

EASTMAN

Eastman AQ™ polymers

for cosmetics and personal care

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Introduction

Eastman Chemical Company manufactures a diverse range of quality ingredients for cosmetics and personal care applications. Among these is the unique product group, Eastman AQ™ water-dispersible polyesters (see Table 1). Eastman AQ™ 38S, Eastman AQ™ 48 ultra, and Eastman AQ™ 55S linear polyesters serve as film formers in skin care, hair styling, color cosmetics and other personal care products. They also aid the dispersion of hydrophobic ingredients in water-based cosmetic formulations. Eastman AQ™ 48 ultra polymer was designed specifically for low-VOC (volatile organic compound) hair spray.

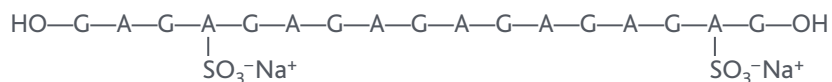
Description

Eastman AQ™ polymers for cosmetics and personal care applications are linear, amorphous polyesters that disperse in water without the assistance of organic solvents, surfactants or amines. This water-dispersibility is mainly attributed to the ionic nature of the sodiosulfo substituents attached to the polymer chain (see simplified structure, Figure 1).

Table 1 Eastman AQ™ polymers

Product name	INCI name
Eastman AQ™ 38S polymer	
Eastman AQ™ 48 ultra polymer	Polyester-5
Eastman AQ™ 55S polymer	

Figure 1 General structure



where: A = dicarboxylic acid moiety
 G = glycol moiety
 SO₃⁻Na⁺ = sodiosulfo group
 OH = hydroxyl group

Eastman AQ™ linear polyesters are similar to each other in physical form, color and molecular weight (see Table 2). They differ from each other chiefly in glass transition temperature (T_g) or softening point. The number in the product name indicates the dry T_g of each polymer. Other differences are the clarity of the Eastman AQ™ aqueous dispersions and their ability to tolerate common organic solvents without precipitating the polymer. Also, films made from the polymer

dispersions have different degrees of water resistance. The relative order of Eastman AQ™ polymers with respect to these properties is as follows:

Aqueous dispersion clarity	AQ 48 > AQ 55 > AQ 38
Solvent tolerance	AQ 48 > AQ 38 > AQ 55
Water resistance	AQ 55 = AQ 38 > AQ 48

Table 2 Typical properties^a of Eastman AQ™ polymers

Property	Eastman AQ™ 38S	Eastman AQ™ 48 ultra	Eastman AQ™ 55S
Percent solids	100	100	100
Physical form	Pellets	Pellets	Pellets
Molecular weight, Mn	10,000	10,000	10,000
Hydroxyl number	<10	<10	<10
Acid number	<2	<2	<2
T_g , °C (dry polymer)	35–38	45–48	51–55
Inherent viscosity, dL/g	0.32–0.40	0.26–0.32	0.29–0.37
Color	Clear, light amber	Clear, light amber	Clear, light amber

^aThese properties are typical of average lots. Eastman makes no representation that the material in any particular shipment will conform exactly to the values given.

Unique properties

- Disperse in water
- Provide low viscosity aqueous dispersions at <30% solids
- Form films at room temperature
- Aid dispersion of hydrophobic materials in water
- Adhere to skin and hair

Applications

The unique properties of Eastman AQ™ linear polymers make them useful in many cosmetics and personal care products (see Table 3). In some instances, they provide a way to differentiate a product line. For example, Eastman AQ™ 38S and 55S seem to impart a good feel to creams, lotions and liquid makeup, especially if a nonoily, nongreasy feel is desired. Eastman AQ™ 38S is preferred over 55S for creams and lotions because its lower T_g provides a softer film and a smoother feel as the cream is rubbed into the skin. Eastman AQ™ 55S has better film integrity when combined with other cosmetic ingredients and, therefore, is the preferred AQ™ polymer for water-based makeup and mascaras. Eastman AQ™ 55S improves water and smudge resistance in these products.

Since Eastman AQ™ 48 ultra was specifically developed as a hair fixative for 55% VOC hair spray, it is compatible with higher levels of alcohol than Eastman AQ™ 38S and 55S. Eastman AQ™ 48 is also less water resistant than 38S and 55S, which facilitates good washout during shampooing. The exceptional dry time and moisture resistance of Eastman AQ™ polymer films are advantageous in all of these applications.

Table 3 Eastman AQ™ polymer applications

Polymer	Primary applications
Eastman AQ™ 38S	Sun and skin care: creams, lotions, sprays
Eastman AQ™ 48 ultra	Hair styling: hair spray, mousse, gels
Eastman AQ™ 55S	Liquid makeup, mascara

Various additives can be used with Eastman AQ™ polymer dispersions to modify the properties of cosmetics and personal care products. Conventional thickeners may be used to adjust the viscosity of Eastman AQ™ dispersions. Selected solvents and/or oils can be added to decrease dry time or provide emolliency. Film flexibility can be adjusted through polymer selection and by incorporating the appropriate level of plasticizer. Additives such as propylene glycol and ethoxydiglycol increase softness, water sensitivity and flexibility.

Characteristics

Moisture Regain

Eastman AQ™ polymers absorb moisture from ambient air because of their ionic nature and the presence of hydrophilic glycols in the polymer chain. Moisture regain of the polymer films is affected predominately by the amount of sodiosulfo substitution and to a lesser degree by the glycol content. Some glycols are more hydrophobic than others and thus tend to decrease moisture regain. As shown in Table 4, moisture regain lowers the T_g of Eastman AQ™ 55S polymer. Eastman AQ™ 48 and 38S behave similarly.

Table 4 Effect of relative humidity on moisture regain and T_g of Eastman AQ™ 55S polymer^a

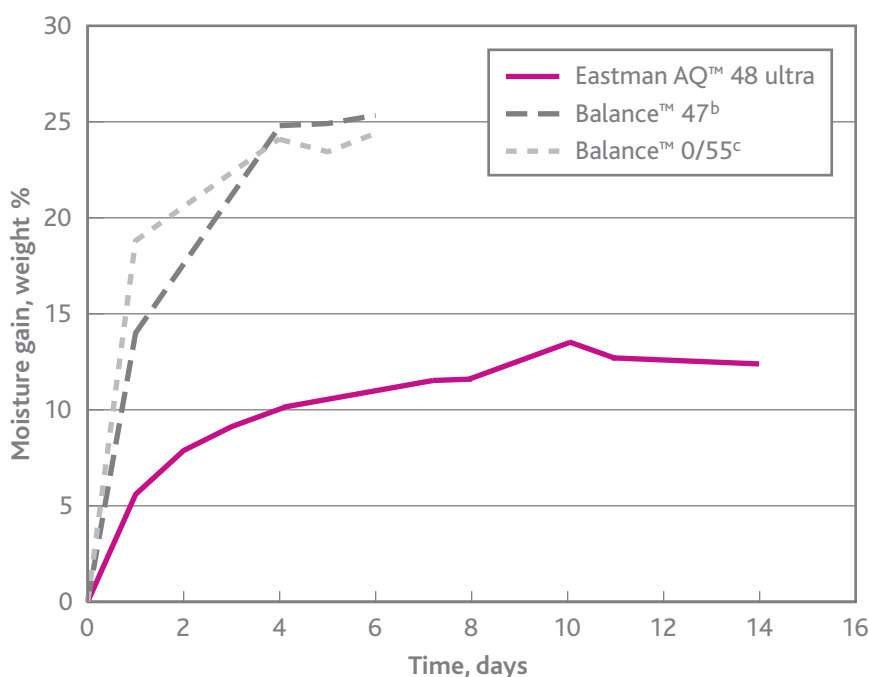
Relative humidity, %	Moisture regain, %	T_g , °C
0	—	55
30	2.3	44
62	3.0	39
80	4.8	37
95	5.0	35

^aTwo-week conditioning of 3-mil film at 21°–23°C (70°–73°F).

Tensile properties of Eastman AQ™ polymers are also affected by moisture uptake. As moisture content increases, the tensile breaking strength and initial modulus decrease; the elongation at break increases.

Under high humidity conditions, Eastman AQ™ polymers absorb less moisture compared with typical acrylic polymers used in hair spray. Figure 2 shows the moisture regain of selected polymers at 90% relative humidity.

Figure 2 Moisture regain of Eastman AQ™ 48 ultra and acrylic polymers^a



^aDry films conditioned at 22°C and 90% relative humidity.

^bNational Starch (Octylacrylamide/Acrylates/Butylaminoethyl Methacrylate Copolymer)

^cNational Starch (Acrylates Copolymer)

Morphology

Eastman AQ™ polymers are thermoplastic and amorphous; they show no detectable crystal melting by differential scanning calorimetry (DSC).

Dispersibility/solubility

Eastman AQ™ polymers are dispersible or soluble in various solvents as shown in Table 5. Eastman AQ™ polymer pellets were combined with various solvents and solvent/water mixtures (1:9 parts-by-weight AQ to solvent), then gently agitated for one week at room temperature. Eastman AQ™ polymers are likely to disperse quicker and more completely at higher temperatures.

Table 5 Dispersibility/solubility of Eastman AQ™ polymers

Solvent	Eastman AQ™ 38S	Eastman AQ™ 48 ultra	Eastman AQ™ 55S
Water	H	C	PD ^{HV}
Glycols and alcohols			
Diethylene glycol	C ^{SV}	C ^{SV}	C ^{SV}
Propylene glycol	U	PD ^V	U
Dipropylene glycol	SW	PD ^{SV}	SW
Glycerin	U ^V	U ^V	U ^V
Ethyl alcohol, anhydrous	U	SW	U
Isopropyl alcohol	U	U	U
Ethoxydiglycol (DE solvent)	C ^{SV}	C ^{SV}	H ^{SV}
Butoxyethanol (EB solvent)	U	SW	U
Esters			
Methyl acetate	PD	PD	PD
Ethyl acetate	SW	SW	SW
n-Butyl acetate	PD	U	U
Butoxyethyl acetate (EB acetate)	U	U	U
Methoxyisopropyl acetate (PM acetate)	U	U	U
Trimethyl hydroxypentyl isobutyrate (Eastman Texanol™ ester alcohol)	U	U	U
Ketones			
Acetone	SW	SW	SW
Methyl ethyl ketone	SW	PD	SW
Hydrocarbons			
Hexane	U	U	U
Mineral oil	U	U	U
1:1 Mixtures with water			
Propylene glycol:water	H	C	PD
Glycerin:water	H ^V	C	SW
Ethyl alcohol:water	H	C	H
Ethoxydiglycol:water	C	C	C

C = Completely dispersed and clear

H = Completely dispersed and hazy

PD = Partially dispersed

SW = Pellets swollen and/or tacky, not dispersed

U = Undispersed, nearly unaffected

^{SV} = Slightly viscous

^V = Viscous

^{HV} = Highly viscous

Aqueous dispersions

Eastman AQ™ polymer pellets are dispersible in hot water without the assistance of cosolvents, surfactants or neutralizing agents. Complete dispersion is normally achieved in 20 to 30 minutes. Dispersions of up to 30% Eastman AQ™ polymer can easily be prepared using deionized water. Typical properties of aqueous dispersions are shown in Table 6.

Table 6 Typical properties^a of Eastman AQ™ polymer aqueous dispersions

Property/polymer	Eastman AQ™ 38S	Eastman AQ™ 48 ultra	Eastman AQ™ 55S
Ionic type	Anionic	Anionic	Anionic
pH	6.0–7.0	5.7–6.0	5.9–6.5
Clarity	Hazy	Clear	Slightly hazy
Turbidity of 30% AQ dispersion, NTU ^b	200–400	5–20	20–40
Maximum alcohol tolerance ^c			
5% AQ dispersion	40%–45%	50%–55%	30%–35%
10% AQ dispersion	30%–35%	40%–45%	25%–30%

^aThese properties are typical of average lots. Eastman makes no representation that the material in any particular shipment will conform exactly to the values given.

^bTurbidity varies with dispersion temperature and rate of mixing.

^cSlight flocculation may occur, which is easily redispersed.

Dispersions of Eastman AQ™ polymers are:

- Solvent-free, if desired.
- Surfactant-free.
- Water-reducible.
- Viscosity-adjustable with thickeners.
- Stable in pH range 5 to 7.
- Compatible with nonionic and anionic surfactants and polymers.
- Generally incompatible with cationic surfactants.

Procedure for dispersing Eastman AQ™ polymers in water

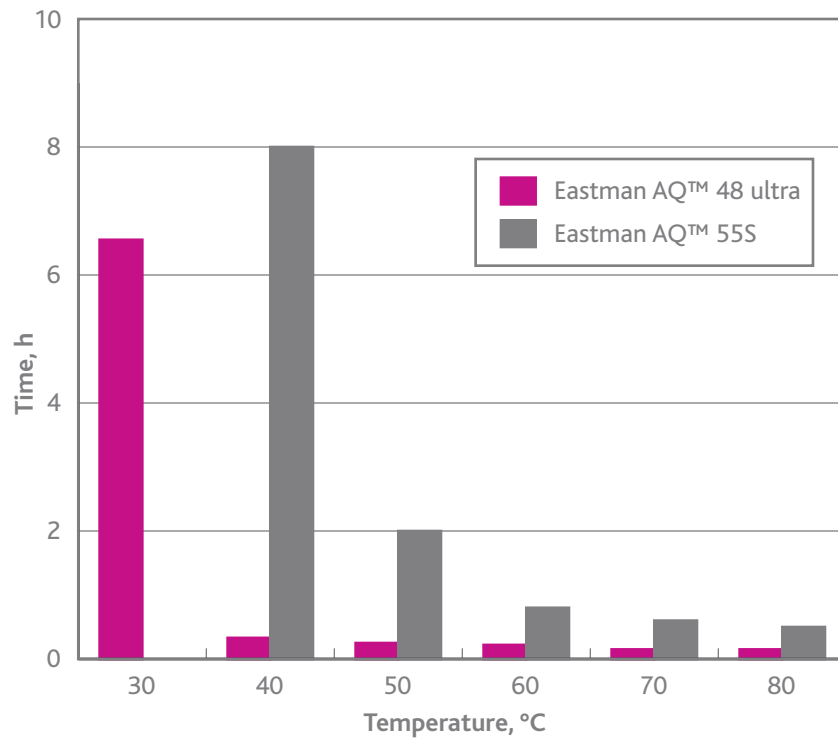
- Heat deionized water.

Eastman AQ™ 38S	60°–80°C
Eastman AQ™ 48 ultra	45°–50°C
Eastman AQ™ 55S	60°–80°C
- Add pellets slowly with rapid stirring.
- Stir until completely dispersed.
- Cool.
- Proceed with formulation.

Dispersion rate

Soft or deionized water (total hardness less than 20 ppm) is recommended for Eastman AQ™ polymer dispersions because hard-water ions (Ca^{+2} , Mg^{+2} , Fe^{+3} , etc.) retard the dispersion rate. Hard-water ions can produce opaque or unstable dispersions if present in sufficient concentration. Dispersion rate is also dependent on water temperature (see Figure 3). Eastman AQ™ 48 disperses faster and at lower temperatures than the 38S and 55S polymers.

Figure 3 Effect of temperature on dispersion rate of Eastman AQ™ 48 ultra and 55S polymers

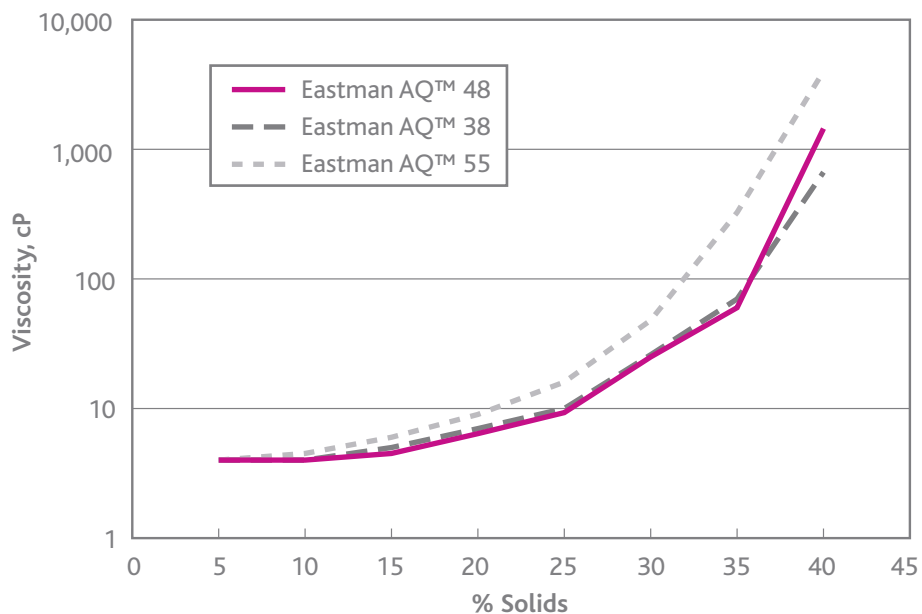


Aqueous dispersion viscosity

Eastman AQ™ polymers are dispersible in water, rather than soluble. Therefore, the viscosity of the dispersions is very low (<10 cP) at 20% solids. As the solids level increases above 30%, the dispersion viscosity increases rapidly (see Figure 4). A solids content of 40% is near the maximum that can be achieved for Eastman AQ™ polymers.

When forming a film from an Eastman AQ™ dispersion, the water evaporates more quickly compared with a polymer solution and the viscosity increases quickly as the polymer film dries. Therefore, formulations containing Eastman AQ™ polymers reach a dry-to-touch state after a relatively short dry time. This is particularly beneficial for Eastman AQ™ 48 polymer, when used as a fixative in hair spray products. Eastman AQ™ 48 provides a very rapid dry time and good hold, even before drying is complete. Conversely, the dried film must absorb a significant amount of moisture from the atmosphere before its properties are adversely affected.

Figure 4 Viscosity of Eastman AQ™ aqueous dispersions



Thickening polymer dispersions

The viscosity of Eastman AQ™ polymer dispersions can be increased by the addition of conventional thickening agents, such as the following.

- Acrylates/C 10-30 alkyl acrylate crosspolymer
- Carbomer
- Cellulose gum
- Polyvinyl alcohol (partially hydrolyzed)
- Silica
- Starch and modified starches
- Xanthan gum

Although mixtures of these thickeners with Eastman AQ™ polymers show good compatibility initially, they may require the addition of other formulation ingredients to maintain long-term stability.

Effect of pH on dispersion stability

Dispersions of Eastman AQ™ polymers in water are most stable at pH 5 to 7. In this pH range, there is no significant change in molecular weight after 1-year storage at room temperature. Below pH 5, acid-catalyzed hydrolysis results in a decrease in molecular weight over time, especially at elevated temperatures. Similarly, above pH 7, base-catalyzed hydrolysis (saponification) can result in precipitation. Both acidic and basic degradation reactions are accelerated by increasing temperature and by increasing acid or base concentration. The presence of an organic solvent in the Eastman AQ™ dispersion can reduce the rate of hydrolysis. Most notable is the increased stability of Eastman AQ™ 48 polymer in 50% to 55% ethanol dispersions in the pH range 7 to 8.

Dispersion of hydrophobic materials and common solvents

Eastman AQ™ polymers have the capability to disperse many hydrophobic ingredients in water; including pigments, waxes, oils, and plasticizers. This property is beneficial for applications where the omission or reduction of solvents and conventional surfactants is desirable.

Solid powders such as common pigments and fillers disperse readily when added to Eastman AQ™ polymer dispersions, without causing coagulation or a significant viscosity change. For color cosmetic emulsions, this means that pigments can be added to the AQ-containing aqueous phase instead of the oil phase, if desired. Alternatively, the pigments themselves can be surface-treated with Eastman AQ™ polymers to provide water-dispersibility. Table 7 illustrates the dispersibility of titanium dioxide and calcium carbonate in an Eastman AQ™ 55S aqueous dispersion.

Table 7 Dispersibility of fillers in Eastman AQ™ 55S dispersion^a

Pigment/filler	Loading phr ^b	Viscosity, cP		pH	
		Initial	7 day	Initial	7 day
Titanium dioxide	50	34	35	5.7	6.1
	25	27	28	7.2	7.7
	50	29	30	7.4	7.7
	75	32	33	7.4	7.8
Calcium carbonate	100	33	35	7.5	7.8

^aEastman AQ™ 55S polymer dispersed at 28% solids in water.

^bDry basis, parts filler per 100 parts Eastman AQ™ 55S polymer dispersion.

Hydrophobic materials that do not readily disperse in Eastman AQ™ dispersions can often be incorporated using a high-shear mixer such as a Kady® mill or Ultra-Turrax® mixer. High loadings of the hydrophobe can be attained. For example, using a high-shear rotor-stator mixer, silicone oil can be dispersed in an AQ aqueous dispersion at an oil-to-AQ ratio as high as 50:1 parts-by-weight. The amount of water in the final dispersion can range from 30 to 90 wt %. Waxes have been dispersed in an AQ aqueous dispersion at a wax-to-AQ ratio of about 10:1 parts-by-weight with 40 to 60 wt % water in the final dispersion. When dispersing waxes, the wax and AQ dispersion are heated separately to a temperature high enough to melt the wax. Then the wax is added slowly while mixing the AQ dispersion under high-shear conditions. Dispersions of hydrophobe/Eastman AQ™ polymer are water-reducible; their rate of separation varies depending on the hydrophobe and its concentration.

The dispersions/emulsions shown in Table 8 were prepared by heating both the “oil-phase component” and the Eastman AQ™ aqueous dispersion to 80°C, then adding the oil phase to the aqueous dispersion with high-shear mixing. Mixing was continued while the emulsions cooled to room temperature. Different types of oil-phase components were selected to show the broad utility of Eastman AQ™ polymers as emulsion stabilizers. In each emulsion, 20 parts of the oil-phase component was dispersed by one part Eastman AQ™ polymer. After 2 weeks, the stability of each emulsion was rated on a scale of 0 to 10. The emulsifying properties of Polysorbate 20 are given for comparison.

Eastman AQ™ polymers are also compatible with many latex products, thus providing a convenient method for introducing plasticizers and other water-incompatible materials into latex systems without additional surfactants.

Table 8 Stability of emulsions^a using Eastman AQ™ polymers as dispersion/emulsion aids

Oil-phase component	Emulsion stability rating, 0 to 10 ^b			
	Eastman AQ™ 38	Eastman AQ™ 48	Eastman AQ™ 55	Polysorbate 20
Castor oil	8	8	8	6
Cetyl alcohol	1	1	0	0
Corn and other vegetable oils ^c	8	8	8	8
Dimethicone ^d	6	3	3	6
Isopropyl myristate	2	2	2	2
Mineral oil	3	3	3	3
Oleic acid	8	9	8	9
Stearyl alcohol	2	1	1	6

^a10% oil phase mixed in 90% Eastman AQ™ polymer dispersion (0.5% AQ in 89.5% water).

^b0 = Complete separation of oil and water phase, with clear water phase

10 = Homogeneous mixture.

^cCottonseed, olive, palm, peanut, safflower, and soybean oils.

^dDow Corning 200® fluid.

Many organic solvents, even those with low water solubility, are dispersible at 10% or more in Eastman AQ™ polymer dispersions. Table 9 shows the viscosity stability of solvent/ Eastman AQ™ dispersion mixtures through 1 month aging.

Table 9 Effect of solvents on Eastman AQ™ 55S dispersion viscosity stability^a

Solvent	Viscosity, ^b cP		
	Initial	7 days	30 days
Acetone	29	29	29
Ethyl acetate	59	51	49
Ethyl alcohol	31	32	32
Isopropyl alcohol	31	32	32
Methyl ethyl ketone	35	36	35

^a10 parts-by-weight solvent mixed with 100 parts Eastman AQ™ 55S polymer dispersion (28% AQ in 72% water) with high-speed mixer for 1 minute.

^bBrookfield™ Viscometer, model RVT, spindle No. 2, 50 rpm.

Compatibility of additives and plasticizing effect on polymer films

Eastman AQ™ polymer dispersions are compatible with many latexes and resins such as acrylics, vinyls, and silicones and other common formulating ingredients. While being compatible with anionic and nonionic surfactants, Eastman AQ™ polymers are generally incompatible with cationic surfactants. However, Eastman AQ™ 48 polymer has been found to be compatible with some of the cationic polymers, such as Polyquaternium-6, -7 and -39. Many cosmetic ingredients modify the properties and behavior of Eastman AQ™ polymer films in the final product.

Typical additives used in personal care products were tested in Eastman AQ™ polymer dispersions to determine compatibility and their plasticizing effect on film properties. Mixtures were prepared by combining 2.5% additive with the Eastman AQ™ dispersion (25.0% AQ and 72.5% water). A mixture was

considered compatible if it was homogeneous (no layer separation or precipitate) after 1 week. Polymer films were prepared from the homogeneous dispersions by making drawdowns on glass plates and drying overnight at 45°C. Surface tension was measured on the dispersions; clarity, hardness and water resistance were measured on the dried films (see Table 10). Under the conditions described, the following additives were found to be incompatible with Eastman AQ™ aqueous dispersions: mineral oil, castor oil, orange oil (Bell Flavor & Fragrance), Silsoft™ 900 dimethicone copolyol (CK Witco), DC 345 cyclodimethicone (Dow Corning), sucrose acetate isobutyrate (Eastman), and octyl dimethoxycinnamate.

Table 10 Additives compatible with Eastman AQ™ aqueous dispersions — effect on dispersion and film properties

Additive	Dispersion surface tension, dyne/cm			Film clarity, Hazegard reading			Tukon™ hardness, Knoop			Water resistance, ^a <u>Good, Partial, or None</u>		
	AQ 38	AQ 48	AQ 55	AQ 38	AQ 48	AQ 55	AQ 38	AQ 48	AQ 55	AQ 38	AQ 48	AQ 55
None (control)	58	56	58	1.7	<0.1	1.7	11.9	15.3	16.1	G	G	G
Diethyl phthalate	50	47	51	2.7	0.1	2.3	<0.1	1.6	2.8	P	P	P
Dimethicone copolyol, Silwet™ L-7657 (Witco)	28	27	29	2.3	0.1	0.5	3.5	4.7	7.5	P	P	G
Dipropylene glycol	57	55	56	3.3	0.1	1.3	<0.1	<0.1	1.2	P	P	P
Ethoxydiglycol, Eastman™ DE solvent	57	55	53	2.9	0.1	0.9	<0.1	<0.1	<0.1	P	N	P
Glycerin	58	56	58	1.0	<0.1	0.8	1.8	<0.1	4.1	P	N	P
Propylene glycol	58	56	58	1.2	<0.1	0.9	<0.1	<0.1	1.2	P	N	P
Triacetin	51	49	51	1.9	0.2	2.1	<0.1	0.8	1.3	P	P	N
Triethyl citrate	43	44	48	1.1	<0.1	1.9	0.6	0.9	2.3	P	P	P

^aDetermined by observing the effect of water dropped on Eastman AQ™ polymer film.

Packaging, storage and handling

Eastman AQ™ linear polyesters are supplied in pellet form and packaged in plastic-lined fiber drums. Eastman AQ™ polymers are hygroscopic and pellets can clump together if exposed to excess moisture or heat. Therefore, drums should be stored in an enclosed area that is protected from moisture and extreme temperatures. When not in use, previously opened drums should be closed and liners resecured to avoid pickup of moisture. Because of their higher bulk density, storage space requirements are less than for many other resins.

Health and safety

The toxicity of Eastman AQ™ linear polyesters has been determined through numerous safety studies. End points evaluated include acute (oral, dermal and inhalation) and subchronic (inhalation) toxicity, mutagenicity potential, dermal (acute and repeat exposure) and ocular irritation, as well as sensitization potential. Most of these studies were conducted only on Eastman AQ™ 55 polymer. However, based on the inherent physico-chemical properties of these polymers and Eastman's experience in conducting toxicity studies of polyesters, it is believed that toxicity data for Eastman AQ™ 55 polymer can be considered representative of data that would be obtained if Eastman AQ™ 38 and 48 were subjected to the same studies. Results from all studies indicate that Eastman AQ™ linear polyesters can be used in many different types of applications with wide safety margins. Please see the respective MSDS or contact your Eastman representative for additional information.

Status in Japan

As of April 1, 2001, premarket approval and licensing are no longer required for cosmetics products in Japan. Companies are required only to provide notification of the product's trade name. The regulations also call for ingredient labeling on or appended to the product package. The industry will also use the International Nomenclature Cosmetic Ingredient (INCI) names as translated into Japanese by the Japan Cosmetic Industry Association (JCIA). The INCI name Polyester-5 has been translated and is available in Japanese.

Related literature

Other publications related to Eastman AQ™ polymers (see Table 11) can be viewed on Eastman's website, www.eastman.com (Markets/Cosmetic & Personal Care/online publications).

Table 11 Eastman publications:
Eastman AQ™ polymers for cosmetics and personal care

Title	Publication number
Eastman™ products for cosmetics and personal care	CB-1
Hair spray formulating tips for Eastman AQ™ 48 ultra polymer	CB-40
Water resistant sunscreen milk spray with Eastman AQ™ 38S polymer	CB-128
Spray gel composition with Eastman AQ™ 48 Ultra polymer	CB-134
High SPF sunscreen milk spray with Eastman AQ™ 38S polymer	CB-135

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It is the responsibility of the cosmetic formulator or manufacturer to determine the suitability of all raw materials, including any Eastman product used in its final product in order to ensure safety and compliance with requirements of all appropriate U.S. and international regulatory agencies.

Material Safety Data Sheets providing safety precautions, that should be observed when handling and storing Eastman products, are available online or by request. You should obtain and review the available material safety information before handling any of these products. If any materials mentioned are not Eastman products, appropriate industrial hygiene and other safety precautions recommended by their manufacturers should be observed.

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