

Advantages of ZemaSol™ over Xylene/Toluene, PCBTF and TBAC

Purpose	This document compares the environmental considerations, safety and effectiveness of ZemaSol vs. Xylene and Toluene. Currently, the most commonly used replacements for these solvents are <i>para</i> -Chlorobenzotrifluoride (PCBTF) and <i>tert</i> -Butyl Acetate (TBAC).				
Factors to consider	A short list of factors to choose ZemaSol as a replacement for Xylene and Toluene over PCBTF and TBAC are: <ul style="list-style-type: none"> • environmental considerations - toxicity and regulatory controls • safety - reduced hazard to the environment and workers • performance - similar physicochemical characteristics that enable the solvent to dissolve the desired substances 				
Environmental considerations	The following table details the environmental considerations between ZemaSol, Xylene, Toluene, PCBTF and TBAC.				
	ZemaSol	Xylene	Toluene	PCBTF	TBAC
VOC Content: US EPA (outside SCAQMD)	0	100%	100%	exempt	exempt (under review)
VOC Content: SCAQMD	1.59* g/L	100%	100%	exempt	100%
Maximum Incremental Reactivity (MIR, g O₃/g organics)	0.079	4.25-10.71	3.97	0.11	0.2
Hazardous Air Pollutants	no	yes	yes	no	no

*ASTM Test Method 313-91. SCAQMD considers <5 g/L VOC content to be "zero VOC". ZemaSol is a blend of VOC-exempt solvents and as such is considered zero VOC by the EPA. ZemaSol is considered comprised of 100% exempt material as per CEPA, NPRI, and SCAQMD.

ZemaSol is far less toxic to the environment than conventional organic solvent alternatives. Toluene and Xylene are designated as Hazardous Air Pollutants (HAPs) and emitters of Volatile Organic Compounds (VOCs). HAPs and VOCs are hazardous to the environment, and regulations are increasingly restricting their emissions. ZemaSol is comprised of 100% VOC-exempt material and is not designated as a HAP.

TBAC and PCBTF are non-HAPS and VOC-exempt in most jurisdictions, but do not perform as well across the broad range of solvent applications.

TBAC, however, has been designated as a carcinogen. Regulators are seeking to de-list this solvent in 2015.

Toluene and Xylene emissions are major contributors to increased levels of VOCs in the environment and have high MIR values. Xylene is the largest contributor to the formation of ground-level ozone and photochemical smog among C₆-C₉ aromatic VOCs.

ZemaSol has a low Maximum Incremental Reactivity (MIR) value, and is thus particularly useful in reformulating aerosol paints and coatings while allowing manufacturers to meet new MIR limitations while maintaining performance properties.

Safety

The following table details the safety considerations between ZemaSol, Xylene and Toluene.

	ZemaSol	Xylene	Toluene
Toxicity: Oral LD₅₀ (rat) (mg/kg)	> 5000	> 4300	636
U.S. ACGIH Threshold Limit Values (8-Hour Time Weighted Average)	> 200 ppm	100 ppm	20 ppm

ZemaSol is far less toxic than conventional organic solvent alternatives. LD₅₀ assesses toxicity derived from acute exposure, and a higher LD₅₀ value suggests reduced acute toxicity. The acute oral toxicity of Xylene and Toluene is lower than that of ZemaSol, which indicates that Xylene and Toluene represent higher acute oral toxicity.

Threshold Limit Values (TLV) are restrictions enforced by the American Conference of Governmental Industrial Hygienists (ACGIH) that quantify in parts-per-million (ppm) the maximum allowable exposure for a certain chemical over an 8-hour time weighted average (TWA). The only ingredient in ZemaSol that contains an ACGIH TLV is listed at 200 ppm, which is higher than the allowable exposures for all other solvents listed.

Furthermore, both Xylene and Toluene are associated toxic effects derived from chronic exposure. Toluene is also designated as a teratogen and potential reproductive hazard, and Xylene has been shown to affect the development of fetuses. The main component of ZemaSol has not been shown to have toxic effects other than those derived from acute toxicity.

Performance

The following table details the performance characteristics between ZemaSol, Xylene, Toluene, PCBTF and TBAC.

	ZemaSol	Xylene	Toluene	PCBTF	TBAC
Solubility	comparable	comparable	comparable	poor	comparable
Viscosity (cP)	0.44	0.81	0.55	0.79	1.2
Surface Tension	24.2	28.7	28.4	25	22.4
Density	1.0	0.87	0.75	1.34	0.86
Hansen Solubility Parameters (MPa)^{1/2}	18.5	17.9	18.2	17.5	17.7
Dispersion (δ_D)	15.3	17.6	18.0	13.7	15.4
Polarity (δ_P)	7.6	1.0	1.4	9.9	6.2
Hydrogen Bonding (δ_H)	7.2	3.1	2.0	4.7	6.2
Hildebrand Solubility Parameter (MPa)^{1/2}	19.2	18.2	18.3	17.6	16.6

ZemaSol was carefully designed to mimic Xylene and Toluene in solubility and solvency, viscosity, surface tension, and physicochemical characteristics. PCBTF is too heavy and has poor solvency, while TBAC is too viscous and has low surface tension.

The performance of ZemaSol is comparable to that of Xylene, Toluene TBAC and PCBTF across many solvent characteristics. ZemaSol can be used across a wide variety of coatings, and ink and adhesive resin systems.

ZemaSol is the only replacement for Xylene and Toluene that is zero-VOC, lower in toxicity than many conventional organic solvent alternatives, and mimics the physicochemical properties of the solvents.

References

- California Division of Occupational Safety and Health. Table AC-1: Permissible Exposure Limits for Chemical Contaminants; https://www.dir.ca.gov/title8/5155table_ac1.html. (Accessed July 16th, 2015)
 - Carter, William P.L. Updated Maximum Incremental Reactivity Scale and Hydrocarbon Bin Reactivities for Regulatory Applications; <http://www.engr.ucr.edu/~carter/SAPRC/MIR10.pdf> Updated January 28th, 2010. (Accessed July 16th, 2015).
 - Na, K., Moon, K.-C., Kim, Y. P. Atmospheric Environment, **39**, 5517-5524.
 - Occupational Safety & Health Administration. Annotated Table Z-1: Limits for Air Contaminants; <https://www.osha.gov/dsg/annotated-pels/tablez-1.html> (Accessed July 16th, 2015)
 - Occupational Safety & Health Administration. Annotated Table Z-2: Limits for Air Contaminants; <https://www.osha.gov/dsg/annotated-pels/tablez-2.html> (Accessed July 16th, 2015)
 - Safety Data Sheet for Megaloid Laboratories Limited Xylenes; <http://megaloid.ca/MSDS/Xylene.pdf> (Accessed August 10th, 2015)
 - Safety Data Sheet for Sigma Aldrich Toluene; <http://www.sigmaaldrich.com/catalog/product/sial/244511?lang=en®ion=CA> (Accessed August 10th, 2015)
 - United States Environmental Protection Agency Technology Transfer Network - Air Toxics Web Site. Xylenes: Mixed Isomers. <http://www3.epa.gov/airtoxics/hlthef/xylenes.html> (Accessed September 18th, 2015)
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