ΕΛSTΜΛΝ

Eastman[™] solvents technical tip

Replacing acetone with Eastman[™] methyl acetate, high purity

Introduction

Eastman Chemical Company has received several requests to provide recommendations for solvents or solvent blends that can be used to replace acetone. The following information was developed using Eastman's Solvent Reformulation Wizard. A thorough evaluation should be made to determine whether a solvent or blend is suitable for use based on the specific applications.

Matching the evaporation rate and solvent activity of the control blend is critical to the success of any solvent reformulation effort. This ensures that the reformulated coating will have the desired flow characteristics and film formation quality when applied to a surface. Methyl acetate is similar to acetone in evaporation rate, VOC exemption, and non-HAP status, but offers a higher flash point and hydrophobic properties which can result in improved cost and performance benefits.

Eastman[™] methyl acetate HP (high purity) was added to the list of compounds excluded from the EPA (Environmental Protection Agency) definition of VOC (volatile organic compound) on the basis that this chemical has been determined to have negligible photochemical reactivity. Methyl acetate is readily biodegradable and relatively nontoxic and nonreactive, making it appropriate for use in environmentally preferred formulations.

Table 1 Physical properties of acetone vs. Eastman[™] methyl acetate, HP

Solvent	Acetone CAS 67-64-1	Eastman [™] methyl acetate, HP CAS 79-20-9	
Evaporation rate, $(n$ -butyl acetate = 1)	6.3	6.2	
Boiling point @ 760 mm Hg	132°–135°F	132.4°–136.7°F	
Freezing point	–95°C	–98°C	
MIR (maximum incremental reactivity)	0.43	0.07	
HAP (hazardous air pollutant)	No	No	
Solubility: In water, @ 20°C	Complete	22.7 wt%	
Water in, @ 20°C	Complete	8.8 wt%	
Wt/vol @ 20°C	6.6 lb/gal	7.78 lb/gal	
Hansen solubility parameters			
Hydrogen bonding	3.4	3.7	
Nonpolar	7.6	7.6	
Polar	5.1	3.5	
Total	9.8	9.2	

Discussion

Key attributes

- •Excellent solvent activity:
- Dissolves a wide range of resins for effective removal of contaminants.
- Yields solutions with low viscosities in coating applications.
- •Fast evaporation rate: Surfaces dry quickly, preventing redeposit of contaminants on cleaned substrates.
- •Versatile: Miscible with most organic solvents.

Applications and performance benefits

Eastman[™] methyl acetate is a viable replacement for acetone in a wide range of applications including:

Aerosol coatings

Cleaners

- Automotive coatings
- Printing inks
- Industrial coatings
- Adhesives
- •Furniture coatings
- Solvents for cosmetics
- •Other paint and coatings
- •Solvents for personal care

Cleaning applications (Metal degreasing, paint removal, precoating cleaning)

Methyl acetate's wide formulation latitude makes it ideal for use as an effective, economical cleaner in a wide range of automotive, marine, and industrial market applications. Its hydrophobic nature is a key performance characteristic in cleaning applications where moisture-related problems can damage or corrode parts, leading to defects or rejects. For example, it can be used to ensure a clean, dry surface prior to coating or painting parts in automotive and aviation applications.

OEM and special purpose applications

The hydrophobic nature of Eastman[™] methyl acetate greatly reduces the likelihood that moisture will be drawn into a coating and can prevent a variety of moisturerelated problems and coating defects. It can also be beneficial in solving shelf stability concerns and reducing surface blush which can occur when coatings are applied under humid conditions. In addition, its low water content makes it suitable for use in moisture-sensitive applications (i.e., 2-K polyurethane).

Electrostatic spray applications

In addition to the performance benefits offered in traditionally applied coatings and cleaners, Eastman[™] methyl acetate provides higher electrical resistance than acetone, which can provide improved transfer efficiency for coatings applied by electrostatic spray. This feature can also translate into reduced cost and lower volatile emissions with improved paint utilization.

Regulations impacting aerosol coatings

The concept of IR (Incremental Reactivity) was developed to measure the relative atmospheric reactivity in VOCs. The most common method of measuring IR in the United States is the MIR (Maximum Incremental Reactivity) scale. In the MIR methodology, each VOC is assigned an individual reactivity value. The MIR value enables the formulator to compare the photochemical reactivity differences of various solvents (including propellants) used in aerosol coatings. A higher MIR value denotes a more reactive compound, which has a greater propensity to create ground-level ozone under appropriate conditions (sufficient NO_v, surface temperature, sunlight, etc.)

CARB (California Air Resource Board) uses the photochemical reactivity-based limits for regulating ozone formation from aerosol coatings (Regs. Tit. 17, Art. 3 §§ 94521–94524 and 94526). This regulation replaced the traditional mass-based VOC emission regulations. It is likely that future air quality policies affecting coatings will contain provisions for using the IR concept and will be more efficient than current mass-based regulations for controlling ground-level ozone formation.

Formulations to balance VOC and cost-effectiveness

Aromatic hydrocarbons such as toluene and xylene tend to be more economical solvents with relatively high MIR values. Methyl acetate's MIR value is 0.07, versus 0.43 for acetone, which makes it particularly useful in reformulating aerosols to meet the reactivity limits while maintaining performance properties.

The control formulation in Table 2 does not meet the targeted MIR value (<1.50) for clear aerosol coatings. Reformulation #1 demonstrates how to achieve the targeted MIR value by decreasing the aromatic hydrocarbons content and introducing *n*-butyl acetate to

maintain an overall balance of properties. Decreasing the MIR value from 2.56 in the control formulation to 1.45 in reformulation #1 required a calculated solvent blend cost increase of 0.136 cents/lb or 37%.

Reformulation #2 shows an aerosol coating formulation using methyl acetate instead of acetone to meet the targeted MIR value. This solvent blend provides a similar evaporation rate and solubility parameter profiles to reformulation #1 with a lower cost/lb. The range of possible cost reduction shown in reformulation #2 is explained by a higher level of more economical toluene.

Table 2 Clear aerosol coating sample reformulations (MIR limit 1.50)

	Control formulation	Reformulation #1	Reformulation #2
Acetone	20	20	_
Eastman [™] methyl acetate, high purity	—	—	20
Xylene	20	7.5	7.5
Toluene	20	10.5	13
<i>n</i> -Butyl acetate	—	22	19.5
Propellant	20	20	20
MIR value	2.56	1.45	1.45
Evaporation rate	1.6	1.7	1.6
Hansen solubility parameters			
Nonpolar	8.3	7.9	8.0
Polar	2.2	2.8	1.9
Hydrogen bonding	2.0	2.8	2.6
Total	8.8	8.8	8.7
Solvent blend, cents/lb	0.384	0.524	0.49–0.504
% Increase ^a		37	28–31

^a% increase can rise or fall based on market conditions.

Eastman[™] solvents technical tip Replacing acetone with Eastman[™] methyl acetate, high purity (Continued)

Regulatory information

- •VOC exempt status: Allows formulators to meet VOC limits.
- •Low MIR value: Helps formulators of aerosol coatings for California meet MIR guidelines.
- •FEMA GRAS: Carries the favorable FEMA GRAS (Flavor and Extracts Manufacturers Association—Generally Regarded as Safe) designation by the Food and Drug Administration.
- •SNAP approved: Significant New Alternative Program.
- •Readily biodegradable solvent.
- •Non-HAP: Use level not restricted by Title III of CAA.
- •Non-ODS: Non-ozone depleting substance.
- •Higher electrical resistance, less hydrophilic, and higher flash point than acetone: VOC-exempt replacement solvent for acetone.
- •Low odor: Suitable for odor-sensitive applications.
- •Urethane grade: Suitable for use with moisturesensitive polymers.

Conclusion

Eastman[™] methyl acetate's VOC-exempt status, in combination with its excellent solvent activity and readily biodegradability, helps formulators meet the demands for environmentally conscious formulations without sacrificing performance.

Eastman is the world's leading producer of methyl acetate with two additional grades available. Contact Eastman Chemical Company to discuss which grade best suits your specific application needs.



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