Product Update

GreenSuite®

Automated Hazard & Risk Assessments

for **Chemicals, Products, Manufacturing Processes & Lifecycle Stages**

2018 PDA Annual Conference

Presented by

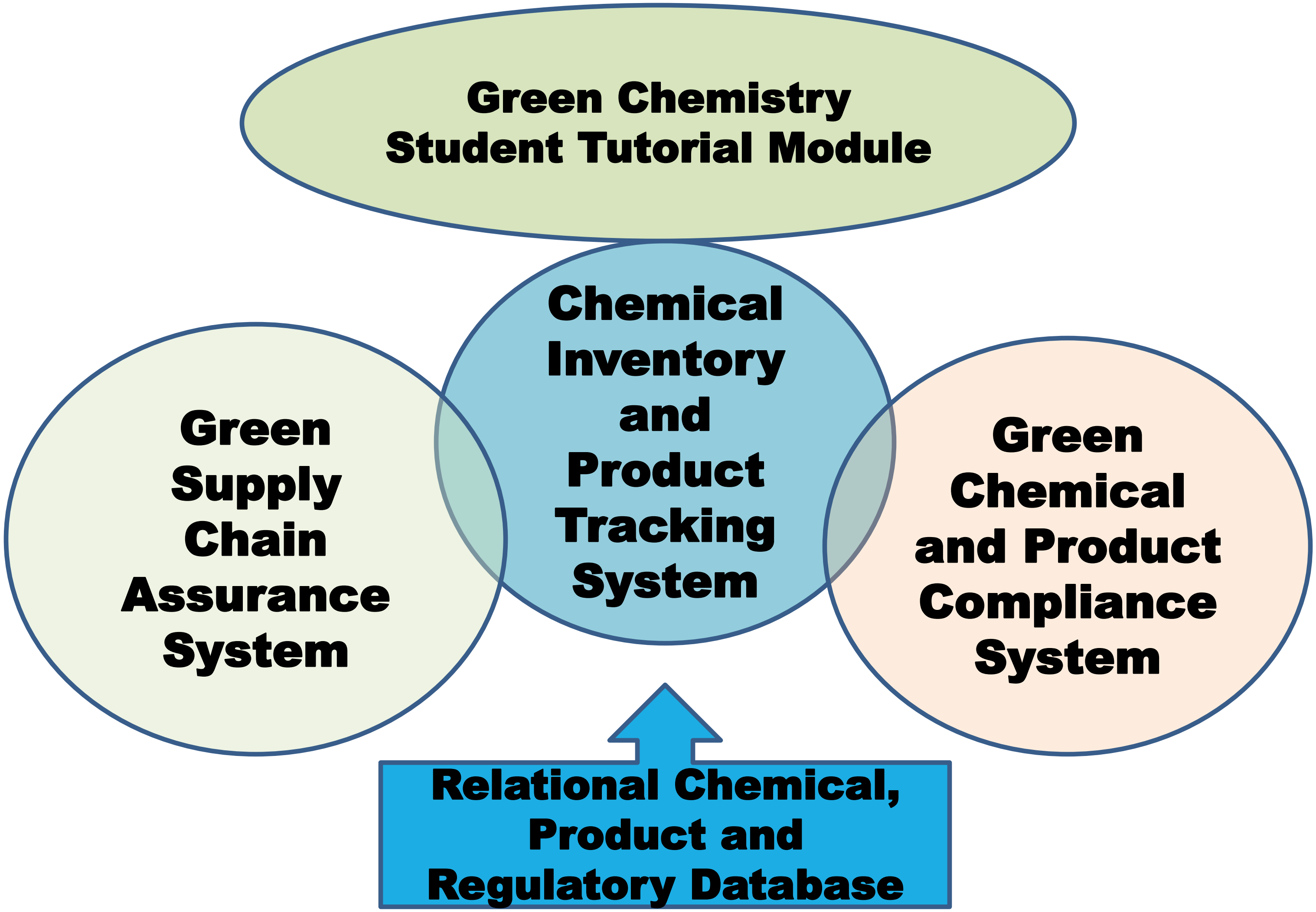
George R. Thompson, Ph.D.

CCS

Chemical Compliance Systems, Inc.

"Anticipating the Unanticipatable"

Chemical and Product Inventory Management Capabilities



What Is The Purpose of Your Inventory?

CCS Relational Chemical and Product Database (R-CPD) Statistics - 2017

Continuous Data Compilation Since 1985

≥ 80,000,000	Data Elements
280,000	Chemicals
>29,000	Chemicals with 44 EHS Endpoints
1,250	*Fracking Chemicals*
1,100	*Munition Chemicals*
1,000	*Cosmetic Chemicals*
200	*PU & SPF Chemicals*
➢1,500,000+	Product MSDSs
> 10,000	Manufacturers
1,000	Public Data Sources
> 800	Chemical Regulatory Lists

CCS Relational Chemical and Product Database (R-CPD)

Chemical

Cross Reference Dictionary
- Chemical Names
- Common Names
- Foreign Names
- Numeric Identifiers

Physical/Chemical
- Elemental Composition
- Redox Potential
- Pka/Pkb
- Log Koc, Log Kow
- BP, FP, VP
- Solubilities

Health
- Acute
- Chronic

Safety
- Incompatibilities
- Storage Codes
- Flammables
- Explosives
- Radioactives

Ecological
- Toxicity
- Pesticides
- Long-term Effects
- Persistence
- Exposure

Exposure

Green
- Ecological
- Health
- Safety

Alternatives
- Acids
- Antioxidants
- Bases
- Binders
- Chelators
- Oxidizers
- Propellants
- Reducers
- Solvents
- Surfactants
- UV Absorbers
- Viscosity Agents
- Other (~30)

Eco-Risk
- Species Factors
- Wildlife Toxicity
- Dietary Considerations
- Ingestion Rates
- Bioconcentration
- Bioaccumlation
- Biotransfer

Human Health Risk
- Biotransfer Animals
  - Biotransfer & Concentration Factors
- Biotransfer Plants
  - Bioconcentration Factors
- Health Benchmarks
  - Cancer Slopes
  - Toxicity Equivalency
- Physical/Chemical Properties
  - Diffusivity
  - Partition Coefficients

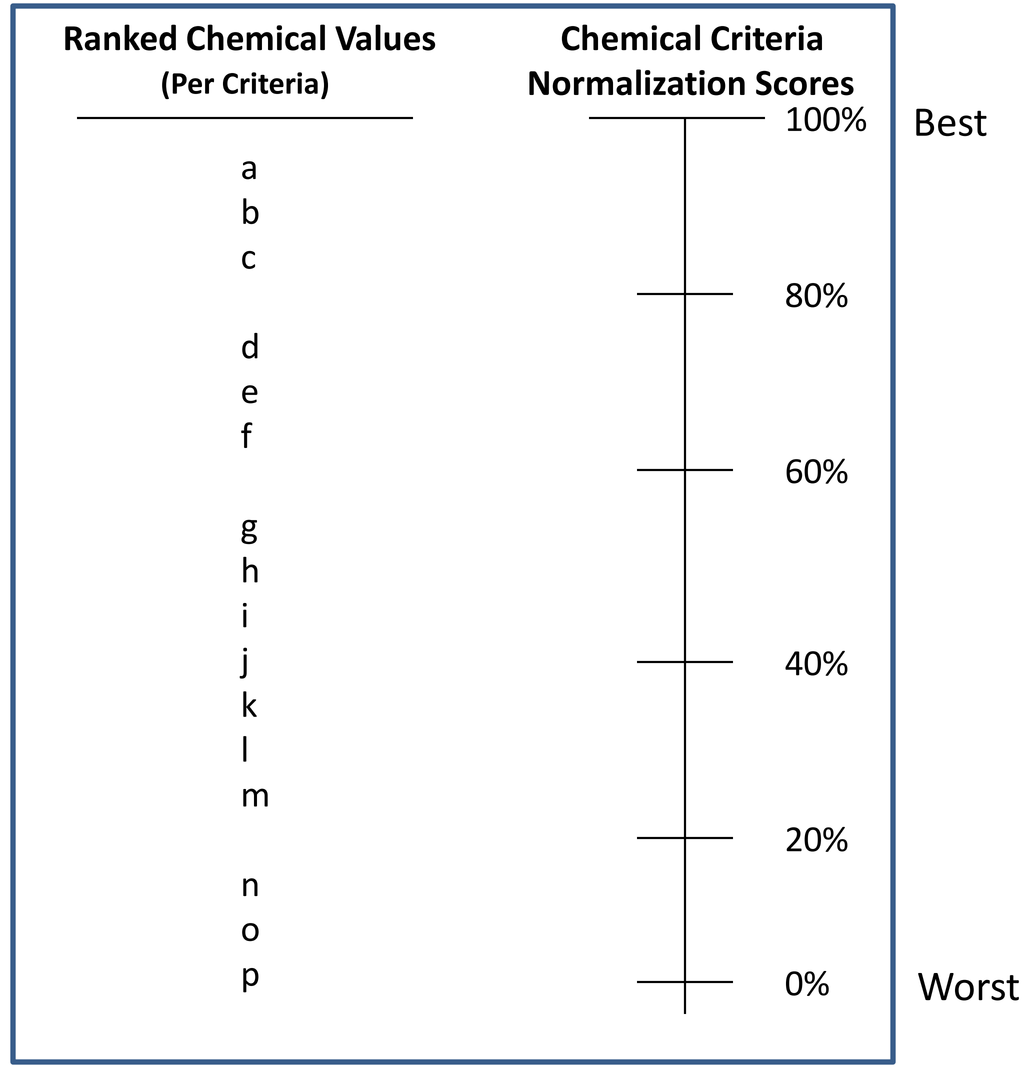
Regulatory
- U.S. EPA
- U.S. DOL
- U.S. DOT
- U.S. FDA
- U.S. Other
- States
- Canada
- Europe
- Pacific Rim
- International
- Compounds
- CCS Compiled
- Textiles
  - AAFA
  - AFIRM
  - H&M
  - NIKE
  - NSF 336 (Current)
  - NSF 140 (Current)
  - Oeko-Tex
  - PUMA
  - SAC

Product
- Manufacturers
- Composition
- Description
- Generic Categories
- Inventories
- Alloys
- MSDS Links

Supplier
- Product Dictionary
- Mfr.- Supplier Links
- Supplier-Supplier Links
- CBI

Hazard Characteristic Ranking and Normalization Process[a]

- Each chemical criteria value, with unique units of measure (e.g., mg/kg, hours, ppm, etc.), were individually ranked from highest to lowest (i.e., “a” to “p”).
- The worst value was assigned 0% and the best value was assigned 100%. Values between were assigned a proportionate %, depending upon their value ranking/position
- Approximately 27,000 chemicals were randomly selected for the initial normalization.
- By normalization , disparate units of measure are converted to an equivalent scale that facilitates direct value comparisons and integrations.



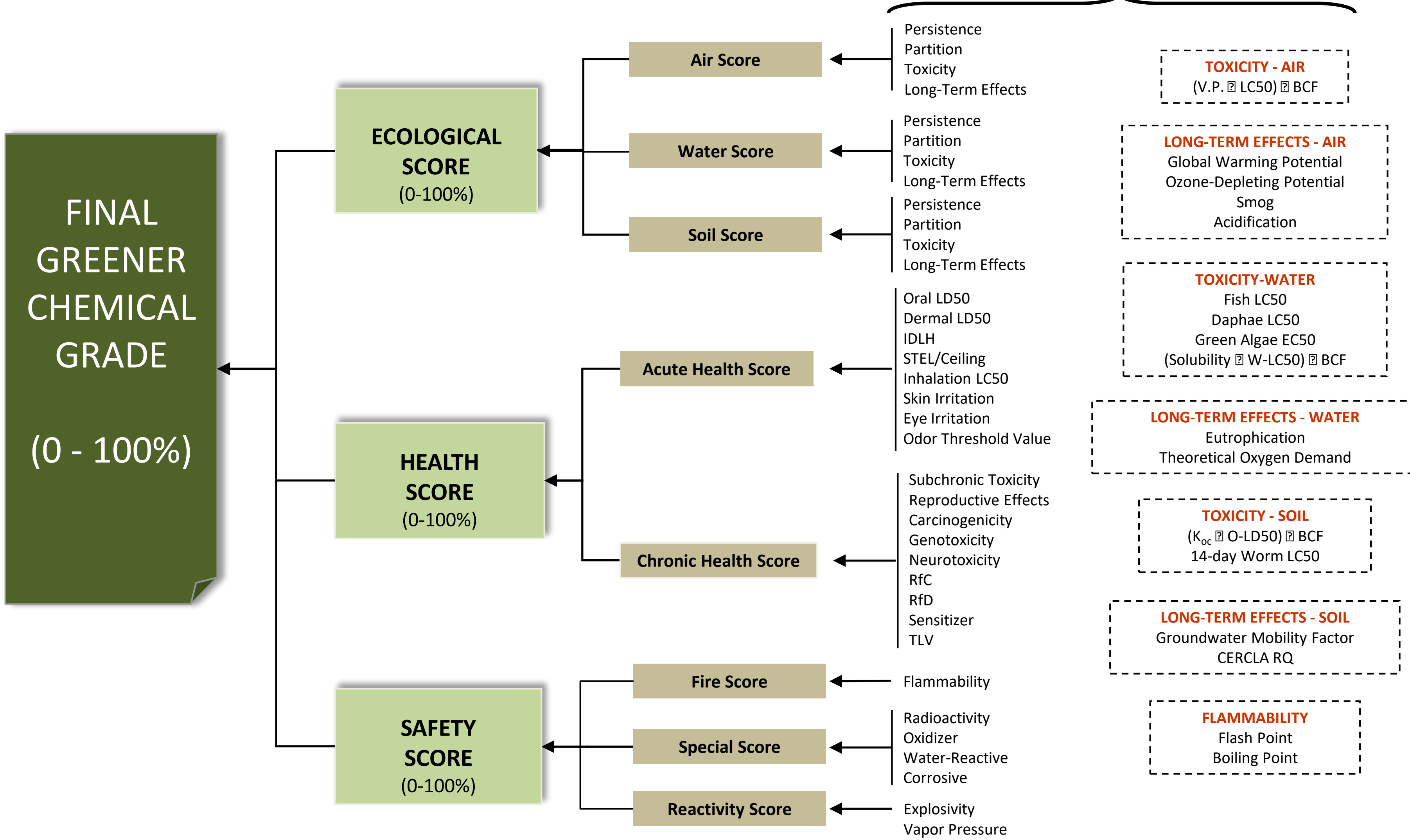
[a]Same process used historically by many agencies : FDA, EPA, NFPA, NPCA

"GREENER" CHEMICAL SCORING PROCESS

Chemicals – Products – Processes – Wastestreams

Significance of each sub-score can be individually weighted

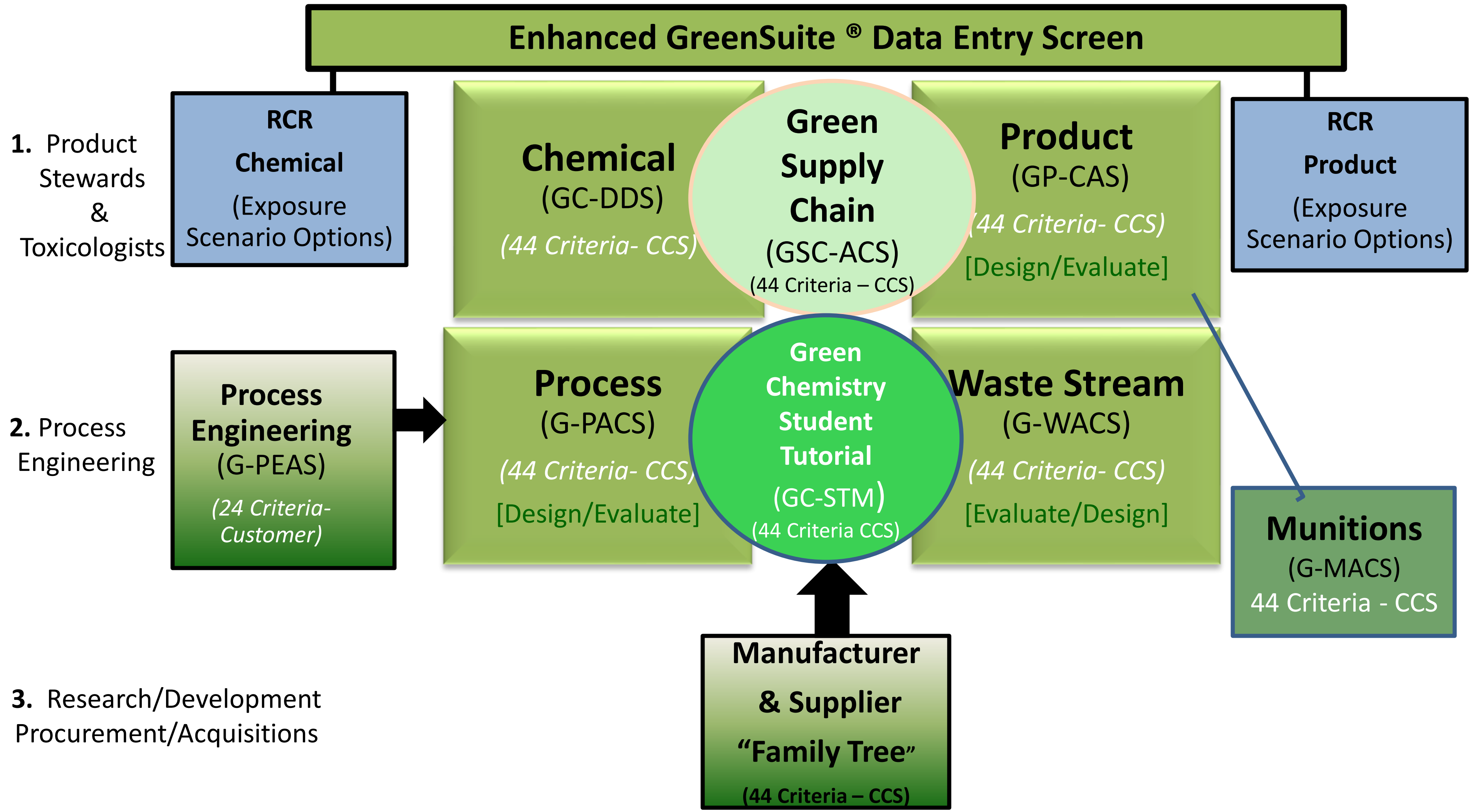
44 "Endpoint" Criteria



44 ENDPOINTS IN THE NSF/GCI/ANSI 355-2011 NATIONAL STANDARD

Enhanced GreenSuite®

"One tool cannot do it all!"



[11 Optional Hazard & Risk Assessments]

Inside the GreenSuite® "Black Box" – Calculation Algorithm Factors

A. Chemical Hazard Green Grade

- Chemical Endpoint Hazard Score
- Weighting Factors (%): Endpoint
  Subcategory
  Category
- Subcategory Hazard Scores
- Category Hazard Scores
- Chemical Hazard Green Grade

B. Product/Process/Wastestream Risk Green Grade[1]

- Chemical Endpoint Hazard Score
- Weighting Factors (%): Endpoint
  Subcategory
  Category
- Constituent Chemical Concentration (%)
- Subcategory Risk Scores
- Category Risk Scores
- Product, Process & Wastestream Risk Green Grade

[1]This first order risk calculation accounts for the product/process/wastestream-specific exposure concentration constraint, but not for other usage exposure constraints (e.g., amount utilized, frequency, duration, ventilation rate, etc.).

GreenSuite® Scoring Hierarchy Descriptors

Green Score	Alpha Score	Text Descriptor	Global Harmonization System (GHS)
97 - 100	A+	Highly Probable Non-Risk	Category 1?
93 - 96	A	Very Probable Non-Risk	Category 1?
90 - 92	A-	Probable Non-Risk	Category 1?
87 - 89	B+	Reasonable Non-Risk	Category 1?
83 - 86	B	Possible Non-Risk	Category 2?
80 - 82	B-	Cautious Non-Risk	Category 2?
77 - 79	C+	Minimal Risk	Category 2?
73 - 76	C	Slight Risk	Category 3?
70 – 72	C-	Moderate Risk	Category 3?
65 – 69	D	Serious Risk	Category 3?
< 65	F	Extreme Risk	Category 3?

Risk Assessment Subsection - Science-Based Stipulations (Draft)

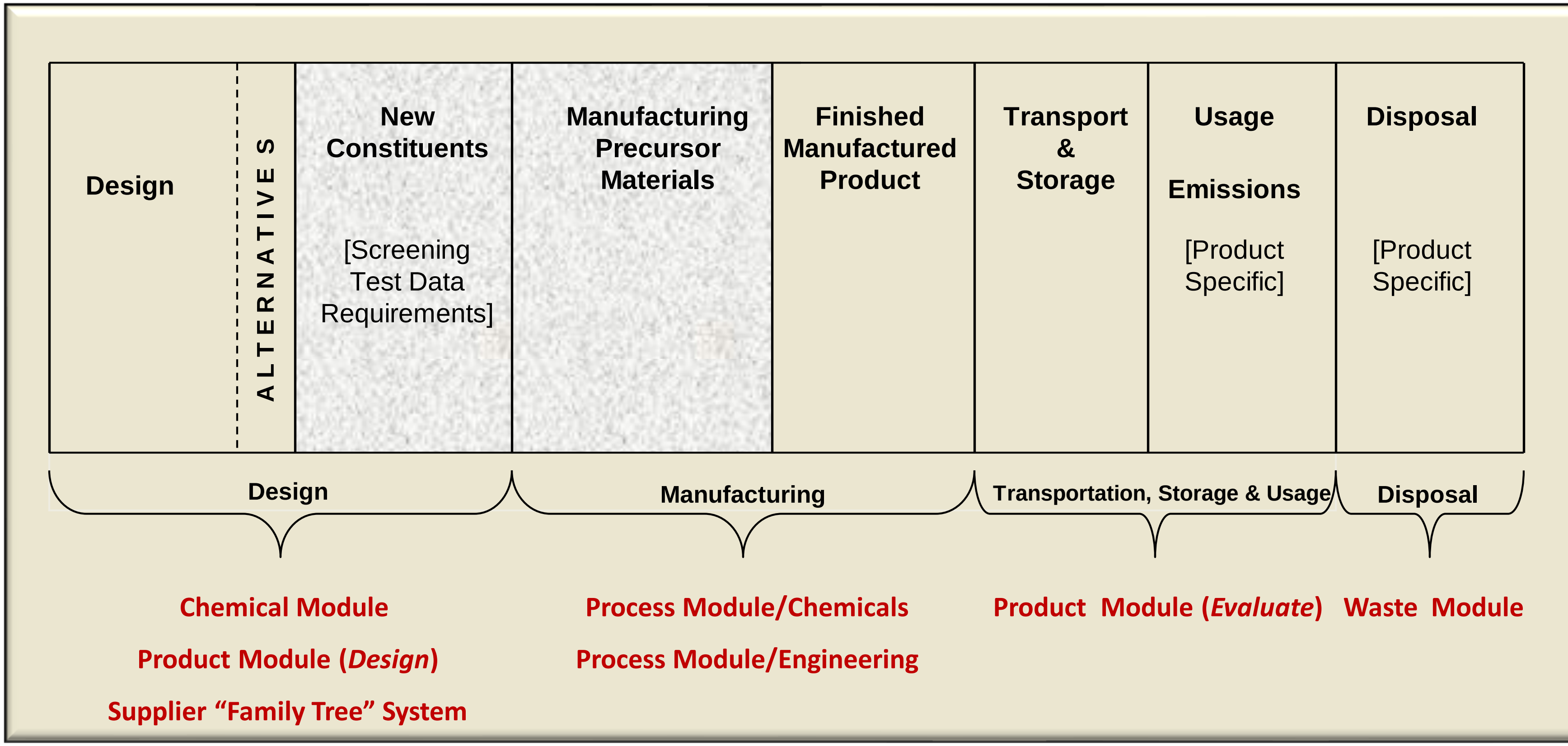
- **Formulated Products and Articles**
    - Add Pure Chemicals (?)
- **Certified to ANSI 355 Greener Chemicals and Processes Information Standard**
    - Human Health
    - Safety
    - Ecologic Impacts
- **Based Upon Chemical Concentrations in the Product/Article – <u>Full Formulation</u>**
- **Includes Exposure Scenario Factors**

Interior	Exterior
Frequency	Frequency
Duration	Duration
Amount Utilized	Amount Utilized
Ventilation Rate	Wind Speed
Room Size	Unlimited

- **Informative References Cited**
    - **GreenSuite®**
    - Other 3rd Party Tools Referencing ANSI 355
- **Risk Reporting Classifications: Green (least), Yellow, Orange, Red (most)**
    - Document Risk Calculation Methodology
    - Underlying Assumptions
    - Conversion to Color Scheme Methodology
    - Exposure Routes and Scenarios
    - Worst Case Constituent Chemical Exposure RCR (I,D, O)

GreenSuite®

Lifecycle Alternative Assessments



How to Avoid (or Win) An SPF/PU Lawsuit

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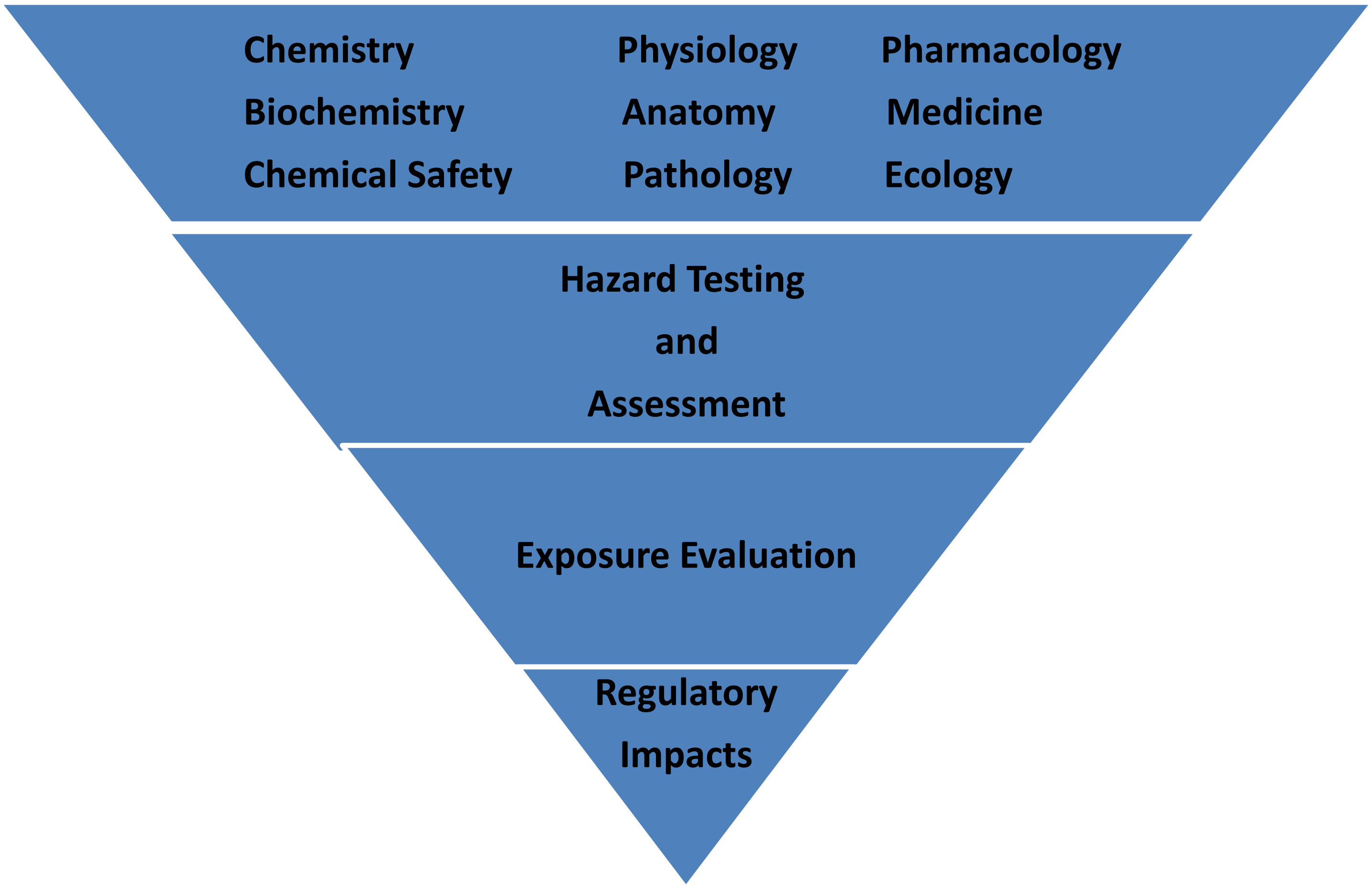
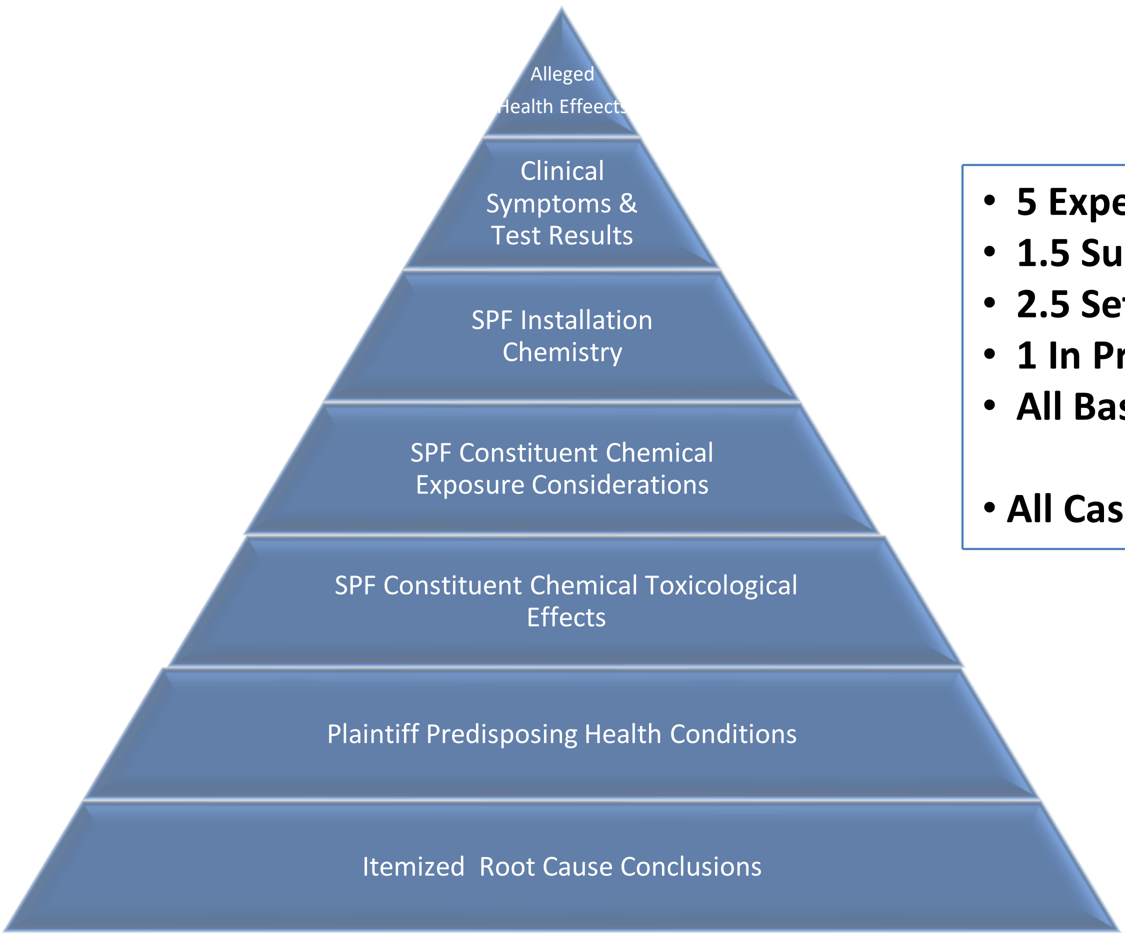
Toxicology – The Regulatory Science of Poisons



Risk Assessment

SPF Chemistry Lawsuit Experiences

Case-Specific *Toxicological Root Cause Analysis Elements*



- **5 Expert Witness Cases - Defendants**
- **1.5 Summary Judgment Wins**
- **2.5 Settled Wins**
- **1 In Progress**
- **All Based Upon Detailed Chemistry Risk Assessments**
- **All Cases Started by Installation Complaint**

SPF and PU General Chemistry Reactions

Side A	+	Side B	----->	Curing SPF/PU	----->	Cured SPF/PU "Article"
Isocyanate Blend	+	Polyol Blend	---->	SPF	---->	SPF

Side A (Isocyanate Blend):

Reacts 100%
Isocyanate chemicals (100%)

Side B (Polyol Blend):

Polyols React 100%
Polyols (20-70%)
Amine/Metal Catalysts (0.1-5%)
Flame Retardants, Reactive (5-8%)
Flame Retardants, Nonreactive (10-30%)
Surfactants (<1%)
Blowing Agent, Reactive – Water (17-20%)
Blowing Agent, Nonreactive (8-14%)
Antimicrobial (<0.5%)

Curing SPF:

SPF (+ CO_2)
SPF (Solid) – No Free Isocyanate
Residual Glycols – V. Low VP
Amine/Metal Catalysts (Intact) – Low VP
Bound 100% to SPF
Flame Retardants, Nonreactive (Intact) – V. Low VP
Surfactants (Intact) – Extremely Low VP
Blowing Agent Reacts 100% to Form CO_2
Blowing Agent, Nonreactive (Intact)
High VP
Antimicrobial (Intact) – V. Low VP
Urea – Low VP

Cured SPF:

SPF (+ CO_2)
SPF (Solid) – No Free Isocyanate
Amine/Metal Catalysts (Intact) – Low VP
Bound 100% to SPF
Flame Retardants, Nonreactive (Intact) – V. Low VP
Surfactants (Intact) – Extremely Low VP
Reacts 100% to Form CO_2
Blowing Agent, Nonreactive (Intact)
High VP
Antimicrobial (Intact) – V. Low VP

Isocyanate Blend	+	Polyamine Blend	---->	PU	---->	PU "Article"

Requires no catalyst
Reactivity temperature independent
Reactivity humidity independent
Chemical, solvent, impact ,temp resistance

“Safe” – Dictionary Definitions

1. “free from harm or risk” – different?
2. “secure from threat or danger, harm, or loss”
3. “affording safety or security from danger, risk, or difficulty”
4. “not likely to take risks; cautious”
5. “*successful in reaching base in baseball without being put out*”

Historic Toxicology - Definitions

HAZARD – estimated/measured adverse effect from a chemical under specific conditions

TOXIC – deleterious to man &/or other organisms

POISON – any agent capable of producing a deleterious biological response (every known chemical)

RISK – probability an adverse effect will occur under specified conditions, influenced by

- Exposure amount, frequency, duration
- Exposure route (inhalation, ingestion, dermal)
- Effect severity/usage conditions

RISK = f (Hazard • Exposure)

HAZARD ASSESSMENT (Chemical) – experimentally identify deleterious effects: Health, Environmental, Safety

RISK ASSESSMENT – characterization of potential adverse effects under specified usage and exposure conditions

- Identify hazards
- Evaluate exposure elements & conditions
- Eliminate or control the hazards

Paracelsus – The Father of Toxicology
(1493-1541)

"Alle Ding sind Gift, und nichts ohn Gift, allein die Dosis macht, das ein Ding kein Gift ist"

All things are poisons, and nothing is without poison; only the dose permits something not to be poisonous

"Substances considered toxic are harmless in small doses, and conversely, an ordinarily harmless substance can be deadly if over-consumed"

"'Poisons' were not necessarily something negative…poisons could have beneficial medical effects"
[*toxicology vs. pharmacology*]

The Dose Makes the Poison

Hazard Assessments *vs.* Risk Assessments

HAZARD of CONCERN	RISK MODIFICATION STRATEGIES	RESULTANT BENEFITS
• **Medicines/Vaccines**	**Dosages, Frequency, Duration**	**Prevent/Cure Diseases**
• **Food Constituents** **Potatoes – *Arsenic/Bromine/Nickel*** **Mushrooms, Duck, Pears, Cauliflower - *Formaldehyde*** **Tea – *Fluoride***	**Small concentrations, Vary Diet**	**Nutrition/Health**
• **Vehicle Fuel Flammability**	**Engineering Controls**	**Efficient Transportation**
Product/Process Chemicals	**Exposure Minimization** **Engineering Controls**	**Diverse Product Availability**

All chemicals are hazardous, but prudent management & use can eliminate the risks

GreenScreen vs. GreenSuite

What is the GreenScreen?

- **Identifies hazard of substance only**
- Evaluates chemicals ranked on 18 hazard endpoints (human health, ecological, physical)
- Rankings are consolidated into a single benchmark score from 1-4 (1 = ”Do not use” to 4= ”Preferred”)
- Cannot be used for an overall assessment of a mixture (hazard score for any ingredient is applied to the whole product)
- Cannot be used to determine risk
- Resins typically have limited data and generally receive a relatively low score
- Evaluations are subjective

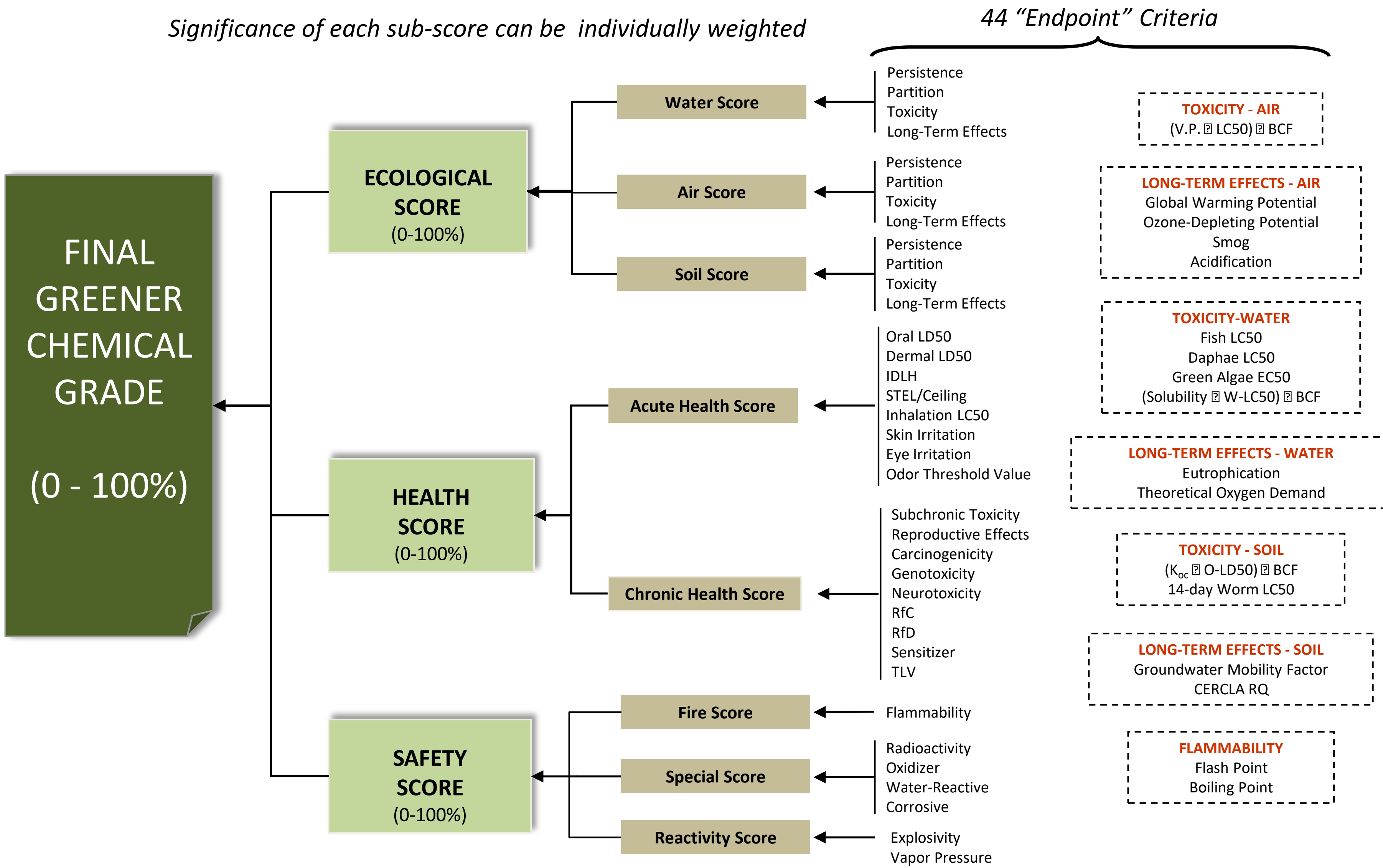
What is the GreenSuite?

- **Tool developed in 2003 for the U.S Department of Defense munition analyses - hazard and risk**
- In 2011, the logic used in the tool was accepted as an ANSI standard (ANSI-355: “Greener Chemicals and Processes Information Standard)
- **Evaluates chemicals on 44 hazard endpoints (ecological, health, and safety) utilizing chemical database with over 80 million data elements**
- Green score classification follows an easy to understand report card grading system (90-100% = A, 80-89%=B, etc.)
- Can be utilized for single chemicals or mixtures of chemicals (e.g., a coating) – objective evaluations
- **Takes into account the amount of a chemical in the mixture - risk of the product can be assessed**

Tool	Hazard Assessment	Overall Product Score	Risk Assessment	Resins Evaluated Accurately	Full Automated
GreenScreen					
GreenSuite					

"GREENER" CHEMICAL SCORING PROCESS

Chemicals – Products – Processes – Wastestreams



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73 - 76	C	Slight Risk
70 – 72	C-	Moderate Risk
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Side A - Isocyanate GreenSuite® Hazard Assessment Comparisons

Chemical Name	CAS #	Green Grade	Ecological	Health	Safety
Hexamethylene diisocyanate	28182-81-2	89	84	87	97
P-Toluenesulfonyl isocyanate	4083-64-1	74	77	83	63
Polymethylene polyphenylisocyanate	9016-87-9	72	70	59	85
Methylene bisphenyl isocyanate	26447-40-5	68	59	60	85
Metheylene diphenyl diisocyanate	101-68-8	65	59	51	85
Toluene-2-diisocyanate	584-84-9	64	69	47	77
Isophorone diisocyanate	4098-71-9	63	65	54	72

Primary Isocyanate Health Hazards

(Two Lowest Health Scores: TDI = **47** & MDI = **51**)

- **Acute Health Hazards** (Scores = **30** & **30**)
  - IDLH = **0** & **0**
  - STEL/Ceiling = **0** & **5**
  - Inhal LC50 = **2** & **7**
  - Skin Irrit. = **25** & 80
  - Eye Irrit. = **0** & **25**
- **Chronic Health Hazards** (Scores = **64** & **73**)
  - Carcinogencity = **50** & 90
  - Sensitizer = **0** & **0**
  - TLV = **0** & **9**

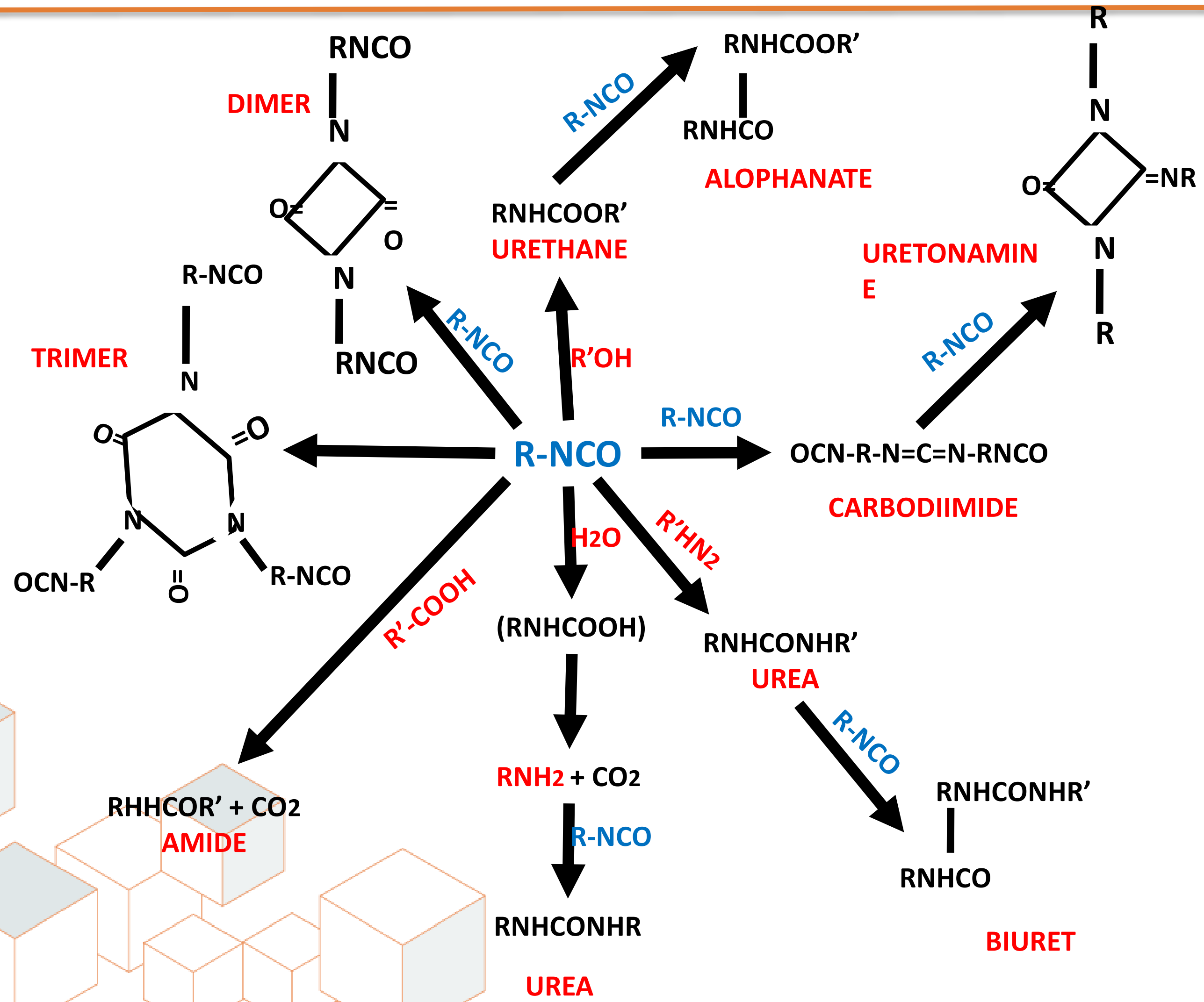
Scores < 65 in Red

CPI recommends full personal protective equipment to prevent skin, eye & inhalation exposure

Side A - Isocyanate GreenSuite® Hazard Assessment Comparisons, Vapor Pressure & Density

Chemical Name	CAS #	Green Grade	Ecological	Health	Safety	Vapor Press. (mmHg)	Density (g/cm3)
Water/Air	7732-18-5/---	100/---	100/---	100/---	100/---	23.8	1.225 E-3
Hexamethylene diisocyanate	28182-81-2	89	84	87	97	1 E-3	1.14
P-Toluenesulfonyl isocyanate	4083-64-1	74	77	83	63	9.44 E-5	1.29
Polymethylene polyphenylisocyanate	9016-87-9	72	70	59	85	5.4 E-13	1.23
Methylene bisphenyl isocyanate	26447-40-5	68	59	60	85	4.8 E-5	1.24
Metheylene diphenyl diisocyanate	101-68-8	65	59	51	85	1.89 E-4	1.23
Toluene-2-diisocyanate	584-84-9	64	69	47	77	2.38 E-2	1.22
Isophorone diisocyanate	4098-71-9	63	65	54	72	3.0 E-4	1.06

Isocyanate Chemical Reactions in Polyurethanes



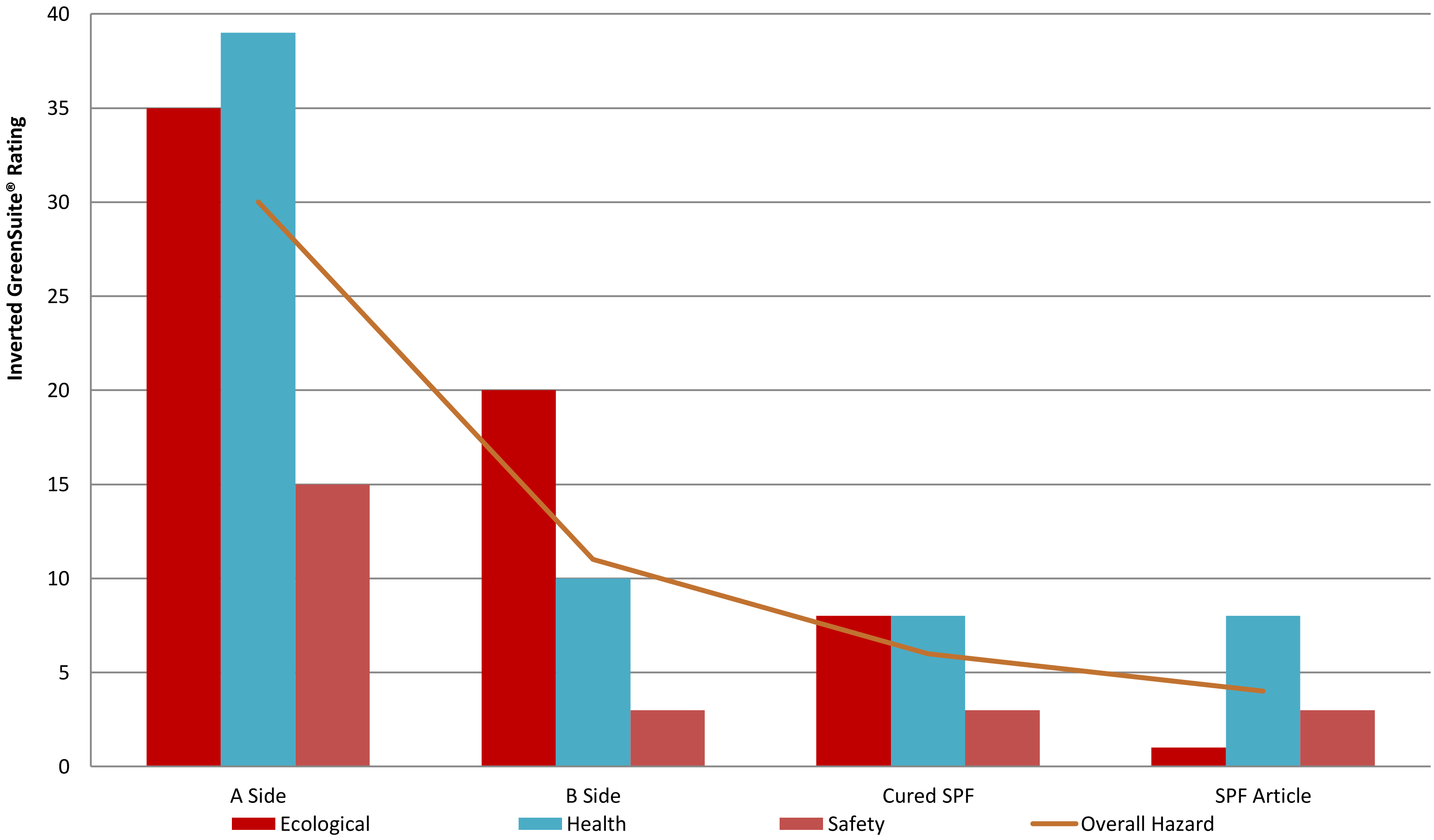
Side B – Polyol Blend GreenSuite® Hazard Assessment Comparisons (15-30 CAS #s)

Chemicals	Conc. (%)	Green Grade	Ecological	Health	Safety
Blowing, Reactive (1)	1	100	100	100	100
Blowing, Nonreactive (1)	9	86	77	91	92
Polyether Polyols (3)	0.8-15.2	85-88	75-84	78-90	92
Polyol, Sucrose (1)	6	85	74	89	92
Polyol, Aromatic (1)	39	86	78	89	92
Flame Retardant (2)	6-17	87	77	91	92
Surfactant (3)	0.03-4.8	79-86	74-81	70-86	92
Catalyst, Metal (6)	0.002-5.6	37,77-86	53, 62,76-78	26, 61, 84-89	30, 83-92
Catalyst, Amine (7)	0.2-0.8	71-83	68-73	50, 55, 81-88	83-92

Curing/Cured SPF Constituent Risk Assessments
(11/9 CAS #s)

Constituent	Conc. (%)	Ranking	Green Grade	Ecological	Health	Safety
Polyurethane Foam (SPF)	78	1	95	95	92	97
Polyol-1	0.04	2	89	83	86	97
Surfactant	0.36	3	88	78	89	97
Catalyst, Metal	5	4	88	77	91	97
Flame Retardant, NR	4	5	88	76	91	97
Blowing Agent	3.1	6	86	73	85	100
Catalyst, Amine-1	1	7	83	78	74	97
Reaction Product-1	7.3	8	82	69	77	100
Catalyst, Amine-2	1	9	81	68	86	88
Catalyst, Amine-3	0.05	10	77	66	84	82
Catalyst, Amine-4	0.2	11	72	74	**52**	90

Decreasing SPF Systems Relative Risk



Spray Polyurethane Foam (SPF) Chemistry

Side A	+	Side B	----->	Curing SPF	----->	Cured SPF "Article"
Isocyanate Blend	+	Polyol Blend	---->	SPF	---->	SPF
Reacts 100%		Polyols React 100% Amine/Metal Catalysts 50% Dilution Flame Retard., Nonreactive 50% Dilution Blowing Agent, Nonreactive 50% Dilution Antimicrobial 50% Dilution		SPF (+ CO_2) SPF (Solid) – No Free Isocyanate Residual Glycols – V. Low VP Amine/Metal Catalysts (Intact) – Low VP Bound 100% to SPF Flame Retard., Nonreactive V. Low VP Surfactants (Intact) – Extremely Low VP Blowing Agent, Nonreactive (Intact) High VP Antimicrobial (Intact) – V. Low VP Urea – Low VP		SPF (+ CO_2) SPF (Solid) – No Free Isocyanate Amine/Metal Catalysts (Intact) – Low VP Bound 100% to SPF Flame Retard., Nonreactive (Intact) – V. Low VP Surfactants (Intact) – Extremely Low VP Blowing Agent, Nonreactive (Intact) High VP Antimicrobial (Intact) – V. Low VP

- **Full PPE required during installation**
- **All occupants vacated during & 24-48 hours after**
- **Ventilate to outside during installation**

- **Maintain vacancy for 24-48 hours after install**
- **Aggressively ventilate to outside during curing**

- Document thorough final project inspection
- Walk through with customer

OSHA Hazard Communication Standard (HazCom)

- **Aligned with UN Global Harmonization System (GHS) 2012**
- **Classified Potential Chemical Hazards, including A & B Side constituents**
- **Employee Communication of Potential Chemical Hazards & Protections**
  - *Written Hazard Communication Plan (WHCP)*
  - *List of Chemical Hazards Present*
  - *Container Labeling – Workplace & Shipped*
  - *Safety Data Sheets (SDSs)*
  - *Employee Training Program*

OSHA Safety Data Sheet (SDS) Elements

1. Product Identification – Chemical/Mixture
2. Hazard(s) Identification
3. Product Hazardous Composition
4. First Aid Measures
5. Fire Fighting Procedures
6. Accident Release Measures
7. Handling and Storage
8. Exposure Controls/PPE
9. Physical/Chemical Properties
10. Stability/Reactivity
11. Toxicological Information
12. Ecological
13. Disposal Consideration
14. Transportation Information
15. Regulatory Information
16. Other Information (Prep Date/Last Revision)

Exposure Prevention Strategies

- **OSHA Hazard Communication required employee training**

  Written Hazard Communication Program
  Product & chemical Safety Data Sheet (SDS) review
  Product hazard awareness training
  Container labeling
  Exposure prevention strategies & equipment
  Personal Protective Equipment (PPE) requirements

- **Installer certification with SPF/PU manufacturer**

- **Worksite preparation procedures**

  Ventilation during & 24-48 hours after installation
  Airflow barriers & site protection coverings
  Restricted access placards – outside, inside

- **Building vacancy 24-48 hours post installation**

  Humans & pets
  Written & signed documentation of this requirement

Safe SPF - Conclusions

- **SPF is safe for consumers, but potentially hazardous for workers**
  - SPF chemistry protects the customer when properly installed
  - PPE and best business practices keep workers safe from SPF constituents

- A **Side is very hazardous (Health Scores = 47-60) – Risk is controllable**
  - Full body PPE & air supply
  - Rapidly reactive – binds to anything/everything
  - Heavier than air – settles quickly
  - Isocyanates undetectable within < 1 hour; don't evaporate
  - Isocyanates not in cured SPF

- B **Side is much less hazardous (Health Scores mostly 70-100)**
  - Protected by full body PPE & air supply
  - Zero to minimal residues in cured SPF – diluted 50%
  - Predominant polyols minimal hazards, mostly/entirely reacted

- **SPF system initial hazards essentially gone in properly cured SPF**
  - Isocyanate 100% reacted
  - B Side constituents diluted 50%
  - Proper chemistry during installation & curing is key

Safe SPF/PU - Recommendations

- **Manufacturers develop SPF/PU complete system risk assessments**
  - Evaluate A Side, B Side, Curing SPF/PU, & Cured SPF/PU
  - Use proprietary reports for internal constituent alternative assessments & sales literature
  - Provide nonproprietary reports to distributors & installers
  - Train product development chemists regarding “green” chemistry, i.e., hazards & risks
  - Add “green” chemistry SPF system awareness to installer certification program
  - Distribute SDSs for entire SPF/PU system – A & B Sides, Curing & Cured SPF/PU – to customers
  - Maintain liability insurance in case of lawsuits

- **Installers request mfr nonproprietary SPF/PU system risk assessment reports & SDSs**
  - **Reject potential customers with asthma, known chemical sensitivities, or COPD**
  - Train & test installers & sales staff regarding constituent hazards & formulation risks
  - Maintain SDSs for all SPF/PU system components
  - Inspect/grade/evaluate completed SPF projects - with pictures
  - Maintain detailed records for each SPF/PU project – specific process, issues, equipment
  - Annually monitor installer health
  - Maintain liability insurance in case of lawsuits

How to Avoid (or Win) An SPF/PU Lawsuit

Questions?

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