

# DEQUEST® 2000, 2010 and 7000 product series for industrial water treatment applications





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## 1 INTRODUCTION

The Italmatch Chemicals S.p.A. DEQUEST® Business is offering unique specialty additives to meet the needs of these industries involved in water management or deal with processes or applications where water plays a crucial role.

More than 40 years ago, DEQUEST® pioneered the development of phosphonate based antiscalants. DEQUEST® phosphonates have been the product of choice for antiscalants / dispersants / corrosion inhibitors / chelants in various applications for many years. Today DEQUEST® offers a broad range of water management additives including DEQUEST® phosphonates, DEQUEST® P acrylic / maleic based (co-) polymers, DEQUEST® PB biological polymers and tailor made products for specific applications.

DEQUEST® phosphonates and polymers are used worldwide in a broad spectrum of markets and applications, including industrial water treatment, household & industrial detergents, industrial cleaners, enhanced oil recovery operations and various industrial processes such as desalination, pulp production & bleaching of paper as well as textiles.

DEQUEST® 2000, 2010 and 7000 series are members of the family of organophosphonates marketed under the Italmatch Chemicals S.p.A. registered trademark DEQUEST®. All three series are excellent scale inhibitors with corrosion inhibiting and dispersing properties perfectly suited for severe water treatment operating conditions. This bulletin provides a detailed overview of physical, chemical and performance properties of

DEQUEST® 2000 series

DEQUEST® 2010 series

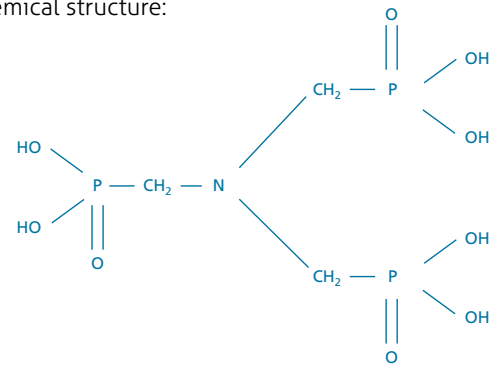
DEQUEST® 7000



## 2 Physical and Chemical Properties of DEQUEST® 2000, 2010 and 7000 product series

### 2.1 - DEQUEST® 2000 series

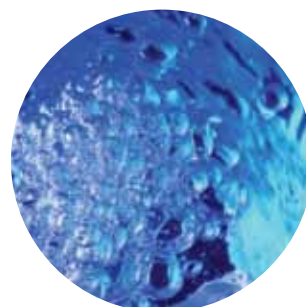
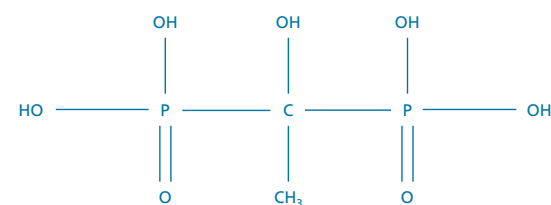
- Chemical name: Aminotri (methylenephosphonic acid) - ATMP
- Chemical structure:



PRODUCT	DEQUEST® 2000	DEQUEST® 2006
<b>Abbreviation</b>	ATMP	Na <sub>3</sub> ATMP
<b>Product form</b>	Acid solution	Pentasodium salt solution
<b>Appearance</b>	Clear water white to pale yellow aqueous solution	Clear water white to pale yellow aqueous solution
<b>Physical &amp; chemical Properties</b>		
<b>Active [%] content</b>	50 (as acid)	29 (as acid) 40 (as salt)
<b>Molecular weight</b>	299	409
<b>Specific gravity @ 20/20°C</b>	1.33	1.42
<b>pH (1% at 25°C)</b>	< 2	10 - 11
<b>Freezing point [°C]</b>	-15	-21
<b>Chloride as [%Cl]</b>	< 1	< 1
<b>Iron [ppm Fe]</b>	20 max	20 max
<b>Phosphorus as "P"</b>	15.5%	9%

### 2.2 - DEQUEST® 2010 series

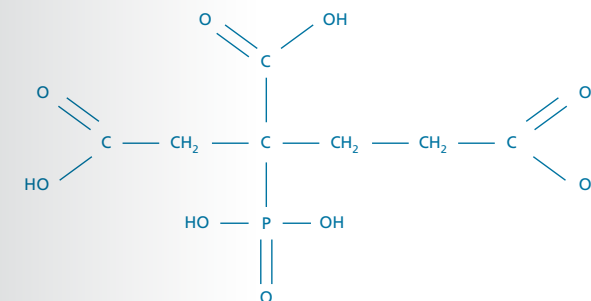
- Chemical name: 1-Hydroxyethylidene (1,1 diphosphonic acid) - HEDP
- Chemical structure:



PRODUCT	DEQUEST® 2010	DEQUEST® 2016
<b>Abbreviation</b>	HEDP	Na <sub>4</sub> HEDP
<b>Appearance</b>	Clear water white to pale yellow aqueous solution	Clear water white to pale yellow aqueous solution
<b>Physical &amp; chemical Properties</b>		
<b>Active [%] content</b>	60 (as acid)	21 (as acid) 30 (as salt)
<b>Molecular weight</b>	206	294
<b>Specific gravity @ 20/20°C</b>	1.45	1.31
<b>pH (1% at 25°C)</b>		
<b>Freezing point [°C]</b>	-25	It is recommended that Dequest® 2016 is maintained above +5°C at all times
<b>Chloride as [%Cl]</b>	< 0.1	< 0.1
<b>Iron [ppm Fe]</b>	20 max	20 max
<b>Phosphorus as "P"</b>	18.9%	6.6%

### 2.3 - DEQUEST® 7000

- Chemical name: 2-Phosphono 1,2,4 - butane tricarboxylic acid (PBTC)
- Chemical structure:



PRODUCT	DEQUEST® 7000
<b>Abbreviation</b>	PBTC
<b>Appearance</b>	Clear water white to pale yellow aqueous solution
<b>Physical &amp; chemical Properties</b>	
<b>Active [%] content</b>	50 as acid
<b>Molecular weight</b>	270
<b>Specific gravity @ 20/20°C</b>	1.28
<b>pH (1% at 25°C)</b>	1.8 - 1.9
<b>Freezing point [°C]</b>	- 15°C
<b>Iron [ppm Fe]</b>	20 max
<b>Phosphorus as "P"</b>	5.7%
<b>Iron (Fe), ppm</b>	20 ppm max



### 2.4 - Solubility

DEQUEST® 2000, DEQUEST® 2010 and DEQUEST® 7000 are miscible in all proportions with water and acid solutions. DEQUEST® 2010 is readily soluble in glycol and methanol. The solubility of DEQUEST® 2000, DEQUEST® 2010 and DEQUEST® 7000 in alkaline solutions strongly varies with pH. Neutralization of concentrated solutions of DEQUEST® 2000, DEQUEST® 2010 and DEQUEST® 7000 should therefore be carried out with care. Please contact your representative for guidance.

### 2.5 - Hydrolytic Stability

Inorganic polyphosphates tend to hydrolyze to orthophosphate. This reversion affects scale inhibition properties and can lead to calcium orthophosphate scale formation. DEQUEST® 2000, DEQUEST® 2010 and DEQUEST® 7000 series of phosphonates are hydrolytically stable over a wide range of pH values and operating temperatures. This superior resistance to decomposition is a major advantage of the DEQUEST® phosphonates.

### 2.6 - Halogen stability

The presence of oxidising biocides (hypochlorous, hypobromous acids, ozone, chlorine dioxide) will affect the performance of DEQUEST® 2000 and DEQUEST® 2010. Therefore, appropriate formulatory and application considerations have to be taken. Under the same conditions, DEQUEST® 7000 remains unaffected.

Increasing order of phosphonate stability in the presence of oxidising biocides is as follows:

<b>Chlorine:</b>	DEQUEST® 7000 > DEQUEST® 2010 >>>> DEQUEST® 2000
<b>Bromine:</b>	DEQUEST® 7000 > DEQUEST® 2000 >>> DEQUEST® 2010
<b>Ozone:</b>	DEQUEST® 7000 = DEQUEST® 2010 >> DEQUEST® 2000
<b>Chlorine dioxide:</b>	DEQUEST® 7000 = DEQUEST® 2010 >> DEQUEST® 2000



### 2.7 - Acidity constants

Phosphonates behave as multibasic acids with several inflexion points. Acidity constants are mentioned in the table I below for DEQUEST® 2000 and DEQUEST® 2010:

ACIDITY CONSTANT	DEQUEST® 2000	DEQUEST® 2010
pK <sub>1</sub>	<2	< 1
pK <sub>2</sub>	<2	2.54
pK <sub>3</sub>	4.30	6.97
pK <sub>4</sub>	5.46	11.41
pK <sub>5</sub>	6.66	NA
pK <sub>6</sub>	12.3	NA

Table I: Test conditions for acidity constant determination:

- DEQUEST® 2000: 1 mole KNO<sub>3</sub> (21°C)
- DEQUEST® 2010: in 0.5M tetramethyl- ammonium chloride (25°C)

### 2.8 - Calcium Tolerance

Operating efficiently an industrial cooling system under high alkaline conditions requires a chemical treatment program that includes an organic calcium tolerant organo phosphonates based inhibitor and a polymeric component.

**CALCIUM ION TOLERANCE TEST CONDITIONS- 320 ppm Ca<sup>2+</sup> - 80 °C - pH 9.2 - 20 hrs**

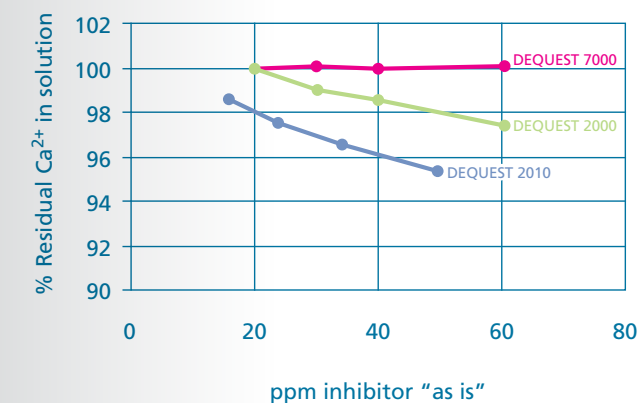


FIG. 1 DEQUEST® CALCIUM ION TOLERANCE



## 3 Functional properties of DEQUEST® 2000, 2010 and 7000 product series

### 3.1 - Sequestration

DEQUEST® 2000, DEQUEST® 2010 and DEQUEST® 7000 are good sequestering agents for most metal ions. A common way of comparing the effectiveness of sequestering agents is the stability of the complex formed. This value is a measure of the extent to which a complex will form from free metal and sequesterant.

For the formation of a given complex:



The equilibrium constant would be:

$$K_e = \frac{[ML^{(n-m)}]}{[M^{+n}][L^{-m}]}$$

where M<sup>+n</sup> is the metal ion, L<sup>-m</sup> the sequestering agent, and ML<sup>(n-m)</sup> the complex formed. The stability constant is then expressed as the logarithm of the equilibrium constant.

Stability constant = log K<sub>e</sub>



A comparison of the stability constants then gives an indication of the amount of unsequestered metal ion in solution. The larger the value, the smaller the amount of free ion.

Table II is presenting the stability constants of the active component of DEQUEST® 2000, DEQUEST® 2010, indicating their sequestering effect with various metals.

	DEQUEST® 2000 (ATMP)	DEQUEST® 2010 (HEDP)
Ion	Log K <sub>e</sub> metal complex	Log K <sub>e</sub> metal complex
Ca <sup>+2</sup>	7.5	6.05
Mg <sup>+2</sup>	7.2	6.55
Fe <sup>+3</sup>	14.6	16.21
Ni <sup>+2</sup>	11.06	9.24
Zn <sup>+2</sup>	16.37	10.73

TABLE II: STABILITY CONSTANTS OF DEQUEST® 2000 AND DEQUEST® 2010

### 3.2 - Crystal Growth Modification

Crystal growth modification is the primary functionality necessary in a sludge modification agent to produce fluid, non-adherent sludge. DEQUEST® phosphonates cause a delayed, altered crystal growth which may give a synergistic effect in formulation with other agents such as polymers.

### 3.3 - Dispersion

DEQUEST® phosphonates are effective dispersants for slurries such as clays, calcium carbonate, barium carbonate, barium sulfate. This efficiency is comparable to sodium triphosphate but organophosphonates offer the advantage of being stable at elevated temperatures.

### 3.4 - Threshold effect

The sum of the above mentioned properties results in a "threshold effect". Threshold scale inhibition is the prevention of precipitation from supersaturated solutions at sub-stoichiometric amounts of scale inhibitor (Fig. 2).

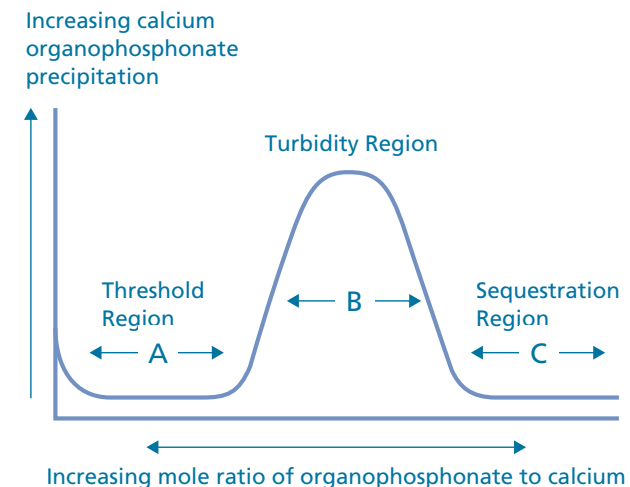


FIG. 2: THRESHOLD EFFECT OF ORGANOPHOSPHONATES

As a result DEQUEST® phosphonates are very effective in a wide variety of precipitating systems at very low use concentrations ( typically 0,2-0,5 ppm level) as outlined in table III below.

	CaCO <sub>3</sub>	CaSO <sub>4</sub>	Ca PHOSPHATE	Ca OXALATE	Cu / Fe OXIDES	CaF <sub>2</sub>	Ba/Sr SO <sub>4</sub>	SiO <sub>2</sub>
DEQUEST® 2000	Good	Excellent	Good	Good	Good	Good	Good	Good
DEQUEST® 2010	Good	Good	Good	Good	Good	Good	Good	Good
DEQUEST® 7000	Good	Good	Good	Good	Good	Good	Good	Good

Good  
Excellent

TABLE III: DEQUEST® PERFORMANCE VERSUS VARIOUS SCALE FORMING SALTS

## 4 Application of DEQUEST® 2000, 2010 and 7000 product series in industrial water treatment systems

The different functional properties of DEQUEST® series are the basis of their application in the following fields:

- cooling water treatment
- boiler water treatment
- off-line/online cleaners

### 4.1 - Cooling water treatment

#### 4.1.1 - Scale Inhibition

In order to minimize operational costs, nowadays, cooling water systems run at high cycles of concentration resulting in high pH and high scaling tendencies. Therefore scale inhibition with avoidance of the use of acid at high stressed conditions is becoming of major importance. This required scale inhibition can be achieved by inclusion of DEQUEST® series in cooling water formulations at dosages of few ppm. DEQUEST® phosphonates are compatible with each other and with most other treatment chemicals used in cooling water treatment such as corrosion inhibition systems like zinc, phosphates. In some cases remarkable technical synergies may be achieved with mixtures of DEQUEST® phosphonates and DEQUEST® P low molecular weight polymers. For more information about the DEQUEST® P product series please, refer to the "Introductory Brochure" and the Product Data Sheets for DEQUEST® P 9000, P9020 and P9030.

#### 4.1.2 - Corrosion Inhibition

Cooling water installations are typically subject to corrosion. Although DEQUEST® provides a reduction of the corrosion, they exhibit beneficial synergy when formulated with zinc, molybdenum or poly-phosphates.

Figure 3A represents synergies between DEQUEST® organophosphates and zinc for corrosion inhibition.

Figure 3B represents synergies between DEQUEST® organophosphates and phosphates for corrosion inhibition.

FIG. 3A: COOLING WATER - ZINC CORROSION PROGRAM CONTROL pH

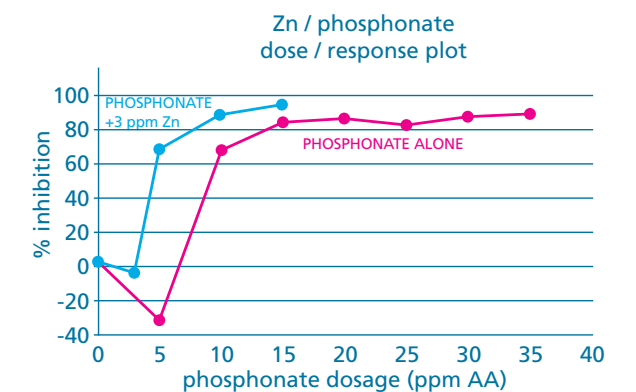
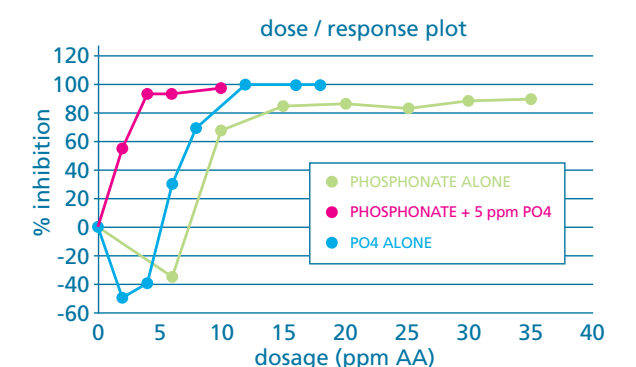


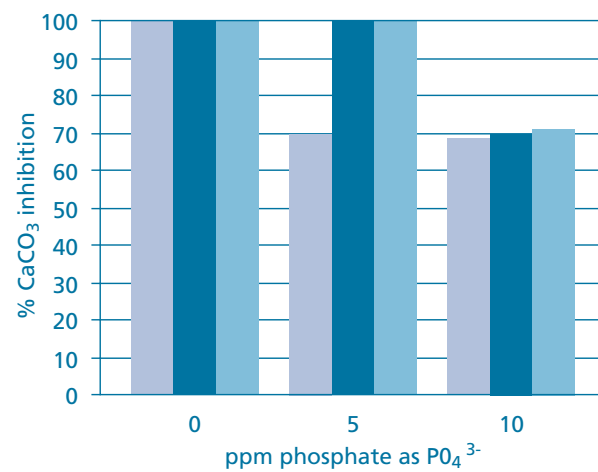
FIG. 3B: COOLING WATER - PHOSPHATE CORROSION PROGRAM CONTROL pH



#### 4.1.3 - Performance in the presence of water contaminants

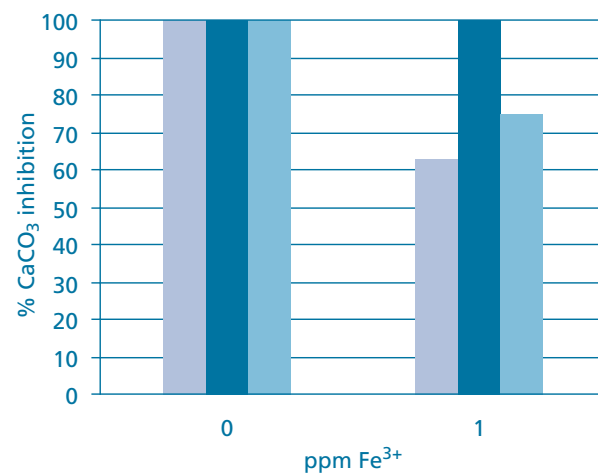
In situations where high cycles and reduced blowdown dictate operations, some interfering species such as ferric ions ( $Fe^{3+}$ ) or phosphates can have an adverse effect on the performance of these inhibitors. FIG.4 indicates impact of phosphate. In FIG.5, the impact of ferric Iron is described.

**FIG 4: EFFECT OF PHOSPHATE CONCENTRATION ON  $CaCO_3$  INHIBITION**  
800 ppm CaH - 800 ppm TAC - 50 °C  
- pH 8.9 - 20 hrs - @ 200 rpm



- Dequest 7000 - 3.0 ppm "as is"
- Dequest 2000 - 3.0 ppm "as is"
- Dequest 2010 - 1.7 ppm "as is"

**FIG 5: EFFECT OF PPM  $Fe^{3+}$  CONCENTRATION ON  $CaCO_3$  INHIBITION**  
800 ppm CaH - 800 ppm TAC - 50 °C  
- pH 8.9 - 20 hrs - @ 200 rpm



- Dequest 7000 - 3.0 ppm "as is"
- Dequest 2000 - 3.0 ppm "as is"
- Dequest 2010 - 1.7 ppm "as is"

#### 4.2 - Boiler water treatment

DEQUEST® 2000 series, DEQUEST® 2010 series and DEQUEST® 7000 are resistant to hydrolytic and thermal degradation to orthophosphate. Since these products function as crystal growth modifiers and as chelating agents, they should be evaluated as synergistic additives for boiler water treatment formulations.

DEQUEST® phosphonate based treatment programs can be designed for low - and medium - pressure (up to 6 MPa) boiler systems. Blends DEQUEST® phosphonates with dispersants and sequestrants will be able to handle a wide range of boiler water system conditions, resulting in clean boiler internals and providing optimum performance.

- Compatibility:  
DEQUEST® 2000 series, DEQUEST® 2010 series and DEQUEST® 7000 phosphonates are compatible with most typically used chelants, sludge modification agents, corrosion inhibitors and oxygen scavengers in boiler water treatment applications.

#### 4.3 - Cleaners

In off-line or on-line, low pressure boiler, chemical cleaning procedures mixtures of sequestrants and dispersants are used. DEQUEST® phosphonates may be included in these mixtures in order to assist in disintegrating deposits and in removal of sludge.

Also in industrial cooling water cleaning applications the DEQUEST® phosphonates enhance the cleaning performance, provide scale inhibition and help to disperse removed solids in order to prevent their redeposition.

## 5 Quality of DEQUEST® products

DEQUEST® products are covered by certification to quality standard ISO 9002.

In addition, the Newport (UK) Dequest® manufacturing site is certified to the Environment Management System Standard ISO 14001. It also participates in the European Community EMAS regulation (Eco Management Audit Scheme) which requires independent verification of environmental performance.



## More information

If you would like to obtain more detailed information about **DEQUEST®** products or are interested in obtaining a sample for evaluation in your system, please contact your nearest **Italmatch Chemicals S.p.A.** representative or visit our website: <http://www.dequest.com>

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