INTEG (IF THEN ELSE("Information Differential (Id)"<=0,0,-"Reception Rate (Rr)") "External Information (Ie)"-"Initial Internal Information (Ii)")

Units: I Units

Information available for reception by the system

(14) "Information Ratio of Emergence (IRE)"= SAMPLE IF TRUE(PULSE TRAIN(0, TIME STEP , SAVEPER, FINAL TIME):AND:"IRE (ΔI/ΔItp)" >=1,1,0)

Units: Dmnl

(15) "Information Tipping Point (ΔItp)"="Activation Information Threshold (Ia)"-"Initial Internal Information (Ii)"

Units: I Units

(16) "Information Transferred (Ix)"= INTEG ("X-mission Rate (Xr)",0)

Units: I Units

Transmitted from the system and received by the environment

(17) "Initial Activation Information Threshold (Ia@t=0)"=2000

Units: I Units [1000,5000,10]

Must be > Initial Internal Information (Ii)

(18) "Initial Internal Information (Ii)"=1000

Units: I Units [100,5000,1]

(19) INITIAL TIME = 0

Units: Minute

The initial time for the simulation.

(20) Int Multiple=0.2

Units: Dmnl [0.01,10,0.01]

(21) "Internal Information (I)"= INTEG ("Reception Rate (Rr)"-"X-mission Rate (Xr)", "Initial Internal Information (Ii)")

Units: I Units

Total information in the system

(22) "Interoperability (Int)"=0

Units: Dmnl [0,1,0.01]

(23) "IRE (ΔI/ΔItp)"=(("Change in Information (ΔI)"/"Information Tipping Point (ΔItp)"))+IRE Noise

Units: Dmnl

(24) IRE Noise=IF THEN ELSE(IRE Pink Noise>MaxNoise,MaxNoise,IRE Pink Noise)
Units: Dmnl

(25) IRE Pink Noise= RANDOM PINK NOISE(Mean Pink, Std Pink, Time Pink, "Seed (IRE)")
Units: Dmnl

(26) "Ix Gap (Ig)"="External Information (Ie)"-"Initial Internal Information (Ii)" "Information Transferred (Ix)"
Units: I Units

(27) MaxNoise=0.99975
Units: Dmnl [0.1,1,0.01]

(28) Mean Pink=0
Units: Dmnl [-1,1,0.0001]

(29) "Reception Rate (Rr)"=IF THEN ELSE("Information Differential (Id)"<=0,0,"Internal Information (I)"*(1-"Internal Information (I)"/("Internal Information (I)"+"Information Differential (Id)"))*(EXP(1*CC Multiple*"Component Concentration (Cc)")*(1*Df Multiple*"Degrees of Freedom (Df)"+1)*EXP(1*Int Multiple*"Interoperability (Int)"))*"Fractional Reception Time (Rt)"/1000)
Units: I Units/Minute

(30) "Reception Xmission Multiple (RXM)"=1
Units: Dmnl [1,5,0.01]

(31) SAVEPER = 250

Units: Minute [0,1000,25]

The frequency with which output is stored.

(32) Seed=0

Units: Dmnl

(33) "Seed (IRE)"=0

Units: Dmnl

(34) Std Pink=0.5035

Units: Dmnl [0.01,2,0.0001]

Best 2nd Order Fit = 0.5035 (1458 sample;w/time =.13;SAVEPER =250) Best 3rd Order Fit = 0.2775 (1458 sample;w/time =.13;SAVEPER =250) Variables in the sensitivity simulation setup are listed in alphabetical order after the IRE seed. Results impacted by order. Variables are randomly shuffled based on initial order.

(35) Time Pink=0.13

Units: Minute [0.01,5,0.01]

(36) TIME STEP = 0.25

Units: Minute [0,?]

The time step for the simulation.

(37) "Variety of Regulators (Vr)"=1

Units: Dmnl [0.1,1,0.01]

(38) "X-mission Rate (Xr)"= IF THEN ELSE("Internal Information (I)"<="Initial Internal Information (Ii)",0,IF THEN ELSE("Information Ratio of Emergence (IRE)"<1,"Ix Gap (Ig)", IF THEN ELSE("Internal Information (I)"<="Initial Internal Information (Ii)" *(1+Absorption Capacity),0,"Internal Information (I)"*("Internal Information (I)"-"Initial Internal Information (Ii)"*(1-Absorption Capacity))/"Initial Internal Information (Ii)")))*"Fractional X-mision Time (Xt)"/1000

Units: I Units/Minute

D: VERIFICATION AND VALIDATION DATA

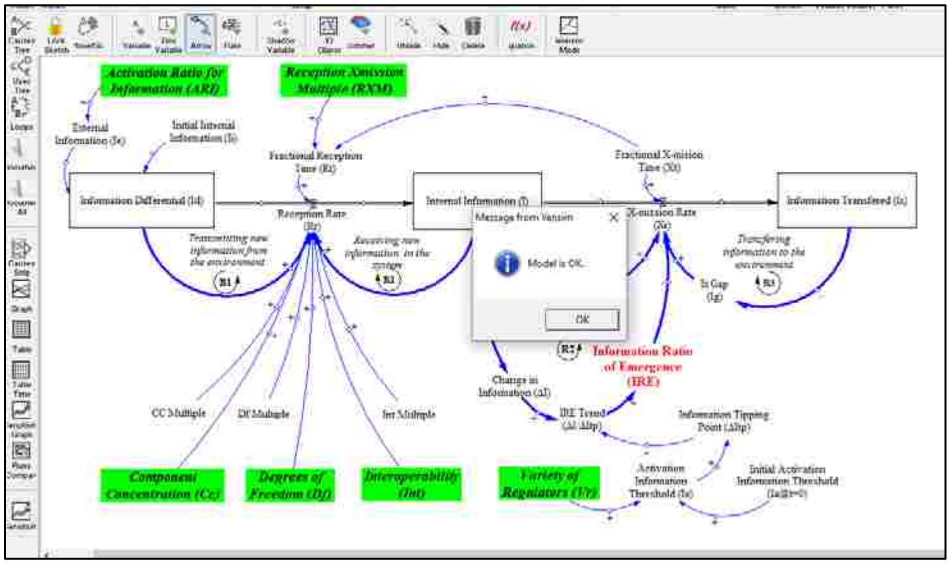

Figure 23. Model Check

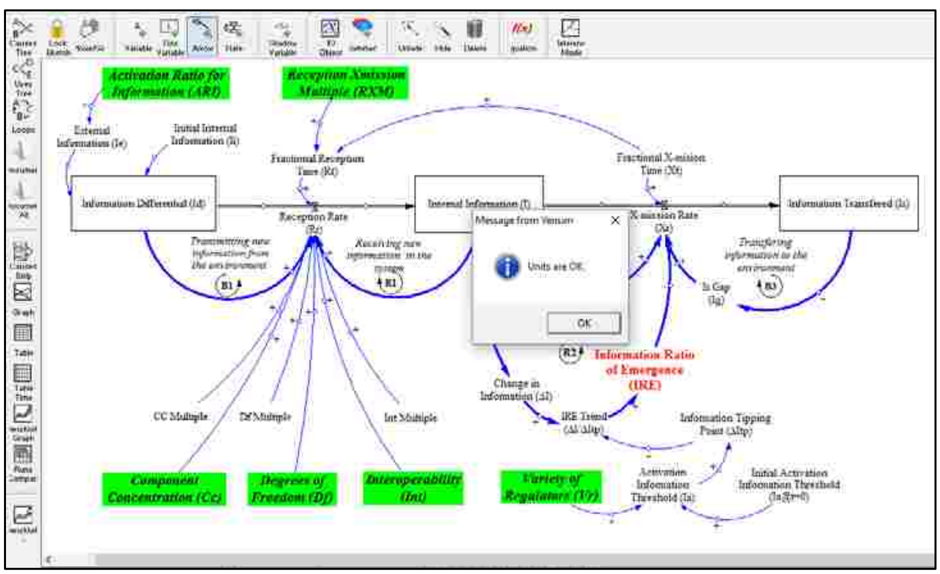

Figure 24. Unit Check

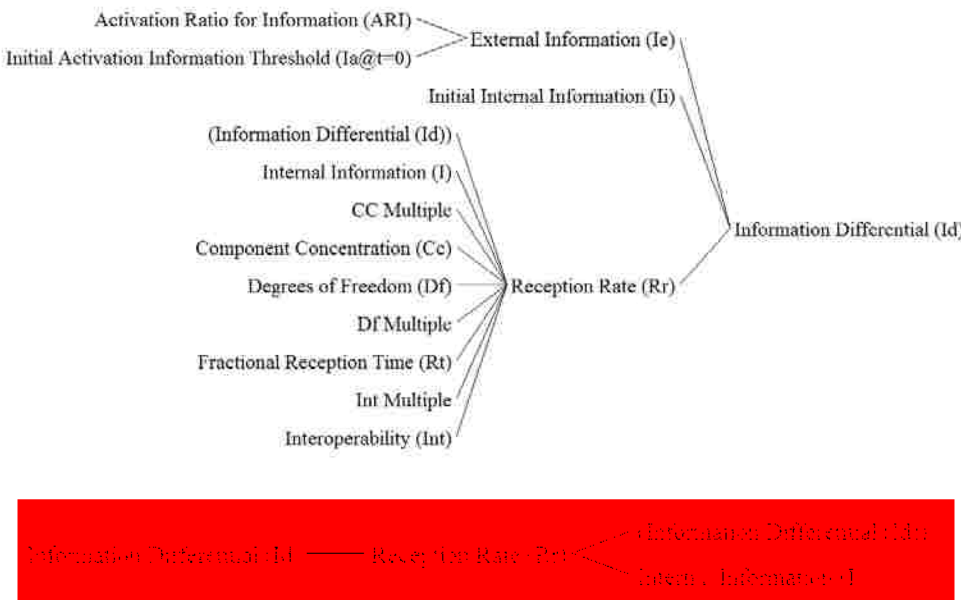

Figure 25. Causal Tree / Use Tree: Information Differential (Id)

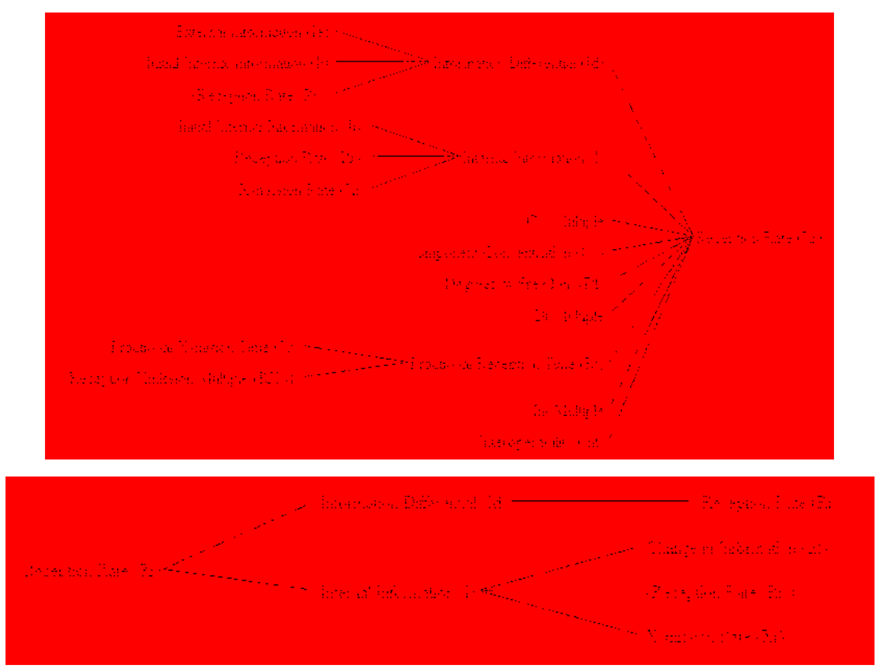

Figure 26. Causal Tree and / Use Tree: Reception Rate (Rr)

Figure 27. Causal Tree and / Use Tree: Internal Information (I)

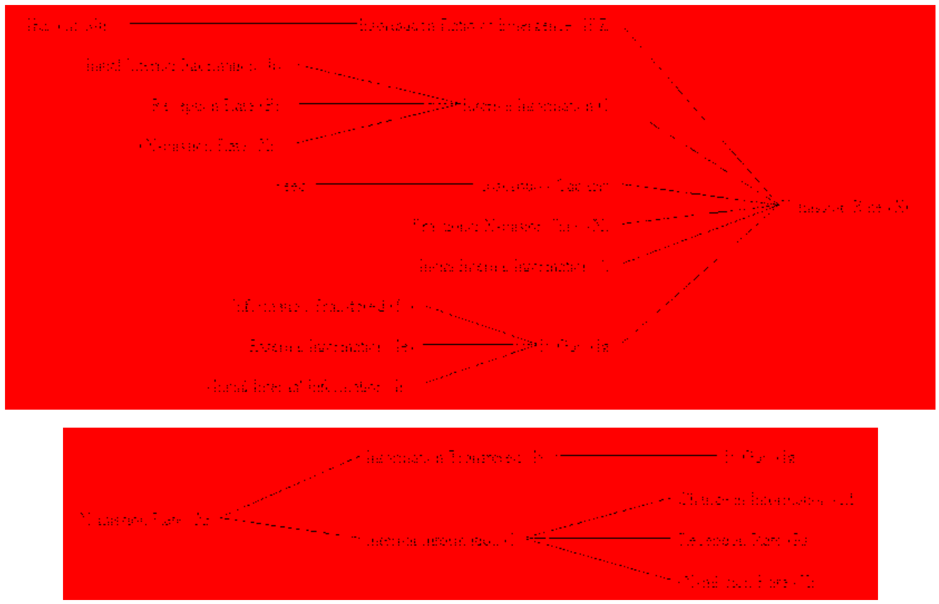

Figure 28. Causal Tree and / Use Tree: X-mission Rate (Xr)

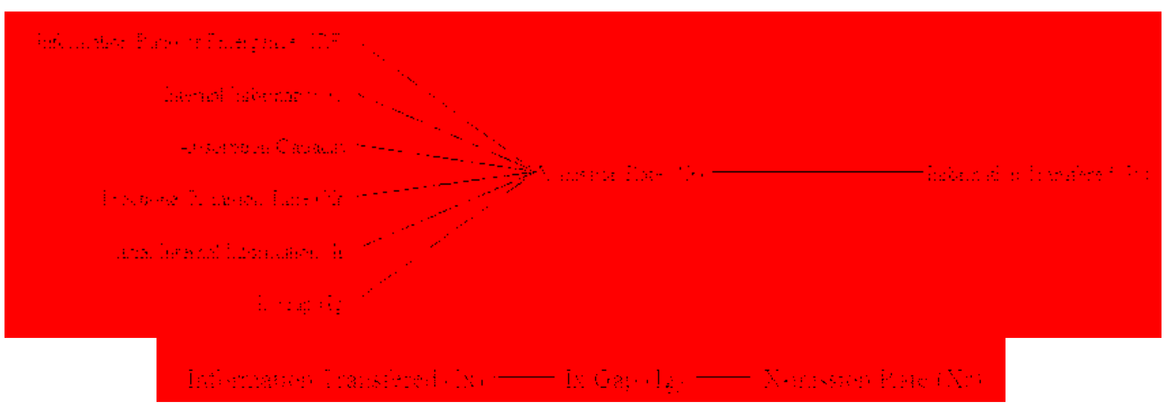

Figure 29. Causal Tree and / Use Tree: Information Transferred (Ix)

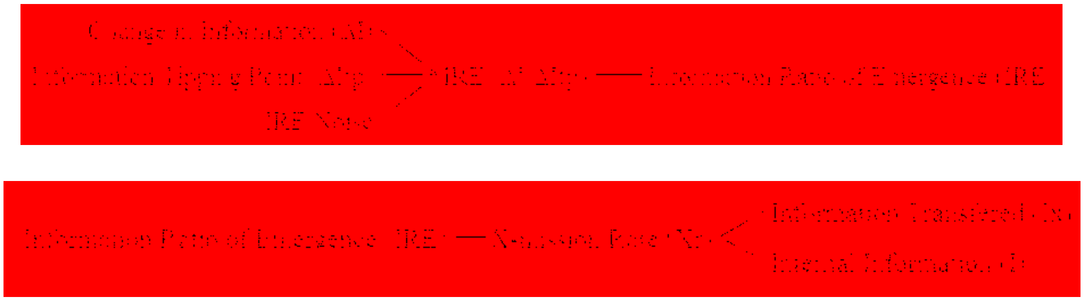

Figure 30. Causal Tree and / Use Tree: Information Ratio of Emergence (IRE)

E: DESIGN OF EXPERIMENTS

E.1 Variables and Assumptions

The independent and dependent variables in the experiments are defined as follows:

Dependent Variable. The Information Ratio of Emergence (IRE) is an indicator that there has been a sufficient change in the system's Information (ΔI) to cause an emergent effect. A sufficient change would be Maximum ΔI > than the Information Tipping Point (ΔItp). From section 5.3, the transition to emergent effects in engineered system is defined by the IRE dependent variable.

$$\mathrm{IRE} = \Delta \mathrm{I} \div \Delta \mathrm{Itp} \qquad [5.2]$$

As ΔI approaches ΔItp, the ratio will approach 1. If IRE ≥ 1 emergent effects will occur.

Independent Variables. There are three variables that remain constant throughout the experiment: X-mission Time (Xt); Initial Internal Information (Ii); and Initial Activation Information Threshold (Ia@t=0). The impact of these variables is explained by the derivation for equation [5.4] which shows how: Activation Ratio for Information (ARI) includes the effect of Ia@t=0 and Ii; and X-mission Time (Xt) is captured in the Reception/X-mission Multiple (RXM). The remaining independent variables are the six experiment factors in the IRE tuple.

$$\mathrm{IRE}\ [\mathrm{ARI}, \mathrm{RXM}, \mathrm{Df}, \mathrm{Cc}, \mathrm{Int}, \mathrm{Vr}] \qquad [5.6]$$

The independent variables (i.e., factors) and their levels are listed in Table 22.

Factor	Low (-)	Nominal (0)	High (+)
Activation Ratio for Information (ARI)	.5	1	1.5
Reception/X-mission Multiple (RXM)	1	3	5
Degrees of Freedom (Df)	0	.5	1
Component Concentration (Cc)	0	.5	1
Interoperability (Int)	0	.5	1
Variety of Regulators (Vr)	0	.5	1

Table 22. Independent Variables

Assumptions. Values were selected for each of the initial value constants in order to initialize the simulation. The values remain constant throughout the simulation: X-mission Time (Xt) = .10 minutes; Initial Internal Information (Ii) = 1000 information units (I-Units); and Initial Activation Information Threshold (Ia@t=0) = 2000 information units (I-Units).

E.2 Monte Carlo Experiment Design

Sampling. Monte Carlo experiments estimate the value of a dependent variable by examining samples from its distribution at random values of the independent variables. One of the recommended approaches for determining samples size in Monte Carlo simulations is based on the Central Limit Theorem (Driels & Shin, 2004; Oberle, 2015). The Central Limit Theorem (CLT) basically states that as the sample size increases, the sample distribution is approximately normal and the mean of the sample distribution approaches the mean of the actual distribution (Albright et al., 2010). The sample size for Monte Carlo experiments based on CLT is determined by [6.5]

$$n = ((z \times \sigma_{\text{estimate}}) \div B)^2 \qquad [6.5]$$

Where:

z = Standard normal distribution multiple for the confidence level

σ_{estimate} = Estimate of dependent variable standard deviation

B = Half-length of the confidence interval

The modeling questions are related to detecting IRE >=1. Therefore, we are interested in the maximum value for IRE. An estimate for the standard deviation for Max IRE is made by randomly varying the independent variables in Table 13 for 100 simulation runs over an extended time period (50,000 minutes). The IRE distribution is depicted in Figure 31, and the maximum IRE for each simulation run is depicted in Figure 32.

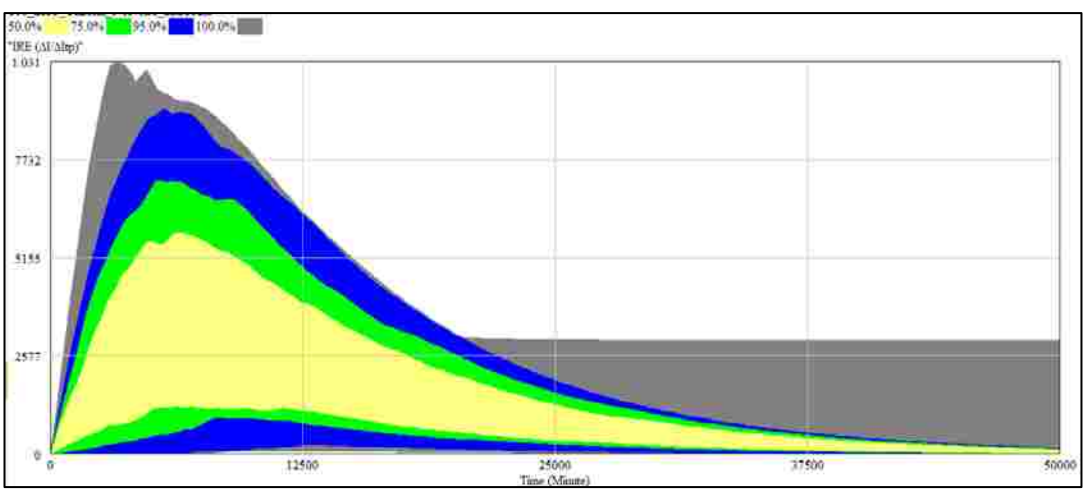

Figure 31. IRE Distribution

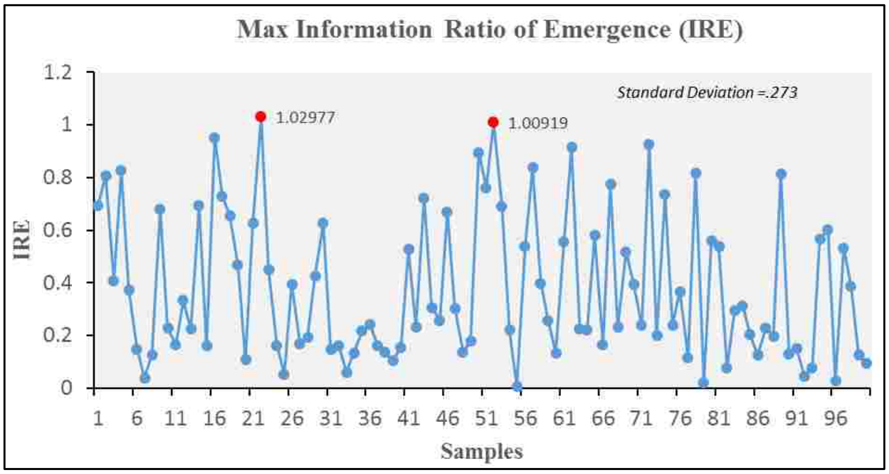

Figure 32. Max IRE

The standard deviation is estimated to be .273. The minimum sample size (n) for estimating IRE with 95% confidence level and a confidence interval of +/5% is:

$$n = ((1.96 \times .273) \div 5\%)^{2} = 115$$

Based on the sample size estimate each Monte Carlo simulation will run for 115 iterations.

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Mr. Johnson's professional experience includes nearly three decades in private and government sectors at various capacities as an engineer and manager. Over his career he has lead manufacturing, quality assurance, and supply chain management operations in domestic and international markets. In 2011, Mr. Johnson co-founded Systems Thinking & Solutions, a Virginia corporation providing consulting and contract support services specializing in acquisition and program management of IT systems.

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