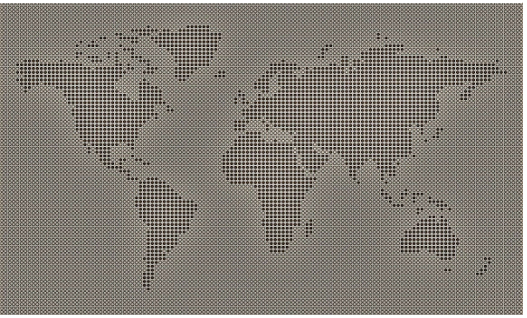
SAND2017-11109PE



Granta MI and Materials at Risk (M@R) at Sandia National Laboratories

GRANTA EMIT Consortium Fall 2017 Meeting

Marseille, France

October 17-19, 2017

Celeste A. Drewien and Richard A. Karnesky

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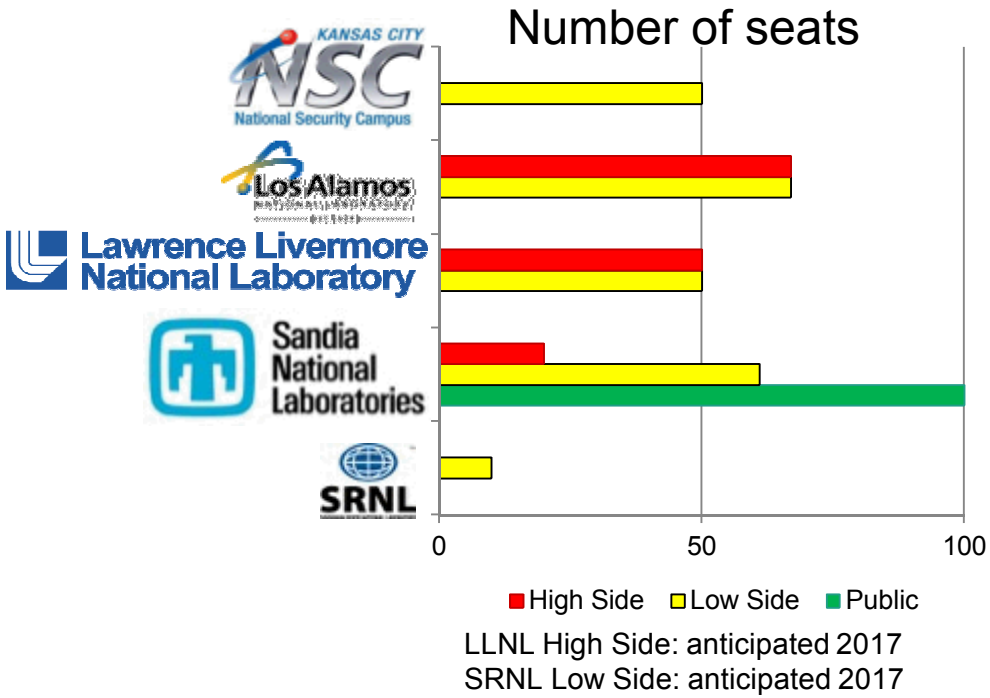
Granta Usage at Sandia National Labs

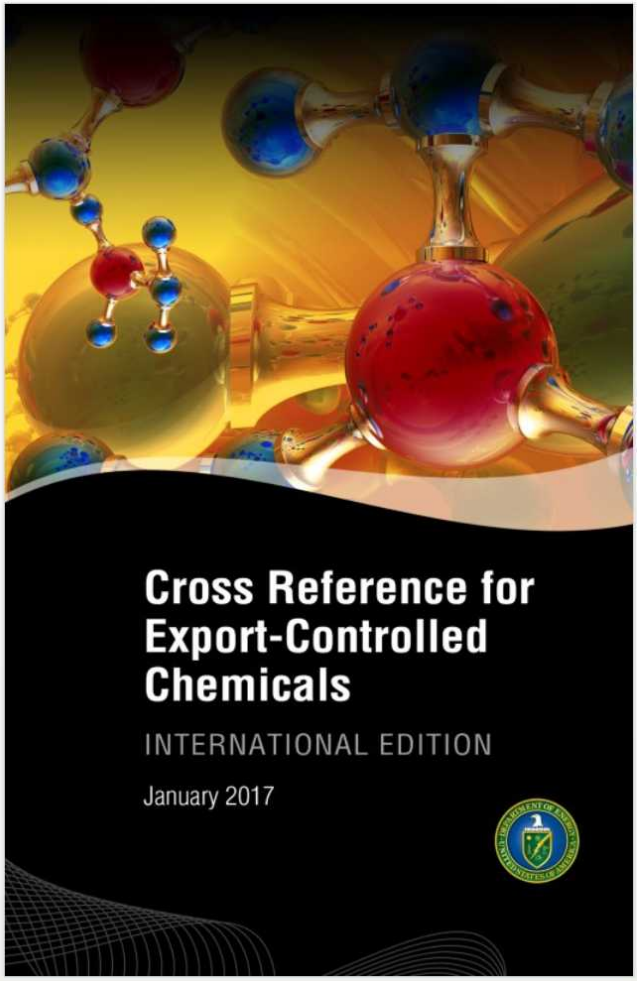
- US Department of Energy (DOE) labs' collaborations
  - Additive Manufacturing (2013)
  - Product Risk (2016)
- Included in SNL's Common Engineering Environment (2017)
  - Tripled low-side number of users
  - Easier to gain access
  - Product Risk database is still being vetted (limited to 10 users now)
- Integration
  - 20x CREO Gateway seats
  - PTC Windchill Product Lifecycle Management (PLM)
    - Exploring Gateway, and
    - Exploring home-grown solution
  - SIERRA/SAW using Granta Software Developer Kit (SDK)



SNL began using Granta in 2010

Product Risk Database at SNL in 2017

- Export Control (+Kansas City National Security Campus (KCNSC))
  - List maintained by Argonne National Lab
  - 261 substances affected
  - Could share with EMIT
- Internal specs (+KCNSC)
  - Some from legacy databases
  - Most manually entered
- Manufacturer information
  - Trade names
  - Company risk factors from Dun & Bradstreet
- Demo'ed "Fallback materials"
  - Demo of mechanical/thermal/etc. properties for internal specs -> PLM



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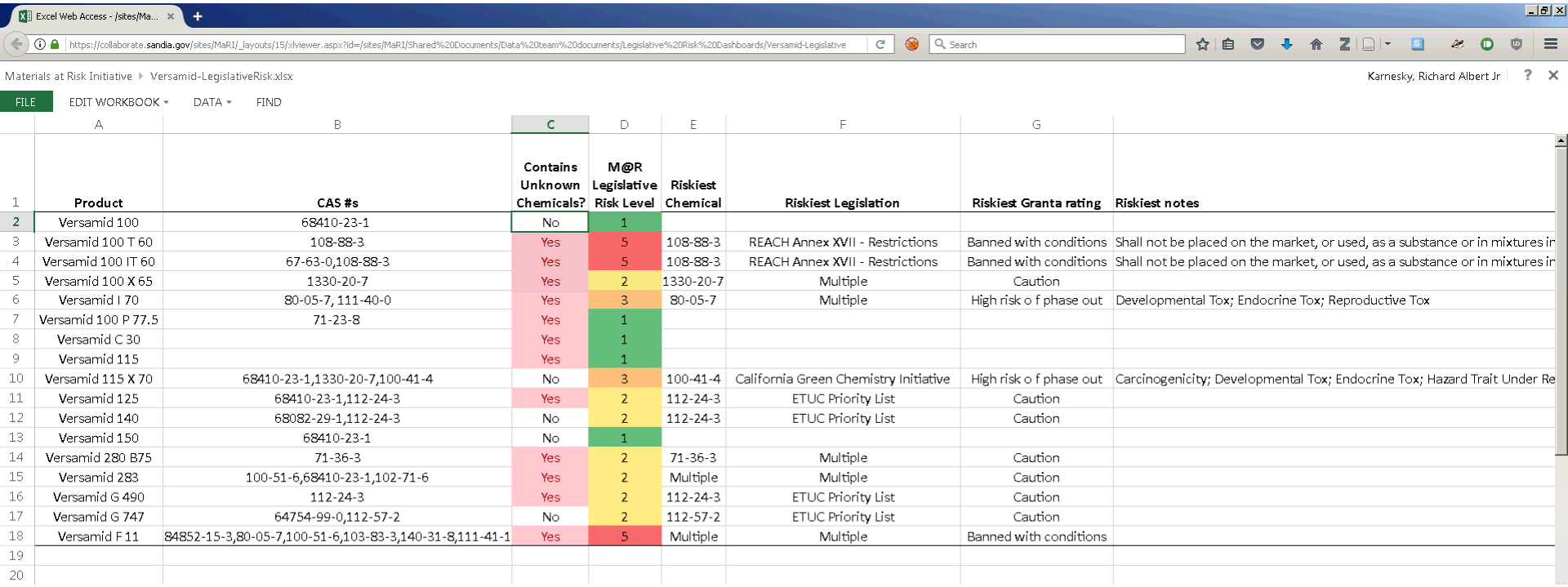
Report Generation Using Python Toolkit



	Product	CAS #s	Contains Unknown Chemicals?	M@R Legislative Risk Level	Riskiest Chemical	Riskiest Legislation	Riskiest Granta rating	Riskiest notes
2	Versamid 100	68410-23-1	No	1				
3	Versamid 100 T 60	108-88-3	Yes	5	108-88-3	REACH Annex XVII - Restrictions	Banned with conditions	Shall not be placed on the market, or used, as a substance or in mixtures ir
4	Versamid 100 IT 60	67-63-0,108-88-3	Yes	5	108-88-3	REACH Annex XVII - Restrictions	Banned with conditions	Shall not be placed on the market, or used, as a substance or in mixtures ir
5	Versamid 100 X 65	1330-20-7	Yes	2	1330-20-7	Multiple	Caution	
6	Versamid I 70	80-05-7, 111-40-0	Yes	3	80-05-7	Multiple	High risk o f phase out	Developmental Tox; Endocrine Tox; Reproductive Tox
7	Versamid 100 P 77.5	71-23-8	Yes	1				
8	Versamid C 30		Yes	1				
9	Versamid 115		Yes	1				
10	Versamid 115 X 70	68410-23-1,1330-20-7,100-41-4	No	3	100-41-4	California Green Chemistry Initiative	High risk o f phase out	Carcinogenicity; Developmental Tox; Endocrine Tox; Hazard Trait Under Re
11	Versamid 125	68410-23-1,112-24-3	Yes	2	112-24-3	ETUC Priority List	Caution	
12	Versamid 140	68082-29-1,112-24-3	No	2	112-24-3	ETUC Priority List	Caution	
13	Versamid 150	68410-23-1	No	1				
14	Versamid 280 B75	71-36-3	Yes	2	71-36-3	Multiple	Caution	
15	Versamid 283	100-51-6,68410-23-1,102-71-6	Yes	2	Multiple	Multiple	Caution	
16	Versamid G 490	112-24-3	Yes	2	112-24-3	ETUC Priority List	Caution	
17	Versamid G 747	64754-99-0,112-57-2	No	2	112-57-2	ETUC Priority List	Caution	
18	Versamid F 11	84852-15-3,80-05-7,100-51-6,103-83-3,140-31-8,111-41-1	Yes	5	Multiple	Multiple	Banned with conditions	
19								
20								

- INPUT: Spec numbers
- OUTPUT: Excel sheet with color-coded risks that make sense for our internal weighting of legislation and supply chain risks

Sandia's M@R Initiative

Broader Scope than Current Product Risk Database

- Conceptual design of M@R tool, including prototype proof of concept demonstration, completed (2017)
- Moving into baseline design phase

- Successes:
  - Multi-site effort
  - Regulatory risk factor identification being performed for new program
- Challenges:
  - Syncing information across sites
  - Ranking relative importance
    - Different risk factors
    - Different regulation/legislation
  - Risk factors exist at:
    - Elemental level
    - Substance level
    - Materials level
    - Other
  - Vendor-substance specific risk factor analyses
  - Establishing technical risk factors

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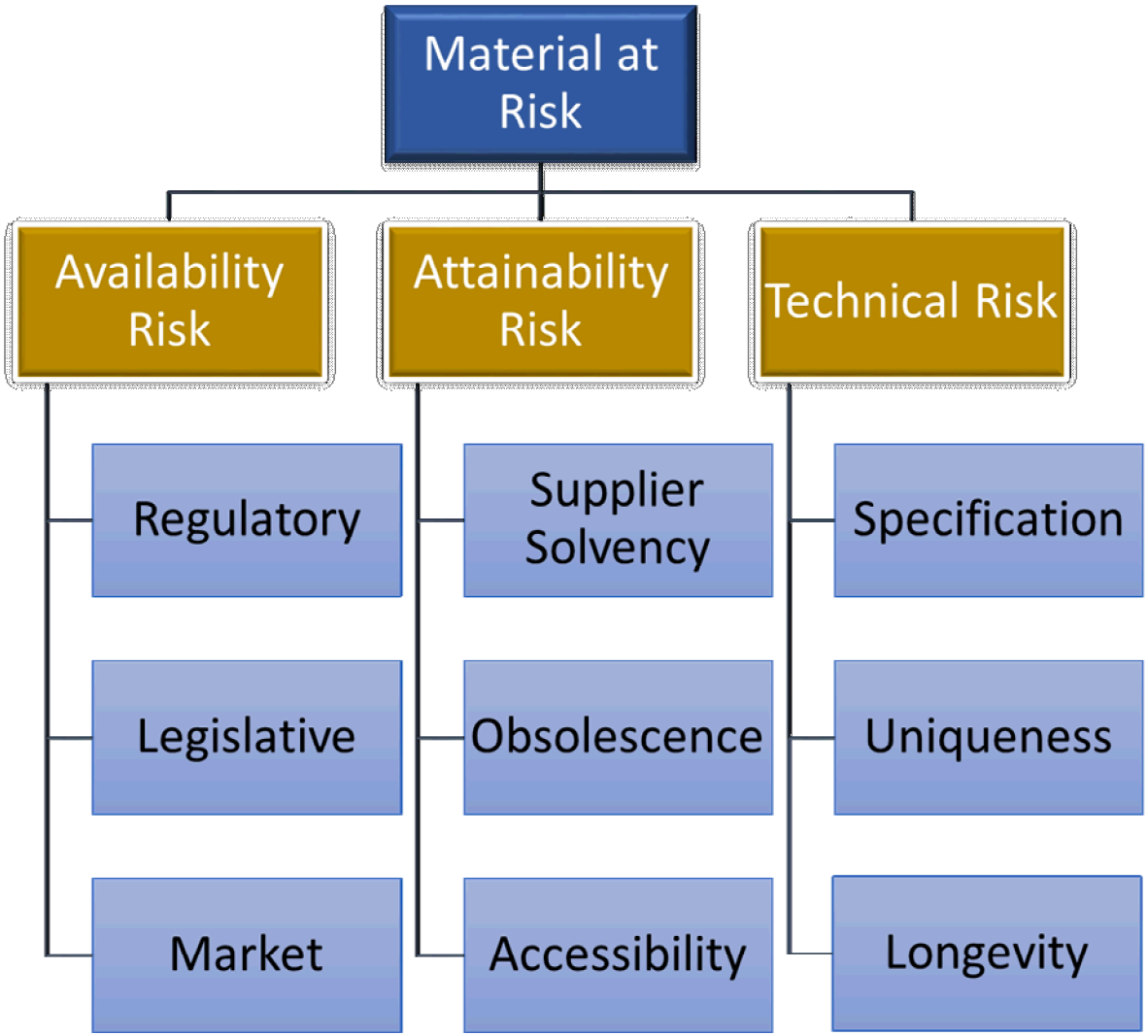
Risk Factor Framework



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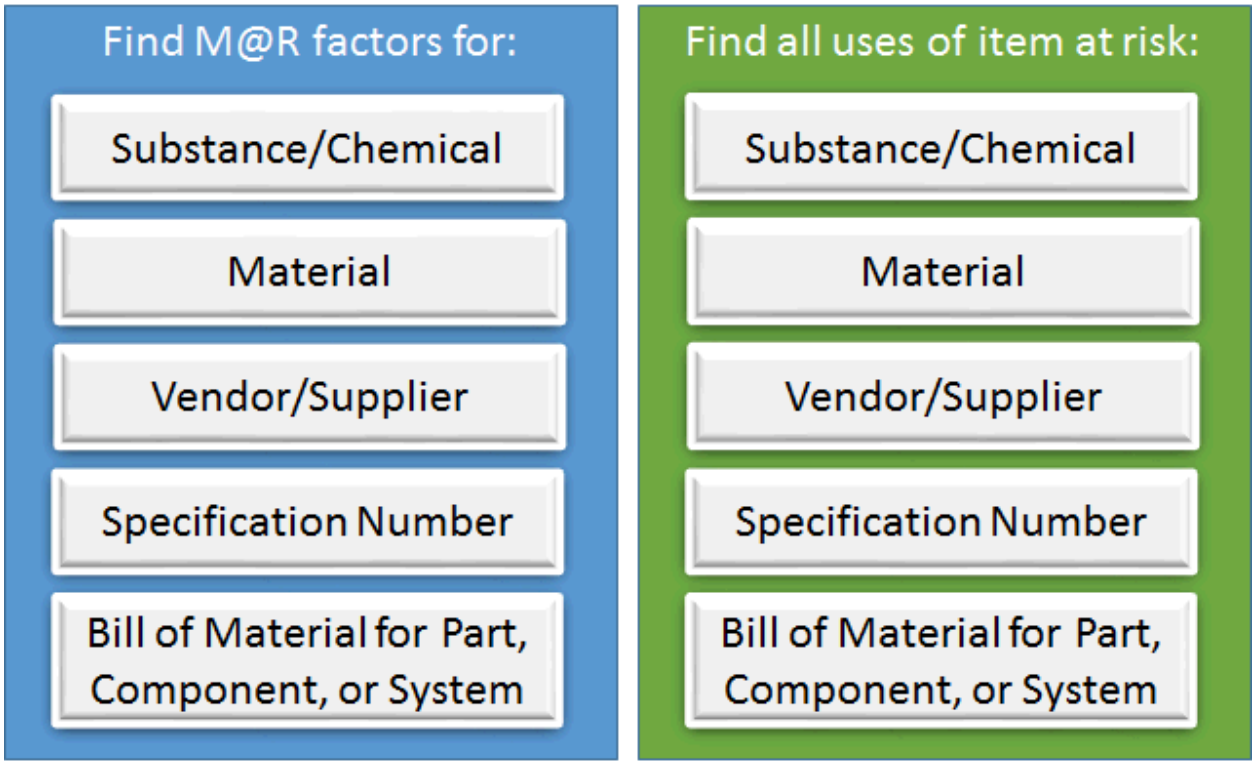
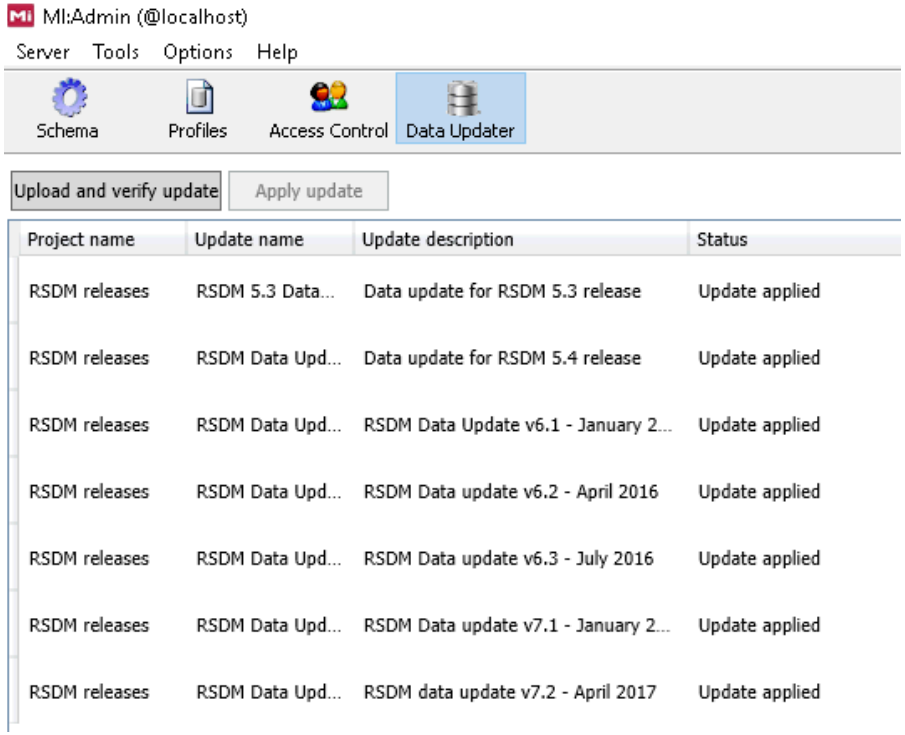
Conceptual User Interface

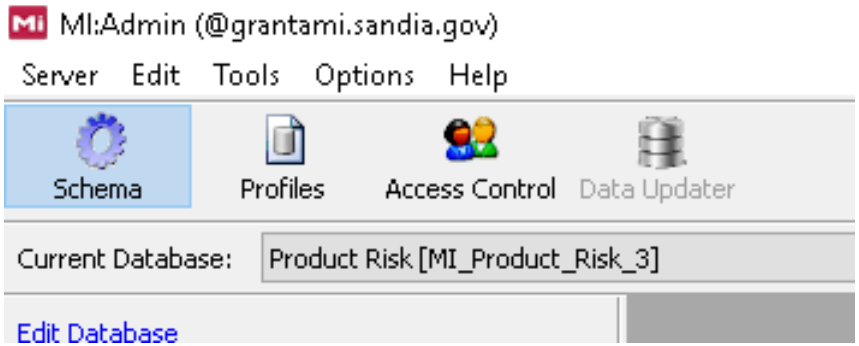


Opportunities for EMIT/Granta to Address M@RI Needs

- Push updates to other DOE labs
  - Use same "data updater" that we use for RSDB updates*
- More risk factor information
  - DOT information [coming soon]
  - Operator hazard risk factor
    - National Institute for Occupational Safety and Health (NIOSH)
    - American Conference of Governmental Industrial Hygienists (ACGIH)
    - National Fire Prevention Association (NFPA)
    - OSHA, GHS (Globally Harmonized System),
    - Other?
  - Market demand risk factor
    - Industry trends and analysis reports
    - Product/substance obsolescence determination

*This data updater doesn't seem to work on our production database for some reason…





Back-Up

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Risk Categories and Questions

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Is the material accessible and available through regulatory, market, and inventory means? Accessibility refers to assets being available to authorized applications at the time needed, without undo effort to obtain approvals, transport the material, or surmount other obstacles.

1. Material Legislative & Political Risks: risk due to (change in) environmental, safety, and hazard regulations and other legislation that might affect industry or business	**1.1. Government ES&H Regulations** 1.1.1. Environmental 1.1.2. Safety & Health	**Do regulations limit the availability of the material?**
	1.2. Site-related regulations and compliance concerns 1.2.1 Environmental 1.2.2 Safety & Health	Do DOE, NNSA, or NSE sites allow the use of this material?
	1.3 Transport or Disposal Regulations 1.3.1 DOT, UN code 1.3.2 Other	Is the process to obtain the material free of transportation regulations?
	1.4 Operator Hazard	Is the process or material hazards to the operator, whether within NSE or the vendor/supplier realm?
	1.4 Export Control Regulations 1.4.1 ECI	Do export control limitations affect market options?
	1.5 Political Risks 1.5.1 Frank-Dodd Act for Conflict mineral	Are constituents or materials conflict free?
	1.5.2 Other Geopolitical Risk	Are constituents or materials from politically sound locations worldwide? Or is it a critical material?

Continued

2. Elemental Material Market Risk: risk due to changes in market usage, limitations in world production or reserves, abundance in earth, etc.	**2.1 Abundance/Supply**	Is there a risk of limited material availability?
	2.2 Market Demand	Does Market Demand impact material availability?

Do we understand the material specifications and properties? Understandability refers to the developers and users comprehending the material specifications sufficiently for the use intended, and to recognize when a procurement problem might be present. Specifications must be accompanied with appropriate contextual information to show who, what where, how and why the material was used.

4. Material Technical Risk: risk in knowledge base, manufacturing aspects (complexity, reproducibility), lifetime, etc.	**4.1 Specification Readiness**	Is the material specification current?
	4.2 Producibility Rating	Is the processing of this material difficult?

Continued

Can the material be obtained from a qualified vendor or any vendor? Qualified vendor refers to a qualification of the vendor's location, financial stability, and past compliance with regulations, as well as the vendor's ability to comply with the details of the specification and meet NNSA qualification requirements.

Vendor Name		
3. Supplier/Vendor Risk: risk due to numbers, locations, and viability of suppliers, and product consistency and availability	**3.1 Intellectual Property**	**Does the material contain Intellectual Property?**
	3.2 Supplier Availability 3.2.1 Number of Producers	**Are there several producers or is this a sole source vendor?**
	3.2.2 Vendor location	Is the vendor located domestically? Or in the sensitive country list?
	3.3 Supplier Qualification	Does a qualified vendor exist?
	3.4 Supplier Reliability 3.4.1 Supplier Evaluation Risk Rating (SER)	**Is the vendor risk acceptable as defined by the supplier evaluation rating (SER)?**
	3.4.2 Supply Chain Risk Index (SCRI)	Is the vendors supply chain at risk?
	3.5 Product Obsolescence	Does vendor still produce product?

Risk Factor Definitions

- Government ES&H Regulations: risk of substance unavailability due to governmental regulation based on environmental, safety, and health (ES&H) hazards
- Site-related regulations and compliance concerns: limitations on substance use or availability due to site restrictions or other site-specific factors
- Transport or disposal regulations: restrictions on substance due to transportation regulations or disposal limitations, including lack of disposal path. National, state, and local regulations should all be considered
- Operator Hazards: risk of substance, material, or process restriction due to cost and/or difficulties associated with operations. This factor could fall under Technical risk but relies on government ratings, so it has been placed in under Regulatory risk factors.
- Export Control Regulations: regulations on shipment or transfer of substance or material or service out of the US
- Political Risks: limitations on availability due to existing legislation, such as the Frank-Dodd Act for conflict minerals; embargoes, controls, or prohibitions due to national security concerns; or conflict or war in a region
- Geopolitical Risks: risk of unavailability due to limited geographical distribution of source material or manufacturing facilities, especially in regions of the globe that experience violence, political instability, corruption, etc.
- Abundance/Supply: risk of inability to attain substance due to low abundance or supply shortage
- Market Demand: risk of inability to attain substance due to declining market demand

Risk Definition Continued

- Intellectual Property (IP): risk from lack of complete knowledge of material or process. While this factor could fall under Technical Risks or Understandability, IP is coupled with the vendor who processes or produces the material.
- Supplier Availability: risk of inability to attain material due to:
  - Number of suppliers or sole source supplier
  - Lack of supplier qualification
  - Sensitive country supplier location
- Supplier Reliability: risk of supplier incompetency and inconsistency that influence supplier's reliability and hence livelihood:
  - Supplier Evaluation Risk Rating (SER)—likelihood supplier will cease business operations
  - Supply Chain Risk Index—assesses the financial/operational risk and other exposures of first tiers of the supply chain using factors, such as Major Financial Distress / Bankruptcy, High Risk Country, Debarment, Office of Foreign Assets Control (OFAC), and Mergers & Acquisition.
- Product Obsolescence: risk that product (substance, material, service) will or has become obsolete
- Specification Readiness: risk due to obsolete or outdated material or process specification rendering the required material vulnerable
- Producibility Rating: risk of material production or process shutdown due to poor producibility or low production yield