TECHNICAL OVERVIEW 13

AEROXIDE®

AEROXIDE® – Fumed Metal Oxides

EVONIK
Leading Beyond Chemistry

AEROXIDE® – Fumed Metal Oxides

Apart from AEROSIL® fumed silica, Evonik has been manufacturing AEROXIDE® fumed metal oxides on a large scale for many years, specifically fumed aluminum oxide and fumed titanium dioxide. Because of their high level of purity, their structure, and their valuable properties for technical applications, these oxides differ considerably from metal oxides that are produced using different methods.

This brochure provides an overview of the manufacturing process, properties, and the applications for these products. It has been fully revised and replaces the earlier Technical Bulletin no. 56, "Highly dispersed metal oxides manufactured according to the AEROSIL® process" and Technical Bulletin no. 80, "Titanium dioxide P 25 Manufacture – Properties – Applications".

Like the AEROSIL® brand, AEROXIDE® also stands for experience, the spirit of research, and a value-added product philosophy. This philosophy is also characterized by excellent customer service, a global production and sales network, a high degree of safety and reliability, innovative technologies, a wide range of products and innovative strength, trust and long-term business relationships and, last but not least, our pursuit of continuous improvement.

Contents

All fired up
about metal oxides …

Introduction

1. Introduction

Evonik is one of the largest manufacturers of nanostructured metal oxides, which are marketed under the product name AEROXIDE®. The company has extensive experience in this field and developed the manufacturing process, high-temperature flame hydrolysis, more than 75 years ago, initially to produce AEROSIL® fumed silica. The process has been continuously optimized over the years and is now used for many other vaporizable metal compounds.

These days, Evonik markets a wide range of pure and mixed oxides on an industrial scale, including oxides of silicon, aluminum, and titanium. The introduction of small quantities of other oxides opens up additional areas of application (Table 1). Because the oxides are produced with high-temperature flame hydrolysis (see Section 2), all compounds have a high degree of purity. Nowadays, the parameters of the manufacturing process can be controlled so precisely that the size and morphology of the resulting particles can be adjusted. For example, various AEROXIDE® types differ in primary particle size distribution, structure, and specific surface area. Initially, the fumed oxides are always hydrophilic products. On their surface, the particles have OH groups, which gives them a high degree of affinity for water and means that they can be completely wetted.

Fumed metal oxides can be treated subsequently by converting the hydroxyl groups on the surface with organosilane compounds. Table 2 shows a selection of the resulting hydrophobic metal oxides and their applications.

These days, fumed metal oxides are available on a large scale. They fulfill important tasks in many different applications: As auxiliary materials, they ensure the functional reliability of processes and products. As additives, they improve and extend existing properties. As pure raw materials, they enable completely new products.

Table 1
Selection of fumed hydrophilic metal oxides and their applications

Fumed metal oxides	Product names	Example of applications
Fumed silica (SiO_2)	AEROSIL® fumed silica	Free-flow additive, rheology control in coatings and colorants, polyester resins, reinforcement for silicones, adhesives, thermal insulation, cosmetics, etc.
Fumed aluminum oxide (Al_2O_3)	AEROXIDE® Alu C, AEROXIDE® Alu 65, AEROXIDE® Alu 130	Photo ink jet paper coating, fluorescent lamps, ceramic binder, powder coatings, additives for Li-ion batteries, flow improver in powders, polymer films
Fumed titanium dioxide (TiO_2)	AEROXIDE® TiO_2 P 25, AEROXIDE® TiO_2 P 90	Catalyst carrier, photocatalysis, toners, silicones, additives for Li-ion batteries
Fumed silicon dioxide-aluminum oxide mixed oxides	AEROSIL® MOX 80, AEROSIL® MOX 170	Textile and paper coatings, foundry technology, cellophane, catalysts
Physical mixtures of fumed silicon dioxide and fumed aluminum oxide	AEROSIL® COK 84	Pigment pastes, water-based paint systems, water-based adhesives
Titanium dioxides doped with iron oxide	AEROXIDE® TiO_2 PF 2	Heat stabilization for silicones

Table 2
Selection of hydrophobic fumed metal oxides and their applications

Hydrophobic fumed metal oxides	Product names	Examples of applications
Fumed silica (SiO_2)	AEROSIL® R types	Adhesives and sealants, colorant and coating systems, toners, defoamers, silicones, greases, etc.
Fumed aluminum oxide (Al_2O_3)	AEROXIDE® Alu C 805	Powder coatings, toners, additives for Li-ion batteries, plastic powder, polymer films
Fumed titanium dioxide (TiO_2)	AEROXIDE® TiO_2 T 805, AEROXIDE® TiO_2 NKT 90	Toners, silicones
Fumed silicon dioxide-titanium dioxide mixed oxides	AEROXIDE® STX 501, AEROXIDE® STX 801	Toners, silicone printing media

Outstanding features of fumed metal oxides are their high degree of chemical purity and large specific surface area.

In this context, it must be mentioned that the specific surface area is also a function of the oxide density. In comparison to SiO_2, fumed metal oxides have a higher true density (actual material density of the respective oxide). Therefore, the primary particles have to be smaller in order to achieve the same specific surface area.

Table 3 shows different oxide types with their respective densities.

Table 3
Connection between oxide type and density. These are typical values and not specifications.

Fumed oxide	BET surface area in m^2/g	Density in g/cm^3
AEROSIL® 90	90	2.2
AEROXIDE® Alu C	100	3.4
AEROXIDE® TiO_2 P 90	90	3.9

Nowadays, fumed metal oxides are available not only as powders but also as compacted powders with a high bulk density, as granules, and as dispersions, which increases the range of applications and simplifies processing.

Are you looking for high-quality particles that are produced in a unique quality process?

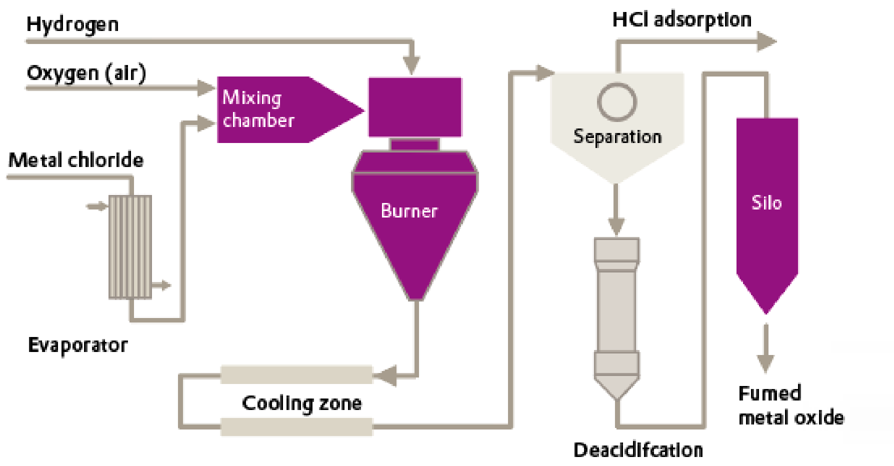
Production

Production process | Mixed oxides and oxide mixtures | Surface-modified products | AEROPERL® – granulated fumed oxides | Dispersion of AEROXIDE® fumed metal oxides

2. Production

2.1 Production process

Figure 1



Process to manufacture AEROXIDE® fumed metal oxides (flowchart)

In the classic flame hydrolysis process, all educts are converted into the gas phase and are then fed to the oxyhydrogen flame as a homogeneous gas mixture. Generally, to manufacture fumed silica, chlorosilanes, such as silicon tetrachloride, are vaporized and converted to silicon dioxide through hydrolysis at high temperatures in the oxyhydrogen flame. Other metal chlorides can also be vaporized and hydrolyzed to form metal oxides in a procedure similar to the AEROSIL® process (Figure 1).

Similar to the production of silicon dioxide, simple reactions can also be formulated to produce other fumed oxides in the oxyhydrogen flame ($2\,H_2 + O_2 \rightarrow 2\,H_2O$), as shown here using titanium dioxide and aluminum oxide as examples:

$$TiCl_4 + 2\,H_2 + O_2 \rightarrow TiO_2 + 4\,HCl$$

$$2\,AlCl_3 + 3\,H_2 + 1.5\,O_2 \rightarrow Al_2O_3 + 6\,HCl$$

In both examples, hydrogen chloride gas is formed as a secondary product.

The process is shown schematically in Figure 1. In the first step of the process, the metal halide, usually a metal chloride, must be converted to the gas phase and then the gaseous raw material is mixed with air and hydrogen. The homogeneous gas mixture is fed to the burner and the metal halide is hydrolyzed. The fumed metal oxide is formed in the flame in a fraction of a second. The fumed oxide is produced as a solid in a mixture of hot gases. The aerosol is then cooled before the solid is separated from the corrosive gases in the next step of the process. In a final step – deacidification – remaining hydrogen chloride is removed from the surface of the metal oxide. The hydrophilic end product can then be packaged. The hydrogen chloride gas in the exhaust gas flow can be used as a raw material to synthesize chlorosilanes. Consequently, there are no by-products in the process to manufacture metal oxides.

In various research work, the procedure has already been transferred to numerous metals and metalloids. A requirement is always that the metal halide used as an educt can be vaporized. At present, oxides of aluminum and titanium are available on a commercial scale.

The most important properties of AEROXIDE® products are already determined in the flame. The production process can be controlled by varying the concentration of the reaction partners, the flame temperature, and the dwell time of the gas in the combustion chamber. This affects the particle size, particle size distribution, the specific surface area, and the surface properties of the fumed hydrolysis products. In other words, different AEROXIDE® products can be manufactured depending on how the process is controlled.

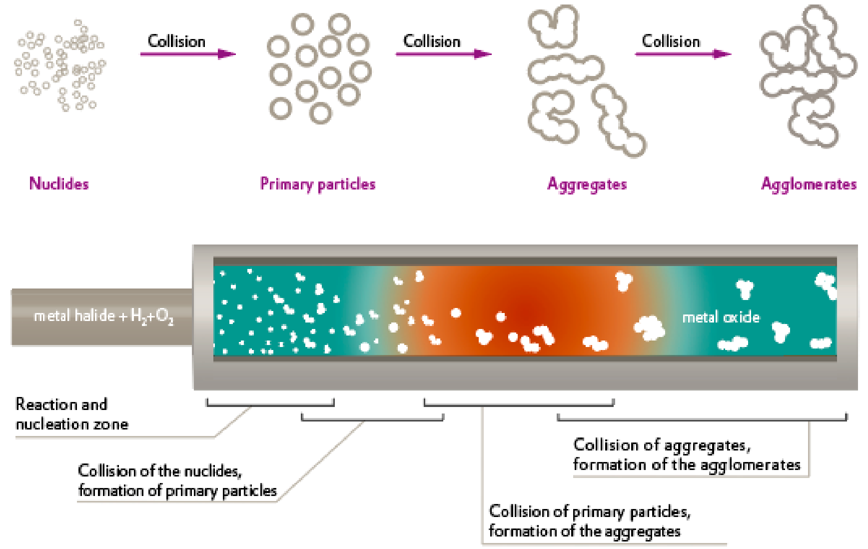
The structure of fumed oxides can be explained simply with a “droplet model” (Figure 2). This extremely simplified model assumes that the reaction gases pass through the flame as a region that imposes a sharp increase in temperature followed by a decrease.

When hydrolysis begins, very small droplets (nuclides) form from the respective metal oxide. According to the model, the nuclides collide with each other and melt into larger droplets. These larger droplets can also collide and gradually become larger and heavier. The number of droplets declines and, consequently, also the collision frequency. It is assumed that the flame is hot enough so that the droplets coalesce completely in the liquid state. More information on the formation mechanism of fumed oxides can be found in the literature [1] [2]. As soon as the droplets enter a colder area of the flame, they partially solidify. When these droplets (= primary particles) collide, they no longer completely merge to form larger droplets. The primary particles melt only partially. Aggregates consisting of primary particles (the initial droplets) form. The aggregates solidify completely in colder areas of the flame. When aggregates collide, they can then no longer even partially coalesce. Instead, the aggregates attach to each other, held together by weak interactions. Agglomerates are formed.

With suitable process control, high purity metal oxides with special property profiles can be produced. As opposed to fumed silica, which is amorphous, aluminum and titanium oxides are (partially) crystalline. The composition of the crystal phases can be controlled largely by adjusting the process.

Evonik understands and uses the flame hydrolysis as a flexible and variable process. With the corresponding precursors, fumed oxides of many elements in the periodic table can be manufactured with special properties and a high degree of purity.

Figure 2



Simple model of particle formation in the flame

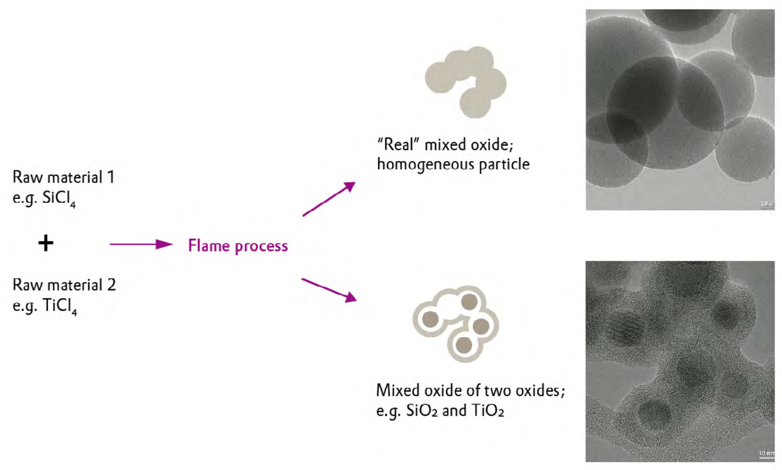
2.2 Mixed oxides and oxide mixtures

The flexibility of the flame hydrolysis process also enables real mixed oxides to be produced directly in a simultaneous process step. To do this, several educts are fed to the flame (e.g. $SiCl_4$ and $TiCl_4$), which are then hydrolyzed simultaneously and form a mixed oxide. Depending on the choice of educt and the flame parameters, it is possible to manufacture very different products with special properties.

The composition of the mixed oxides can be adjusted across wide areas of the mole fraction. The structure of the oxide particle is influenced strongly by the chosen composition. In most cases, homogeneous particles are created by adding just a small quantity of a second starting material. The resulting mixed oxide contains a minor fraction of metal ions of the second starting material homogeneously distributed in the base oxide matrix (Figure 3, top photo).

Mixed oxides with higher proportions of a second metal oxide can also be produced if the second component is fed to the flame in a correspondingly higher proportion. Homogeneous particles (primary particles or aggregates) or also particles containing areas with different stoichiometries can then be obtained. It is also possible to create special morphologies in the flame. Best known are core-shell structures, such as in silicon dioxide-titanium dioxide mixed oxides. A crystalline titanium dioxide core is surrounded by an amorphous layer of silicon dioxide (Figure 3: bottom photo).

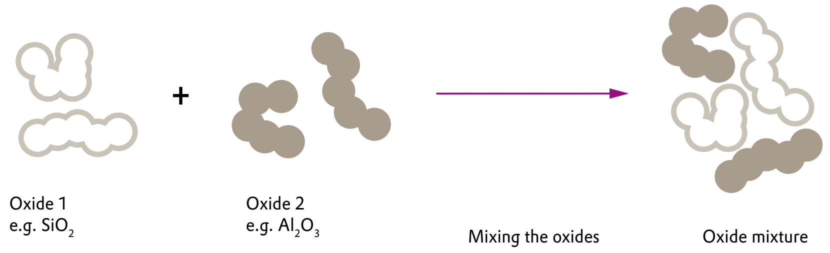
Figure 3



Mixed oxides and core-shell morphology

As mentioned above, mixed oxides, which are formed in the flame, differ from oxide mixtures. Oxide mixtures are physical mixtures of fumed oxides. The oxides are produced independently of each other and are then consolidated to form an oxide mixture. The two starting oxides do not coalesce; therefore, the primary particles and aggregates consist of just one oxide type. The agglomerates, on the other hand, can consist of both oxide types. Figure 4 shows the manufacture of an oxide mixture. The main difference between mixed oxides and oxide mixtures is shown in Figure 5.

Figure 4



An oxide mixture is formed by mixing two fumed oxides

Figure 5

Comparison of mixed oxides and oxide mixtures

Examples of mixed oxide products are the Al_2O_3/SiO_2 mixed oxides AEROSIL® MOX 80, AEROSIL® MOX 170 and the SiO_2/TiO_2 mixed oxides VP TiO_2 1580 S and VP TiO_2 545 S. AEROXIDE® TiO_2 PF 2 contains titanium dioxide with 1-3 % iron oxide.

One example of an oxide mixture is AEROSIL® COK 84, which consists of 84 % fumed silica and 16 % fumed aluminum oxide.

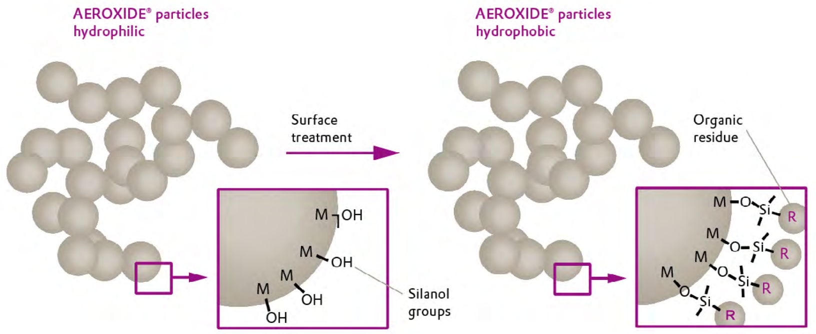
Details about the properties of the mixed oxides can be found in Sections 3.2 and 4.2.

2.3 Surface-modified products

The products described above are compounds that are recovered directly from the flame hydrolysis process. Because of the freely accessible hydroxyl groups (e.g. Si-OH, Ti-OH, or Al-OH) on the particle surface, products manufactured in this way are hydrophilic – in other words, they can be wetted with water. Many applications where special properties are needed require a subsequent treatment step: hydrophilic fumed oxides can be converted to repel water and to become hydrophobic.

The hydrophobic behavior is achieved through the reaction of hydrophilic hydroxyl groups with organic molecules (Figure 6). After being modified, the organic groups are firmly anchored on the surface (covalent bond). This surface modification cannot be reversed without changing the entire structure of the fumed oxide.

Figure 6



Conversion of a hydrophilic metal oxide to a hydrophobic where M = Al or Ti.

At first glance, there is no difference between hydrophilic and hydrophobic fumed metal oxides – both are fine, white powders. However, the difference is evident when mixing with water: while hydrophilic products can be wetted completely with water, hydrophobic products cannot be mixed with water (Figure 7).

The water-repelling behavior is created by anchoring organic residues on the surface of the fumed metal oxide. Figure 8 shows the surface groups of the hydrophobic metal oxides AEROXIDE® Alu C 805 and AEROXIDE® TiO_2 T 805.

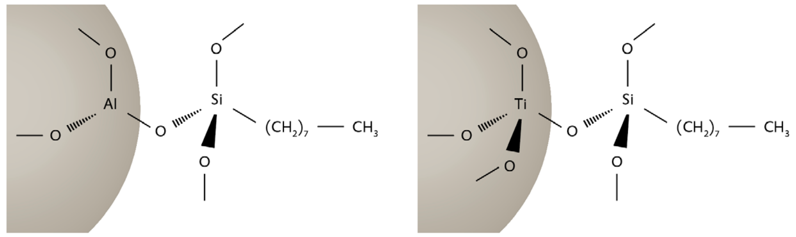
But more complex organic compounds, which may have functional groups, can also be anchored to the surface.

Surface modification produces completely different physico-chemical properties compared with non-modified AEROXIDE® products. This extends the areas of application for fumed metal oxides and opens up opportunities in many different areas of industry, such as for silicones, toner products, powder coatings, plastic powder, and many more.

Figure 7

Water with hydrophilic (left) and hydrophobic (right) fumed metal oxide

Figure 8



Two hydrophobic AEROXIDE® types with the respective surface groups.

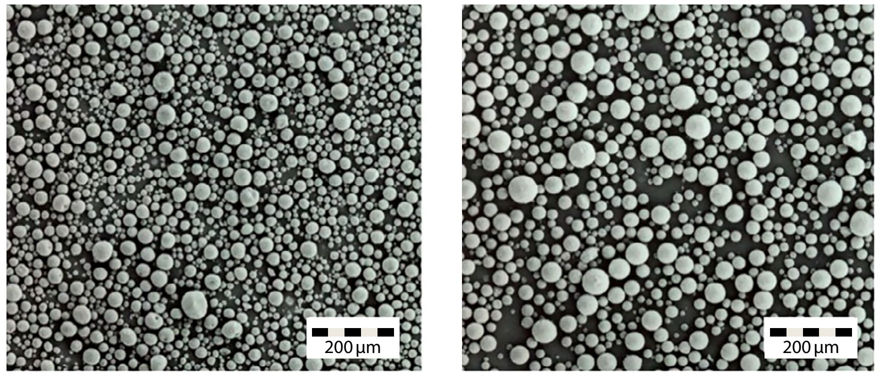
2.4 AEROPERL® – granulated fumed oxides

AEROPERL® types are another product group from Evonik's extensive portfolio of fumed oxides. Using a granulation process, which has been especially designed for fumed oxides, it is possible to manufacture these granules with an average particle size of approx. 10-40 µm. The spherical shape of the granules, regardless of the chemical composition, can be seen clearly in Figure 9 (the material based on titanium dioxide on the left and the one from aluminum oxide on the right).

AEROPERL® types are especially characterized by outstanding flow properties, good incorporation, and low dust handling, which considerably extends the areas in which fumed oxides can be used. Figure 10 shows the flow properties of AEROXIDE® TiO_2 P 25 and the corresponding granules VP AEROPERL® P 25/20.

The manufacturing process guarantees that the granules have a high degree of purity. As opposed to powder AEROXIDE® starting materials, AEROPERL® products have a pore structure. Because of this "inner porosity" they are able to absorb large volumes of substances and can be used, for example, as a carrier material. The porosity is created by mesopores and macropores, the proportion of micropores is below the detection limit (Table 4).

Figure 9



Scanning electron microscope images of VP AEROPERL® P 25/20 (left) and
VP AEROPERL® Alu 100/30 (right)

Figure 10

Flow properties of AEROXIDE® TiO_2 P 25 (left) and VP AEROPERL® P 25/20 (right)

Compared to the corresponding AEROXIDE® products with the same specific surface area (BET), the tamped density is up to ten times higher, which is an advantage for transportation and storage. Better handling and faster incorporation extend the applications for these products. Applications for AEROPERL® fumed metal oxide granules are, for example, in catalyst production and in the ceramic and paper industries. More information about AEROPERL® products can be found in Sections 3.4 and 4.4 of this brochure and in Technical Information 1341 [3].

Table 4
Pore volume of selected AEROPERL® products. These are typical values and not specifications.

Pore volume	Unit	VP* AEROPERL® P 25/20	VP* AEROPERL® Alu 100/30	AEROPERL® 3375/20
Mesopores, determined with BJH (2-50 nm)	cm^3/g	approx. 0.4	approx. 1.0	approx. 1.0
Macropores, determined with Hg intrusion (50 nm - 1 µm)	cm^3/g	approx. 0.2	approx. 0.3	approx. 0.1

*VP = development product. Commercialization depends on feedback from the market.

2.5 Dispersion of AEROXIDE® fumed metal oxides

In many applications, the fumed metal oxide is used in a liquid formulation. In these cases, the material in powder form must be dispersed homogeneously in a liquid phase. Dispersion of AEROXIDE® fumed metal oxides is described in detail below. Evonik also markets commercial quantities of dispersed AEROXIDE® types under the brand name AERODISP®. Details about the respective AERODISP® types can be found in Sections 3.5 and 4.5 for the respective metal oxides.

Because of the special particle structure, the tamped density of fumed metal oxides is relatively low. To prevent dust, these loose powders must be handled very carefully. In principle, powder can be added manually to the liquid phase, such as from bags, but an adequate extraction system must be ensured for the dust. The products can be transferred to suitable batch vessels with a suction pipe, which produces a lot less dust. Suitable units are available from Ystral (jetstream mixer with product suction, or from the Conti TDS series). To prevent dissolved gases in the dispersion and for safety considerations within the scope of explosion protection, it is advisable to use a vacuum dissolver. Detailed information can be found in our Technical Information 1279 [4].

Energy is needed to disagglomerate the product during dispersion. (For information about the structure of AEROXIDE® fumed metal oxides, refer to Figure 2). This energy can be in the form of shearing energy or direct impact; a mild stirring process provides only a low energy input. With the right mode of operation, a dissolver is suitable for disagglomeration. For this purpose, the optimum viscosity must be set. On the one hand, the viscosity of a dispersion depends on the liquid that is used and, on the other, on the concentration, the specific surface area, and the structure of the powder.

With the dissolver dispersion, optimum viscosity is achieved when the "donut effect" occurs. If the dissolver is properly dimensioned (diameter of the tank, diameter of the dissolver disk and the distance of the dissolver disk from the base), the speed is adequate and the concentration increases, a product bead in the shape of a "donut" appears on the surface of the dispersion in the tank (Figure 11).

When dispersing with other machines, such as a rotor-stator, ball mill, homogenizer, or kneader, attention should also always be paid to the viscosity range that is ideal for the process and the machine that is used.

If the energy density is sufficiently high, even part of the aggregate structure of the powder can be broken, which causes smaller aggregates. Suitable machines for this are bead mills with very small beads (< 0.5 mm), which, with a sufficiently long milling time and high milling energy, are able to produce dispersions with a mean particle size of less than 100 nm. In many practical examples, the aggregate size is between 100 and 500 nm.

Figure 11

Dissolver dispersion with visible "donut effect"

However, the surface of the beads must also be considered to ensure that the bead material cannot contaminate the product.

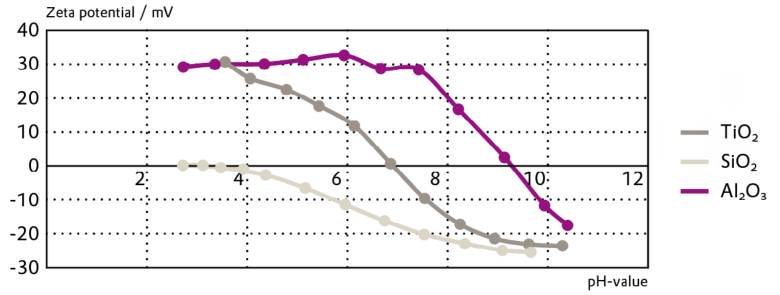
A good dispersion process alone is not enough to manufacture a dispersion with long term stability. Among other things, the surface charge of the dispersed particles plays an important role as regards stability. Figure 12 shows the zeta potentials for silicon dioxide, aluminum oxide, and titanium dioxide in relation to pH. At the isoelectric point, there is no repulsion of the dispersed particles due to the same electrical charge and, as a result, there is a greater risk of reagglomeration. Often additives are needed to make sure that the particles retain their fineness even after milling and that they do not reagglomerate. These additives can change the zeta potentials of the dispersed particles or also induce steric stabilization.

This additional effort and locating suitable additives is not worth it for all customers. This is why Evonik offers a wide range of dispersed fumed silica and metal oxides in an aqueous or solvent-based phase under the brand name AERODISP®.

With a specific combination of dispersing technologies, expertise in using additives as stabilizers, and substances for surface modification, it is possible to offer a wide range of stable dispersions with high solid content.

Evonik has also developed a special high-energy milling process. This enables us to produce contamination-free dispersions in which the aggregates of the fumed metal oxides are milled to a range below 100 nm. These AERODISP® types are marked with an "X" in the product name. Major advantages of high-energy milled dispersions are high solid content and low viscosity. Examples of this product class are the aluminum oxide dispersion AERODISP® W 640 ZX and the titanium dioxide dispersion AERODISP® W 740 X. Details of these dispersions can be found in Sections 3.5 and 4.5.

Figure 12



Zeta potential curves of pure AEROXIDE® Alu C, AEROXIDE® TiO_2 P 25 and AEROSIL® 200, each in 10 % dispersion in de-ionized water.

The Product Overview of AERODISP® products contains more information about dispersions from Evonik [5].

You need an alumina with the unique properties of a fumed metal oxide?

AEROXIDE® – Fumed Aluminum Oxide Products

Structure and properties | Mixed oxides and oxide mixtures containing aluminum oxide | Surface-treated aluminum oxide | Granulated aluminum oxide | Aluminum oxide dispersions | Application-specific effects

3. AEROXIDE® Fumed Aluminum Oxide Products

3.1 Structure and properties

Aluminum oxide is found mainly in two modifications. In the thermodynamically stable α form and the metastable γ form. From a crystallography aspect, the latter can be split into γ, δ, and θ sub-groups. The α form is created when aluminum oxide is heated to temperatures above 1250 °C. The other forms are created, for example, through eliminating water from aluminum hydroxides at temperatures below 1000 °C. In γ-aluminum oxide, oxygen ions form a cubic close-packing of equal spheres whose octahedral and tetrahedral sites are statistically filled with aluminum ions (spinel-like). On the other hand, α-aluminum oxide is based on a hexagonal close-packing of equal spheres in which 2/3 of the octahedral sites contain aluminum ions.

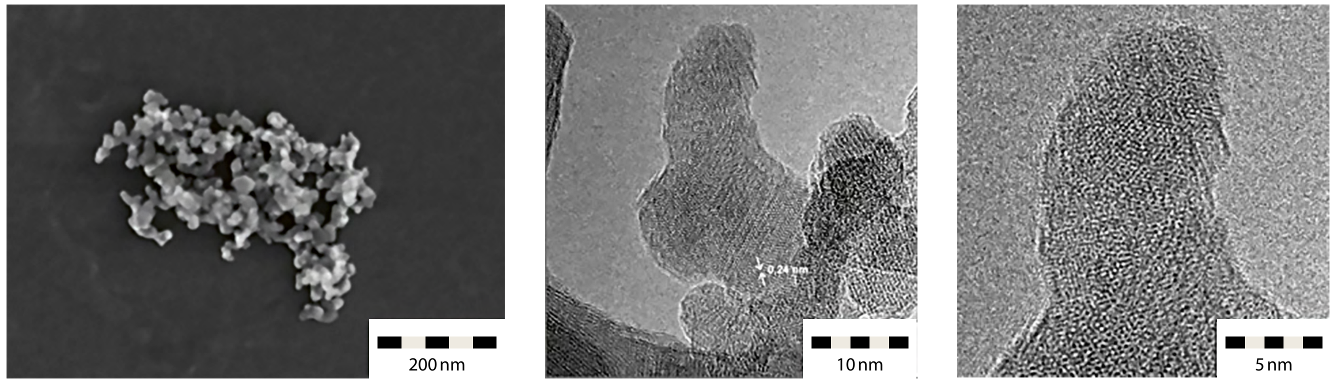
Evonik has been producing AEROXIDE® Alu C according to the flame hydrolysis process since 1953. This material has a specific surface area of about 100 m^2/g and is used for many different applications (see Section 3.6). To address individual customer needs even better Evonik has developed two more grades of fumed alumina: AEROXIDE® Alu 65 with lower surface area and AEROXIDE® Alu 130 with higher surface area. The short dwell times in the oxyhydrogen flame prevent α-aluminum oxide forming. In AEROXIDE® Alu C, AEROXIDE® Alu 65, and AEROXIDE® Alu 130 the transition phases γ, δ, and θ are found in various ratios. These crystal structures are metastable and can convert to α-aluminum oxide if the temperature is sufficiently high.

Table 5 lists the physico-chemical data of the products in comparison.

Figure 13 shows the structure of AEROXIDE® Alu C based on SEM and TEM images. It is clear that the crystalline primary particles are congregated into larger structural units.

The main difference between aluminum oxides produced in the flame hydrolysis process and aluminum oxides produced by alternative means, especially aqueous means, is the fractal structure. The aluminum oxides produced by precipitating aluminum hydroxide from an aluminate solution followed by calcination consists of compact particles in the micrometer scale. As opposed to AEROXIDE® Alu C, aluminum oxide/aluminum hydroxide gels with a high surface area (e.g. pseudo boehmite) have a high proportion of inner surface area and a completely different structure.

Figure 13



SEM image (left) and (HR)TEM images (middle and right) of AEROXIDE® Alu C. The individual crystal layers are quite clear. [6]

Table 5
Physico-chemical data of fumed aluminum oxides. These are typical values and not specifications.

Property	Unit	AEROXIDE® Alu 65	AEROXIDE® Alu C	AEROXIDE® Alu 130
BET surface area	m^2/g	55-75	85-115	110-150
pH (4 % eq. dispersion)		4.5-6.0	4.5-5.5	4.4-5.4
Loss on drying (2 h @ 105 °C)	%	≤ 5.0	≤ 5.0	≤ 5.0
Tamped density	g/l	approx. 50	approx. 50	approx. 50
Concentration of Al_2O_3	%	≥99.8	≥99.8	≥ 99.8

Fumed aluminum oxide has hydroxyl groups on the surface that react mildly alkaline in water. With IR spectrometry, with a hydrated aluminum oxide, five different types of OH groups can be detected, which differ in terms of the number of neighboring oxygen atoms.

When water is completely removed, one finds aluminum ions on the surface of the particles, which are coordinated by five oxygen ions and represent LEWIS acid centers. They can take up LEWIS bases (e.g. pyridine) or form hydroxyl groups again by absorbing water.

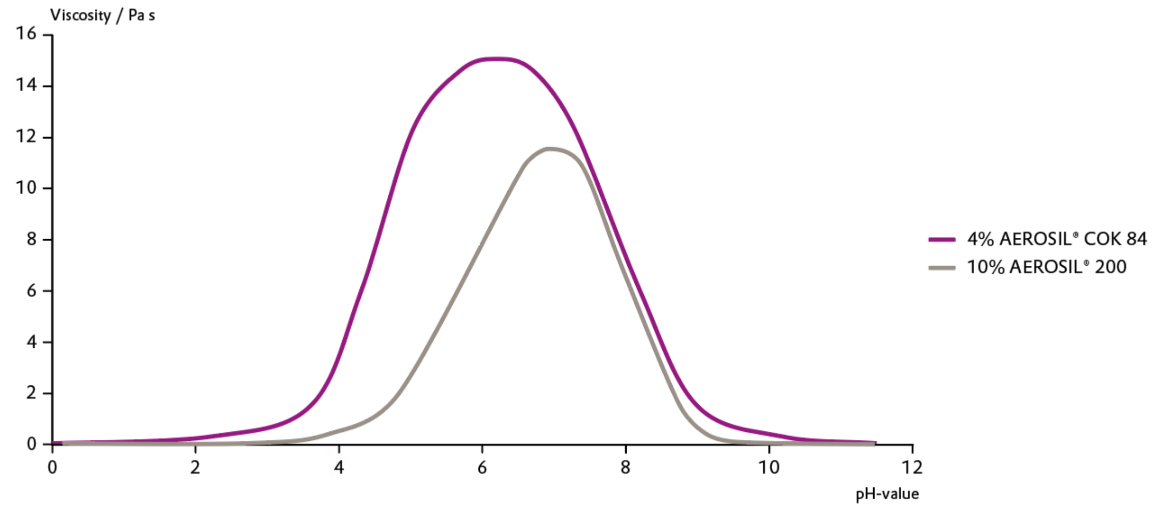
An important difference between fumed aluminum oxide and fumed silica is the cationic (positive) surface area charge across a very large pH range (see Section 2.5, Figure 12). This is used in several applications (see Section 3.6).

The hydroxyl groups on the aggregate surfaces are also responsible for the thickening and thixotropic effect of fumed aluminum oxides in liquids. The individual particles interact with each other via the hydroxyl groups and form a three-dimensional network that can be broken down mechanically by stirring or shaking and recombines when left to settle. This effect is especially pronounced in non-polar liquids. This thickening mechanism was originally observed with AEROSIL® and has proved to be a useful working basis in this regard.

A combination of AEROSIL® and AEROXIDE® Alu C can be used as a thickening agent and to generate thixotropic behaviour for polar liquids. In this case, a network is also formed; however, the interaction between the different particles is likely of an electrostatic nature, as the AEROSIL® particles are negatively charged through dissociation of the acidic silanol groups, as opposed to AEROXIDE® Alu C. The effective forces are especially large here due to the interaction of anionic and cationic surface areas. This effect can be achieved especially well with the help of AEROSIL® COK 84, a prepared physical mixture of fumed silica and fumed aluminum oxide. (Figure 14). In other liquids or liquid systems, the most effective mixing ratio has to be determined on a case-by-case basis.

Even when dry, AEROXIDE® Alu C, as opposed to AEROSIL®, tends towards a positive electrostatic charge. This is explained by the high permittivity of about 5. According to Coehn's rule, when two substances come into contact, the one with the higher permittivity charges itself positively. This effect plays a role in numerous applications. Details are provided in the following sections.

Figure 14



Thickening effect of AEROSIL® COK 84 (4% dispersion) compared to AEROSIL® 200 (10% dispersion)

3.2 Mixed oxides and oxide mixtures containing aluminum oxide

The fumed mixed oxides AEROSIL® MOX 80 and AEROSIL® MOX 170 are manufactured by flame hydrolysis escribed earlier and can be regarded as true mixed oxides of Al_2O_3 and SiO_2 on a molecular level. The aluminum oxide, of which there is approx. 1 %, is incorporated directly into the primary particles of the base oxide (SiO_2) during the production process. The two products differ in respect of their specific surface area (see Table 6).

Because of their lower thickening effect in aqueous systems, these mixed oxides are popular for the production of highly filled dispersions. The dispersions are excellent for the following applications:

- Paper coatings
- Textile coatings
- Foundry technology
- Textile fibers

With VP Alu 560 S and VP Alu 590 S, Evonik also offers two mixed oxides rich in aluminum, which have higher thermal stability than pure aluminum oxide.

As opposed to this, the AEROSIL® COK 84 described in Section 3.1 is a physical mixture of fumed silica and fumed aluminum oxide. The primary particles are either pure SiO_2 or pure Al_2O_3. AEROSIL® COK 84 is suitable for efficient thickening of aqueous and other polar liquids. The oxide mixture is therefore excellent for the following applications:

- Pigment pastes
- Water-based paint systems
- Water-based adhesives

Table 6
Physico-chemical data of some fumed mixed oxides and oxide mixtures produced by flame hydrolysis. These are typical values and not specifications.

Property	Unit	AEROSIL® MOX 80	AEROSIL® MOX 170	AEROSIL® COK 84	VP* Alu 560 S	VP* Alu 590 S
Chemical composition		SiO_2/Al_2O_3	SiO_2/Al_2O_3	SiO_2/Al_2O_3	Al_2O_3/SiO_2	Al_2O_3/SiO_2
BET surface area	m^2/g	60-100	140-200	155-215	40-80	70-110
pH		3.6-4.5	3.6-4.5	3.6-4.3	4.5-6.5	4.5-6.5
Loss on drying (2 h 105 °C)	%	≤ 1.5	≤ 1.5	≤ 1.5	n. a.	n. a.
Tamped density	g/l	approx. 60	approx. 50	approx. 50	approx. 50	approx. 40
Concentration of Al_2O_3	%	0.3-1.3	0.3-1.3	14-18	approx. 95	approx. 95
Concentration of SiO_2	%	≥ 98.3	≥ 98.3	82-86	approx. 5	approx. 5

*Development products have VP in the product name. Commercialization depends on feedback from the market.

3.3 Surface-treated aluminum oxide

A hydrophobic aluminum oxide type called AEROXIDE® Alu C 805 is available. This product has chemically bonded octyl groups on the surface. Table 7 contains the physico-chemical data.

From a technical application aspect, it is an alternative to hydrophobic AEROSIL® and is used, for example, in toners where triboelectric properties are required, which cannot be provided by silica. AEROXIDE® Alu C 805 also can be used in applications in which the properties of AEROXIDE® Alu C are needed but where better compatibility to an organic matrix is required (e.g. polymer films).

Because of its special properties, AEROXIDE® Alu C 805 is used in the following areas:

- In powder coatings to increase the electrostatic charge and to improve the flow properties, especially in systems that are sensitive to moisture
- In plastic powders (e.g. PVC) to reduce electrostatic charge during mixing and processing in order to prevent cohesion and to protect the powder against moisture
- As an additive in Li-ion batteries (e.g. separator films or polymer electrolytes)

Table 7

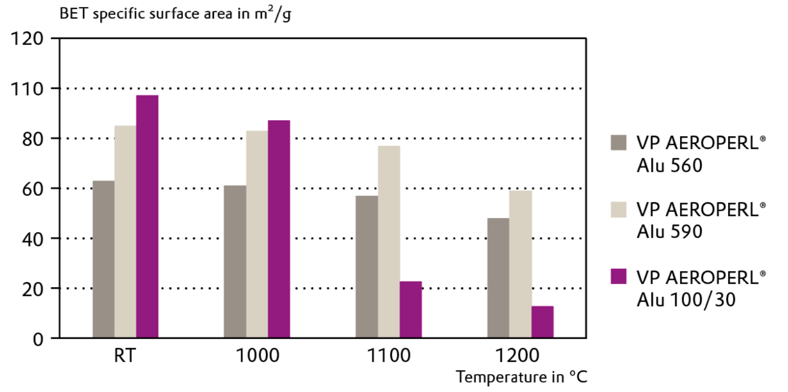
Physico-chemical data of AEROXIDE® Alu C 805. These are typical values and not a specification.

Property	Unit	AEROXIDE® Alu C 805
BET surface area	m^2/g	75-105
pH (4 % eq. dispersion)		3.0-4.5
Loss on drying (2 h @ 105 °C)	%	≤ 2.0
Tamped density	g/l	approx. 50
Concentration of Al_2O_3	%	≥ 95.0
C content	%	3.5-4.5

3.4 Granulated aluminum oxide

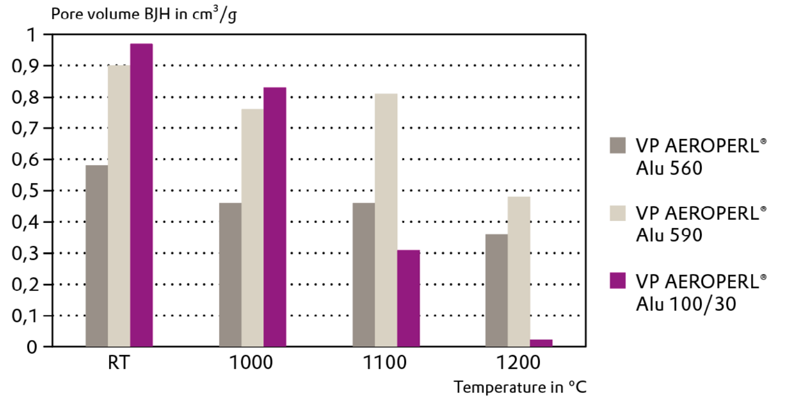
Fumed aluminum oxides and aluminum silicon mixtures are also available as granules. The spherical particles allow easier handling and metering compared to the powder products (see also Section 2.4). Another outstanding feature of these granulated AEROPERL® products is their high degree of porosity. Because of this, these products are also ideal as carrier materials and also for the adsorption of metal solutions, which are then converted further. As a result of these properties, AEROPERL® products are especially interesting for heterogeneous catalysis.

Figure 15



Stability of VP AEROPERL® Alu 100/30, VP AEROPERL® Alu 560, and VP AEROPERL® Alu 590 when heated for 24 h (BET specific surface area).

Figure 16



Stability of VP AEROPERL® Alu 100/30, VP AEROPERL® Alu 560, and VP AEOPERL® Alu 590 when heated for 24 h (pore volume).

Pure aluminum oxide is available in granules as VP AEROPERL® Alu 100/30. It has outstanding flow properties, a high degree of chemical purity, and produces little dust during handling. The average particle size of the spherical granules is approx. 30 µm. It is used in ceramic and paper products and as a catalyst carrier material.

The granulated VP AEROPERL® Alu 560 and VP AEROPERL® Alu 590 were developed on the basis of the aluminum-silicon mixed oxide powders VP Alu 560 S and VP Alu 590 S (see Section 3.2).

The VP Alu 560 S and VP Alu 590 S powder products and also the AEROPERL® products VP AEROPERL® Alu 560 and VP AEROPERL® Alu 590 have excellent thermal stability. When heated to 1200 °C for 24 hours, these new AEROPERL® developmental products have only a slight reduction in specific surface area (BET) and pore volume (see Figure 15 and Figure 16). On the other hand, VP AEROPERL® Alu 100/30 sinters at temperatures above 1000 °C, which results in a marked decline in specific surface area (BET) and pore volume.

Apart from the aluminum-rich aluminum-silicon mixed oxides with higher thermal stability, Evonik also offers a silicon-rich mixed oxide with higher thermal stability:

AEROPERL® 3375/20 consists mainly of silicon dioxide with a small proportion of aluminum oxide, which increases thermal stability up to 1200 °C.

The properties of AEROPERL® products, which are based on aluminum oxide and aluminum-silicon mixed oxides are listed in Table 8.

Table 8

Physico-chemical data of AEROPERL® products based on aluminum oxide and aluminum-silicon mixed oxides. These are typical values and not specifications.

Property	**Unit**	**VP* AEROPERL® Alu 100/30**	**VP* AEROPERL® Alu 560**	**VP* AEROPERL® Alu 590**	**AEROPERL® 3375/20**
BET specific surface area	m^2/g	85-115	50-80	70-100	60-80
pH (4 % eq. dispersion)		4.0-6.0	4.0-6.0	4.0-6.0	3.5-6.5
Loss on drying (2 h @ 105 °C)	%	≤ 2.5	≤ 2.5	≤ 2.5	≤ 2.0
Tamped density	g/l	approx. 500	approx. 575	approx. 500	approx. 600
Concentration of SiO_2	%	–	approx. 5	approx. 5	≥ 99 %
Concentration of Al_2O_3	%	≥ 99.6	approx. 95	approx. 95	0.08-0.30

*Development products have VP in the product name. Commercialization depends on feedback from the market.

3.5 Aluminum oxide dispersions

For some applications, it is beneficial to use a fumed aluminum oxide dispersion. This is the case when, for example, – together with other components – a slurry is to be prepared or a molded body is to be coated or impregnated. Primarily, the application properties and the stability of a dispersion are dependent on the dispersion status, in other words, from the size of the particles that are actually in the liquid, the specific weight of the dispersed oxide, and the stabilization via additives.

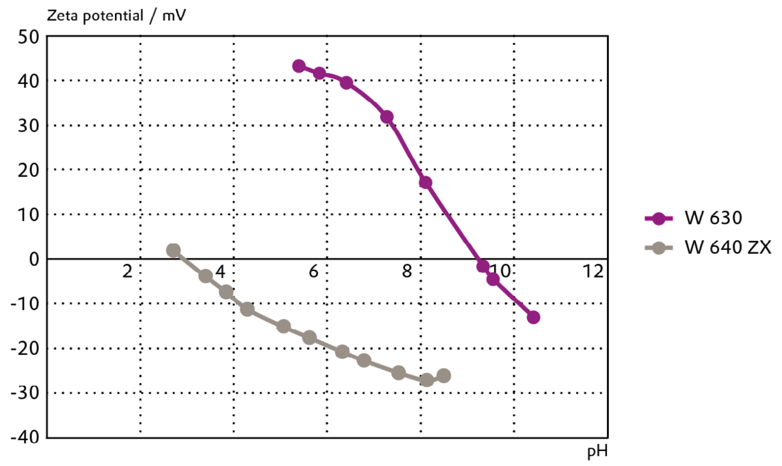
AERODISP® W 630, AERODISP® W 440, and AERODISP® W 925 are three aqueous dispersions based on AEROXIDE® Alu C, AEROXIDE® Alu 65, and AEROXIDE® Alu 130, which can be used as direct alternatives for the corresponding powders. For stabilization, the dispersions contain only a buffer based on acetic acid, which guarantees a constant pH of approx. 4.

At this point, the stability of the dispersions is highest, as the very positively charged aluminum oxide particles repel each other and prevent reagglomeration (see Section 2.5, Figure 12).

But there are also cases where the user needs a dispersion that is stable in basic systems. For these areas, Evonik has developed a special stabilization in which the surface of the aluminum oxide is modified in such a way that anionic – negatively charged – particles are present. AERODISP® W 640 ZX is such a dispersion. Figure 17 shows a comparison of the zeta potential curve of this product and AERODISP® W 630.

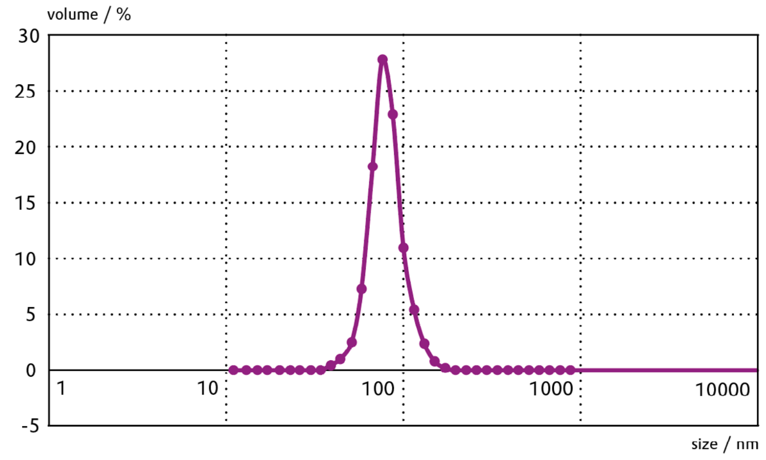
AERODISP® W 640 ZX is a special product in other aspects as well. The average particle size has been reduced to 80 nm through special high energy milling. From a macroscopic aspect, this is obvious in the much lower viscosity of the dispersion. Figure 18 shows the particle size distribution of AERODISP® W 640 ZX measured with static light scattering.

Figure 17



Zeta potential curves of AERODISP® W 630 and AERODISP® W 640 ZX

Figure 18



Particle size distribution of AERODISP® W 640 ZX measured with static light scattering.

The table below shows several examples of aluminum oxide-based AERODISP® types. More information can be found in our product overview AERODISP®.

Table 9

Physico-chemical data of selected aqueous aluminum oxide dispersions. These are typical values and not specifications.

Property	Unit	AERODISP® W 440	AERODISP® W 630	AERODISP® W 925	AERODISP® W 640 ZX	AEROIDISP® W 450 ZX
Al_2O_3 type		AEROXIDE® Alu 65	AEROXIDE® Alu C	AEROXIDE® Alu 130	AEROXIDE® Alu C	AEROXIDE® Alu 65
Solid content	%	40	30	25	40	50
pH		3.0-5.0	3.0-5.0	3.0-5.0	6.0-9.0	6.0-9.0
Viscosity	mPa·s	≤ 1000	≤ 2000	≤ 1000	≤ 70	≤ 100
Density	g/cm^3	1.38	1.26	1.20	1.39	1.53
Aggregate size (d50)	nm	120	140	110	80	80

3.6 Application-specific effects

The most important applications are described briefly below. This information does not claim to be complete and is intended only to illustrate the many different applications that are possible with these products.

3.6.1 Flow aid in powders

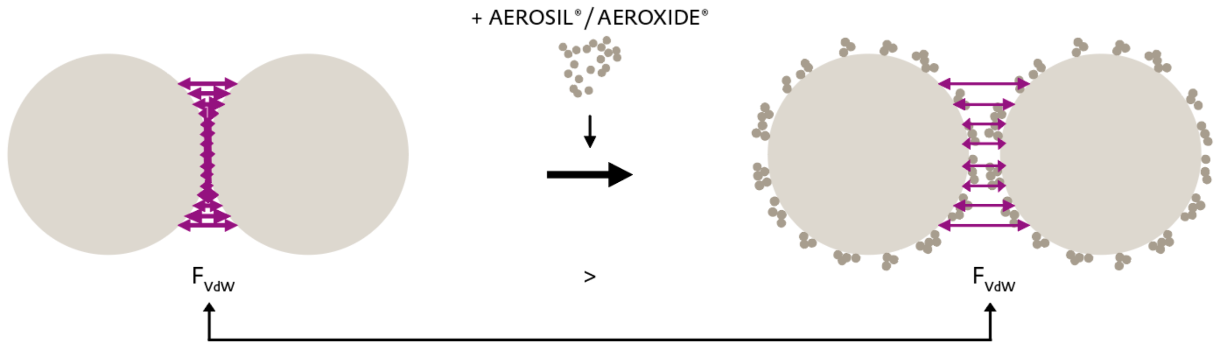
Manufacturers and users of powders increasingly work with automated processes. This requires that the powders flow well to enable clean and even metering. The powders must also not cake during storage. However, there are many powder products that do not flow well and that tend to form lumps during storage, which leads to undesired downtimes. AEROSIL® and AEROXIDE® offer an efficient way to resolve these problems and improve productivity.

The flow properties of powders are influenced by adhesive forces, known as Van der Waals forces, and gravity. Van der Waals forces have an effect on all powders. In relation to the gravitational force, these forces are higher the smaller the particles are. Because of this, fine powders tend to flow worse than coarse ones.

There are other reasons for bad flow properties: liquid on the surface of powder particles, such as water or oil (e.g. in hygroscopic powders or fatty powders), holds it together through surface tension. Unevenly formed particles snag and some powders tend to become statically charged and stick to the walls of pipes or mixers.

Because of their fineness, AEROSIL® and AEROXIDE® are able to encase the particles of the powder (hereinafter called host powder) where flow properties are to be improved. They act as spacers between the individual powder particles, separate them from each other and, consequently, reduce adhesive forces [7] [8].

Figure 19

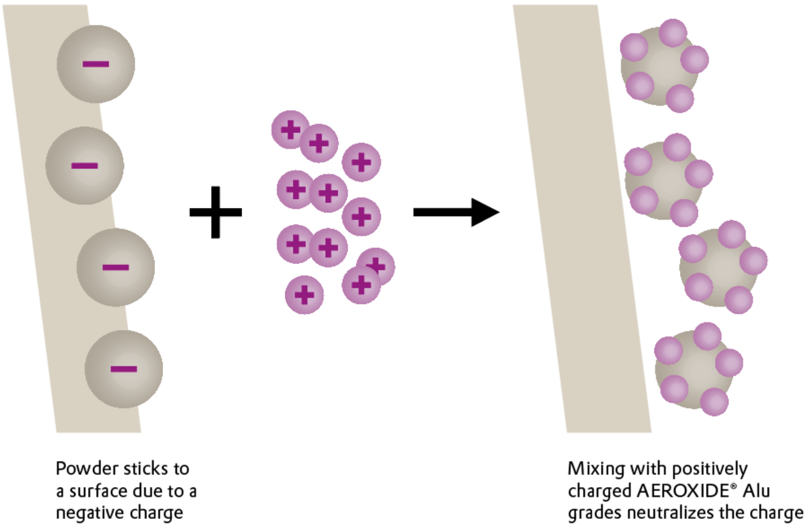


AEROSIL® and AEROXIDE® aggregates act as spacers and reduce Van der Waals forces (F_{vdw}) between powder particles.

If electrostatic charging affects the flow properties of a powder, AEROXIDE® fumed aluminum oxides can help. Many non-conductive powders, especially polymer powders and granules, tend to become negatively charged and, because of this, adhere to surfaces. On the other hand, as explained in Sections 3.1 and 3.6.2, AEROXIDE® Alu 65, AEROXIDE® Alu C, and AEROXIDE® Alu 130 tend to develop a positive electrostatic charge and, in many cases, can compensate for the negative charge of the host powder. On the whole, this produces a neutral powder that sticks much less to surfaces. The effects can be illustrated schematically as follows.

Figure 21 shows the effect described above on a Polypropylenegranulate.

Figure 20



Charge neutralization with AEROXIDE® Alu grades

Figure 21

Polypropylenegranulate without (left) and with 0.5 % AEROXIDE® Alu C (right).

3.6.2 Powder coatings

Because of the continuing trend towards environmentally friendly paint systems, the market for powder coatings is growing at a faster rate than for conventional liquid paints. AEROSIL® fumed silica and the fumed aluminum oxides AEROXIDE® Alu C, AEROXIDE® Alu 130, and the hydrophobic AEROXIDE® Alu C 805 are known to considerably improve the processing properties, quality, appearance, and performance of powder coatings.

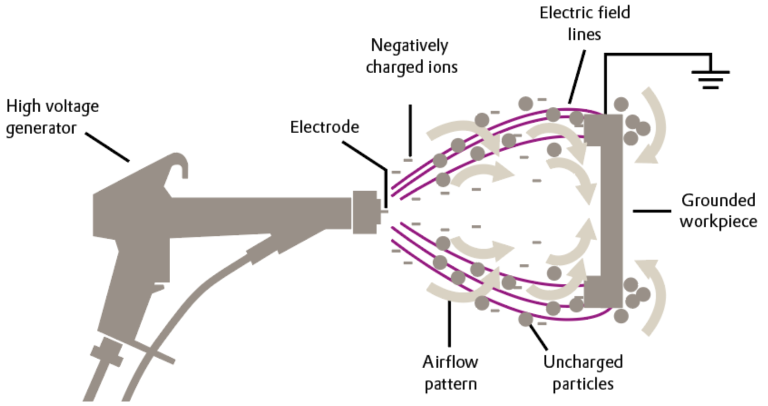
To understand the effect of fumed metal oxides in powder coatings, you have to know the special features of electrostatic deposition. The powder particles are electrostatically charged and deposited on the grounded work piece.

There are three methods of transferring charge:

a) Corona method:
An electrode is installed at the outlet of a spray gun. The high voltage ionizes the surrounding air, which can cause a blue corona from which the method derives its name.

The powder coating particles are conveyed in an air flow through the spray gun and the ionized air and also absorb the negative charge of some air ions. The powder particles then follow the field lines of the electric fields to the work piece, which reduces "overspray".

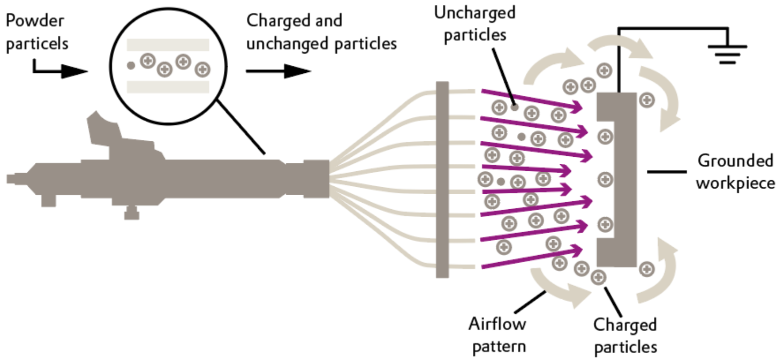
Figure 22



Schematic presentation of the corona method

b) Tribo method:
The spray gun is lined with a plastic (usually PTFE). When the powder coating is conveyed in the air flow, the particles rub against the plastic lining and charge separation occurs. Suitable powder coatings take on a positive charge.

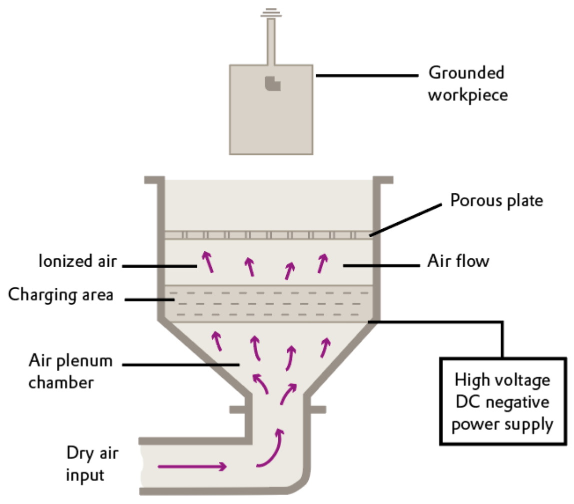
Figure 23



Schematic presentation of the tribo method

c) Fluidized bed method:
In this process, the powder coating is in a container and is fluidized by air, which flows through a porous base plate. When a high voltage is applied to the base plate, the powder coating particles are electrostatically charged. The grounded workpiece is immersed in the fluidized bed and is covered with powder coating.

Figure 24



Schematic presentation of the fluidized bed method

One thing that all these methods have in common is that, after application, the powder coatings are present as a loose layer on the workpiece and, under certain circumstances, can be easily wiped off. Therefore, immediately after coating, the workpieces are placed in an oven where the powder coating melts, forms a closed film and, at higher temperatures, cures and hardens.

Good flow, charging, and film formation properties are important for the manageability, control, and quality of powder coatings.

By just adding 0.1-0.3 % of the fumed oxides, it is possible to improve the following properties of powder coatings:

- Improved flow properties of the raw materials in the production of powder coatings (homogeneous flow of all coating components into the extruder). To adjust the flow properties of the finished powder coating, an anticaking agent has to be added.
- Improved storage stability of the powder coatings (no lumps in the finished powder coating).
- Preventing the powder coating from absorbing moisture (through hydrophobic surface treatment of the fumed metal oxide).
- Improved metering and processing (because of the improved flow properties). The anticaking agent should be added before the powder coating is milled, as it is important to have homogeneous distribution and even coverage of the surface.
- Improved edge coating of the substrates due to more even application.
- Enabling the tribo process (by using metal oxides that can be positively charged).

An internal study in collaboration with the University of Western Ontario (Canada), in which innovative, finer powder coating particles were also investigated (they produce thinner films), showed that the two products AEROXIDE® Alu C 805 and AEROXIDE® Alu 130 have even more benefits in the systems that were examined. In polyester-based conventional and fine-particle powder coatings, AEROXIDE® Alu C 805 had the greatest positive influence on the flow properties of all fumed aluminum oxides that were investigated. In regard to the degree of deposition, AEROXIDE® Alu 130 was rated best in a conventional powder coating.

Detailed information for using AEROXIDE® products in powder coatings can be found in Technical Information 1340 [9].

Figure 25

AEROXIDE® Alu C improves the performance of many powder coatings; the picture shows a powder coated wheel rim as an example

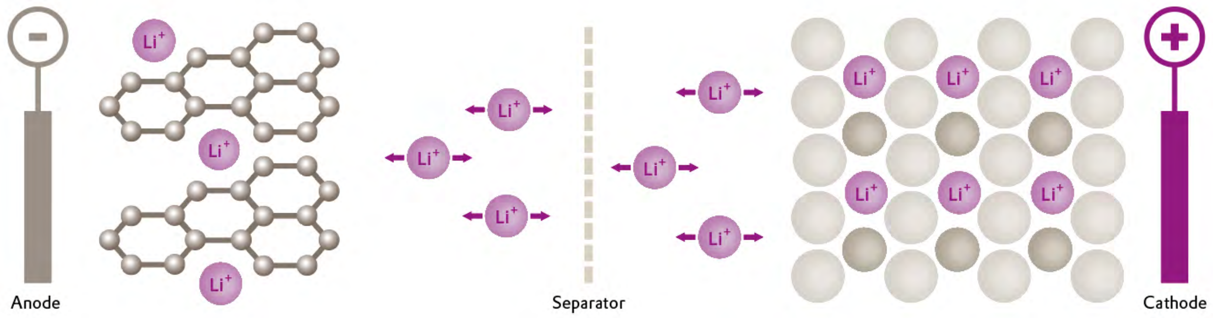
3.6.3 Lithium-ion batteries

Lithium-ion batteries (LIB) are now an inherent part of our everyday lives. Used mainly in consumer electronics and computer technology (notebooks, tablets, smartphones, etc.), they have almost completely replaced the outdated Ni-MH technology. But LIBs are also used increasingly in the advancing field of electromobility and the associated rapidly growing market for storage systems.

No matter whether they are used in a smartphone or an automobile, the function of Li-ion batteries is always the same: When the battery discharges, Li-ions flow from the graphite anode through the separator to the metal oxide cathode, which produces a constant discharge current (vice versa during charging).

This works very efficiently (little charge loss) and extremely constantly over many cycles and years.

Figure 26



Schematic description of a lithium ion battery

High demands are placed on LIBs, especially for electromobility: They have to meet a high safety standard, and high energy density. This especially implies the use of new materials such as for the electrodes, within the separator, or also in the electrolyte.

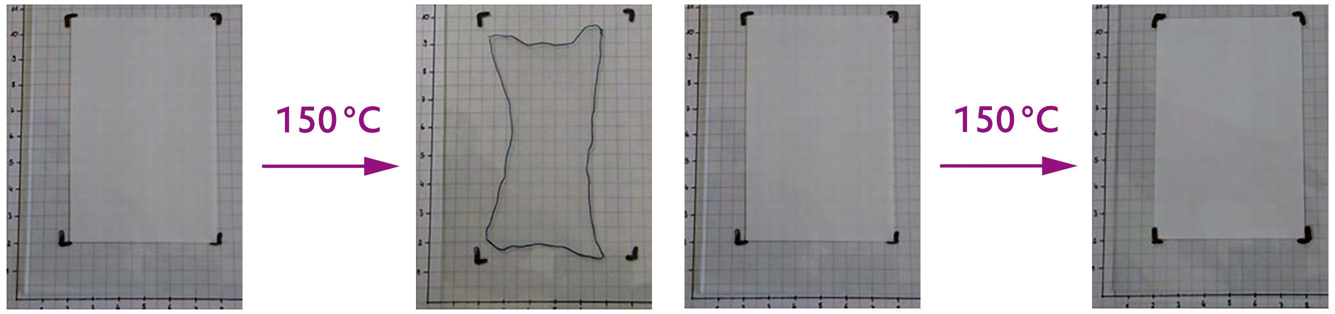
AEROXIDE® Alu and AEROXIDE® TiO_2 fumed metal oxides can be used as additives in lithium-ion batteries in the following components:

- As a ceramic coating on the polymer separator or inside the separator (ceramic filler) to increase safety and battery performance
- As a coating on the cathode and anode material in the form of an Al_2O_3 or TiO_2 layer (= artificial solid electrolyte interface); it also increases battery life and performance
- Inside solid-state polymer electrolytes to improve efficiency and battery life

The separator in an LIB is very thin (approx. 25 µm), very porous, and consists mainly of a polyolefin (e. g polyethylene and / or polypropylene). It is the only component in the cell that prevents direct contact between the cathode and anode, and consequently, a short circuit. However, this polymer separator is very susceptible to sudden temperature increases in the cell (e.g. during a thermal runaway). From about 140 °C, the separator starts shrinking and the electrodes come into direct contact – which causes a short circuit and, in the worst-case scenario, ignition of the flammable electrolyte.

A ceramic coating in the form of a very thin layer of AEROXIDE® Alu C or AEROXIDE® Alu 65 limits shrinkage of the porous membrane at higher temperatures considerably, which helps improve the safety standards of an LIB cell (Figure 27). At the same time, additivation of the separator with fumed aluminum oxide increases battery performance, as the ceramic layer improves the cell's capacity retention for many hundreds of charging and discharging cycles.

Figure 27



LIB separator, uncoated

LIB separator, coated with AEROXIDE® Alu 65

Comparison between two LIB separators before and after the temperature was increased to 150 °C.

In the coming years, we can expect to see new materials being used, especially in cathodes and anodes, which will significantly increase energy density. This will also increase cell voltage, which especially means stress for the electrode material and electrolyte and can ultimately reduce performance and battery life. Coating the electrode materials with fumed aluminum oxide (e.g. AEROXIDE® Alu 130) or also titanium dioxide (AEROXIDE® TiO_2 P 25) improves capacity retention and increases battery life.

The fumed AEROXIDE® aggregates form a Li-ion conductive layer around the electrode particles and create a type of artificial solid electrolyte interface. This layer reduces the decomposition of the electrolyte and also stabilizes the electrode particles against the high cell potential. This positive effect can already be observed in current cathode materials, such as lithium cobalt oxide (used mainly in consumer electronics) and considerably improves battery performance and battery life.

Fumed aluminum and titanium oxides, preferably the hydrophobic variants AEROXIDE® Alu C 805 and AEROXIDE® TiO_2 T 805, can also be used in solid-state polymer electrolytes. In this type of Li-ion battery, liquid electrolyte and separator are replaced by a Li-ion conducting electrically isolating polymer (e.g. polyethylene oxide, PEO). The advantages include an increase in energy density and avoidance of the otherwise liquid, flammable electrolyte. It is now also possible to use pure Li metal as an anode. However, a polymer LIB such as this must be operated at higher temperatures (min. 60 °C). The fumed metal oxides can be incorporated directly into the polymer and then be processed into thin films. Adding AEROXIDE® improves the life and efficiency of polymer batteries. The higher temperature needed for operation can also be reduced.

3.6.4 Inkjet paper coatings

Thanks to modern inkjet technology, everyone can now print digital photographs on high-quality photographic paper in excellent quality. The print result is very dependent on the physical and chemical properties of the surface to be printed.

The requirements of modern photographic paper can be fulfilled ideally by using fumed aluminum oxide in microporous paper coatings. Because of their unique structure, their high specific surface area, their particle size, and the cationic surface charge, the following properties can be implemented at the same time:

- **High gloss**
  Together with a binder, the very tiny aluminum oxide particles (aggregate size approx. 100-200 nm) form a smooth surface with a high gloss.

- **Short drying time for the ink**
  Because of the fractal structure of the AEROXIDE® aggregates, a three-dimensional network of capillaries develops, which directs the water out of the ink into the aluminum oxide layer for water absorption.

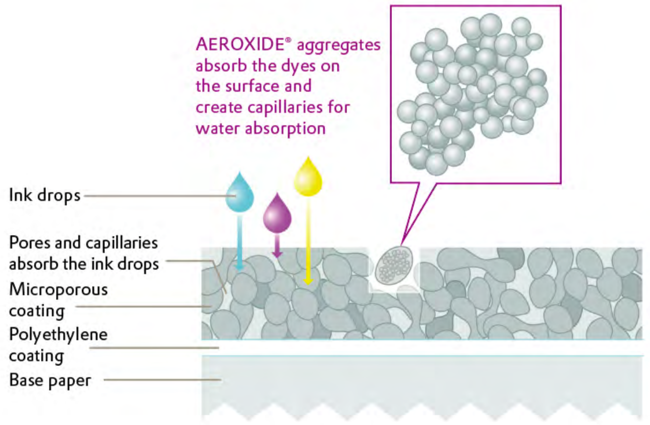
- **Photo-realistic resolution**
  As soon as they impinge on the paper, the dyes in the ink drops are adsorbed by the aggregates on their

surface, the liquid from the ink is directed downward. As a result, the ink droplets do not run and resolutions of up to 2800 DPI are achieved.

- **High color brilliance**
  The dye molecules are very stable when they adsorb on the surface of the aggregates and do not change their color. The dyes are also preferably embedded in the top areas of the color-absorbing layer, which produces a high color density.
- **Compatibility with different inks**
  As opposed to traditional swellable polymer coatings, microporous coatings allow high-quality printouts of pigment inks. As opposed to dye inks, pigment inks are more resistant to environmental influences.

More information can be found in our Technical Information TI 1331 [10].

Figure 28



Structure of a microporously coated inkjet paper

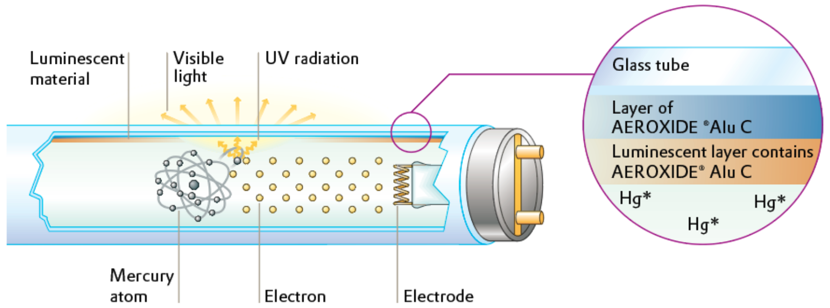
3.6.5 Fluorescent lamps

Fumed aluminum oxide fulfills two different functions in fluorescent lamps and compact fluorescent lamps (energy saving lamps). Figure 29 shows the structure of such a lamp.

Inside, a mercury vapor plasma burns and emits UV light at 254 nm, which is invisible to the human eye. This is converted into visible light by various luminescent materials in the luminescent layer. A fumed aluminum oxide protective layer directly on the surface of the glass prevents mercury atoms diffusing into the glass (function 1). This considerably extends the life of the lamp and also ensures that the light output remains constant. The amount of mercury can also be reduced to a minimum.

Because of the positive surface charge of the aluminum oxide, it also acts as an inorganic binder (function 2) by facilitating adhesion of the luminescent layer (luminescent materials are usually negatively charged) to the negative glass surface. Inside the luminescent layer, fumed aluminum oxide is also used as an inorganic binder to increase the strength of the layer. It plays an important role in the manufacture of the lamp, as it prevents a loss of luminescent particles.

Figure 29



Fluorescent lamp with the functions of aluminum oxide

3.6.6 Other applications

AEROXIDE® Alu C is also used as a ceramic binder in the production of various ceramics (e.g. refractories). It allows coarser materials to be sintered together, is used as a reinforcement in the material itself and also acts as a flow improver while the educts are being mixed.

In metal processing (e.g. continuous metal band coating), fumed aluminum oxide is used as an anti-corrosive adhesion agent between the actual metal and the coating. It also increases the mechanical resistance of the coating (including wear protection).

AEROXIDE® Alu C is also used in flame-retarding polyester and acrylate-based plastics. The positive effect is due mainly to the extreme fineness of the product.

Because of its high degree of purity, fineness, and high specific surface area, fumed aluminum oxide is ideally suited as a raw material for the manufacture of catalysts carriers. The loose structure makes the surface very accessible.

You need a titanium dioxide with a unique structure?

AEROXIDE® – Fumed Titanium Dioxide Products

Structure and properties | Mixed oxide types containing titanium dioxide | Surface treated titanium dioxide | Granulated titanium dioxide | Titanium dioxide dispersions | Application-specific effects

4. AEROXIDE® – Fumed Titanium Dioxide Products

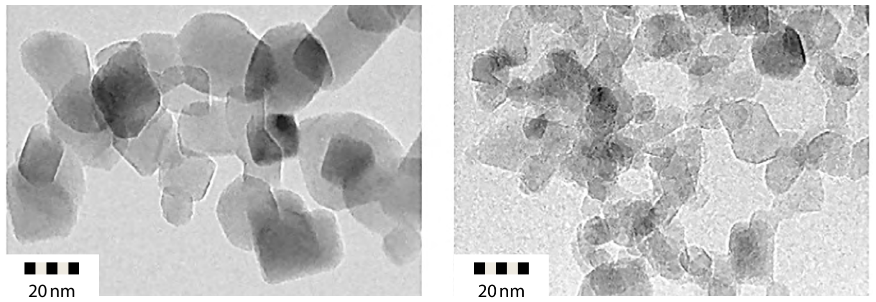
4.1 Structure and properties

Titanium dioxide is found in nature in the modifications anatase, rutile, and brookite. From a technical aspect, anatase and rutile are important as white pigments.

Back in 1940, flame hydrolysis was used to produce a titanium dioxide with a primary particle size 10 times smaller than existing white pigments that were known at that time. The new product was called "highly dispersed titanium dioxide" in the scientific literature. Nowadays Evonik markets a range of fumed titanium dioxide grades under the brand name AEROXIDE®.

AEROXIDE® TiO_2 P 25 is manufactured by flame hydrolysis of titanium tetrachloride and, because of the resulting fineness of the aggregates, has few pigment properties. It is therefore used in applications where the titanium dioxide should not cause white coloring or where a very high specific surface area is required to achieve specific technical effects. AEROXIDE® TiO_2 P 25 is especially used as a catalyst carrier and as an active component in photocatalytic reactions, and as a heat stabilizer for silicones.

Figure 30



TEM images of AEROXIDE® TiO_2 P 25 (left) and AEROXIDE ® TiO_2 P 90 (right).

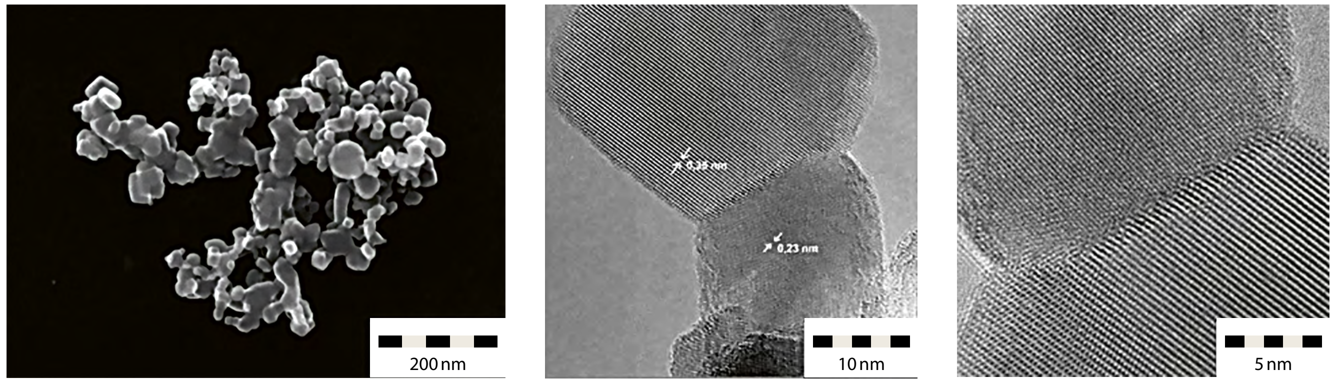
In addition to AEROXIDE® TiO_2 P 25, Evonik also markets AEROXIDE® TiO_2 P 90, a titanium dioxide with an even higher specific surface area of 90 m^2/g. Figure 30 shows comparative TEM images of both oxides.

AEROXIDE® TiO_2 PF 2 is another titanium dioxide product which is also produced according to the flame hydrolysis method and is a mixed oxide based on titanium dioxide and iron oxide. AEROXIDE® TiO_2 PF 2 is used mainly as a heat stabilizer in silicones.

The fractal structure in which there are no defined agglomerate sizes is characteristic for oxides produced with high temperature hydrolysis. However, VP AEROPERL® P 25/20 (see also Section 4.4) can be produced in a special downstream granulation step.

From a radiographic aspect, AEROXIDE® TiO_2 P 25 consists of about 85 % anatase and 15 % rutile. In other words, despite the manufacturing conditions (flame hydrolysis) the thermodynamically more stable rutile modification is present to a much lesser degree, is found mainly on the particle surface, and is intensively interlinked with the anatase phase (see Figure 31). In AEROXIDE® TiO_2 P 90, which has a higher specific surface area, the rutile proportion is even less and makes up just 5 %.

Figure 31



SEM image (left) and (HR)TEM images (center and right) of AEROXIDE® TiO_2 P 25. The different crystal phases and the individual crystal levels can be seen clearly. [6]

Table 10
Physico-chemical data of the different fumed titanium dioxides.
These are typical values and not specifications.

Property	Unit	AEROXIDE® TiO_2 P 25	AEROXIDE® TiO_2 P 90
BET specific surface area	m^2/g	35-65	70-110
pH (4 % aq. Dispersion)		3.5-4.5	3.2-4.5
Loss on drying (2 h @ 105 °C)	%	≤ 1.5	≤ 4.0
Tamped density	g/l	approx. 140	approx. 120
Concentration of TiO_2	%	≥ 99.5	≥ 99.5

The physico-chemical data of fumed titanium dioxide types marketed by Evonik is aggregated in Table 10.

The surface chemistry of titanium dioxide is characterized by hydroxyl groups, which lead to an energetic preferred hexacoordination of the titanium atoms on the phase boundary. Half of these hydroxyl groups react acidically, while the other half have a basic character and can be replaced with certain anions.

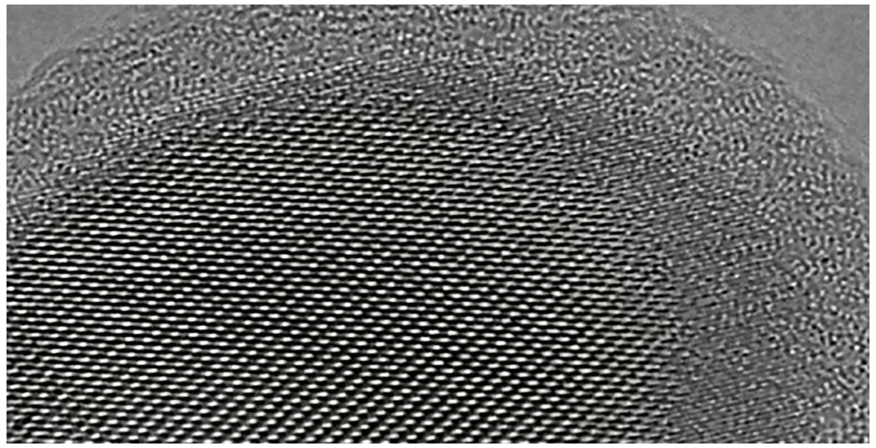
Fumed titanium dioxides are produced from titanium tetrachloride, which can be purified easily through distillation. Therefore, the product, which is manufactured using flame hydrolysis, is very pure and has a titanium dioxide concentration of more than 99.5 %, based on the substance calcined at 1000 °C for two hours. This pre-treatment is necessary to obtain a constant reference point since, due to the high specific surface area, weights of the physically adsorbed water (loss on drying) and the chemically adsorbed water (loss on ignition) have to be taken into account. The high degree of purity is very important in many applications.

4.2 Mixed oxide types containing titanium dioxide

As well as the pure titanium dioxide powders, silicon titanium mixed oxides are also produced by the flame hydrolysis process (see also Section 2.2). Depending on the process control, "real" mixed oxides and core-shell mixed oxide particles can be produced. With the "real" mixed oxides, titanium dioxide is statistically incorporated in the SiO_2 matrix, while with the core-shell particles an amorphous SiO_2 layer surrounds a crystalline titanium dioxide core (Figure 33). The crystalline titanium dioxide core is composed of the anatase and rutile phases.

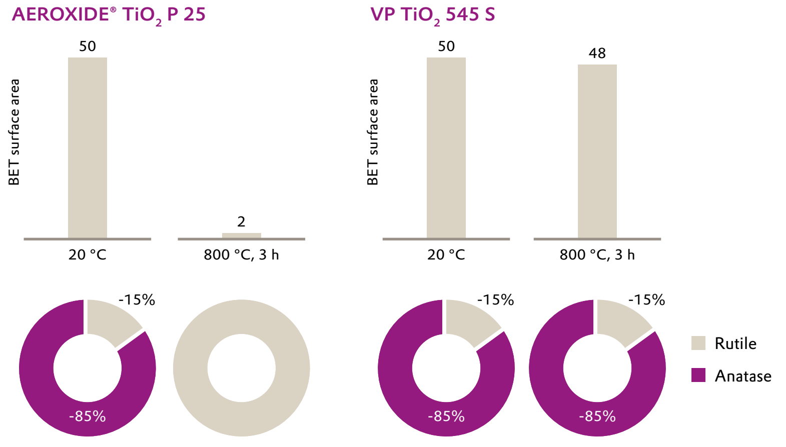
Examples of silicon dioxide-titanium dioxide mixed oxides are VP TiO_2 545 S and VP TiO_2 1580 S. They are characterized by improved thermal stability. For example, the surface area of AEROXIDE® TiO_2 P 25 is reduced from 50 m^2/g to just 2 m^2/g when it is heated to 800 °C over three hours, and there is an almost complete phase conversion to rutile. As opposed to this, the anatase / rutile phase composition of the mixed oxide VP TiO_2 545 S does not change with thermal stress. In addition, there is practically no change in the specific surface area at a temperature of 800 °C over a dwell time of three hours.

Figure 32



HR-TEM image of a fumed mixed oxide with core-shell morphology: an amorphous SiO_2 layer surrounds a crystalline TiO_2 core.

Figure 33



Comparison of the specific surface area before and after temperature treatment of AEROXIDE® TiO_2 P 25 and VP TiO_2 545 S.

These mixed oxides are used mostly as catalyst carriers. This effect is described in more detail in Section 4.6.1.

AEROXIDE® TiO$_2$ PF 2 is a titanium dioxide containing iron oxide which is used for thermal stabilization of silicones (see Section 4.6.3).

Table 11
Physico-chemical data of fumed mixed oxides containing titanium dioxide. These are typical values and not specifications.

Property	Unit	VP* TiO$_2$ 1580 S	VP* TiO$_2$ 545 S	AEROXIDE® TiO$_2$ PF 2
BET specific surface area	m^2/g	65-95	40-55	45-70
pH (4 % eq. dispersion)		3.0-4.5	3.5-4.5	3.5-4.5
Loss on drying (2 h @ 105 °C)	%	n.a.	n.a.	≤ 2,0
Tamped density	g/l	approx. 60	approx. 100	approx. 80
Concentration of SiO$_2$	%	approx. 15	approx. 5	n.a.
Concentration of TiO$_2$	%	approx. 85	approx. 95	≥ 94.0
Concentration of Fe2O$_3$	%	n.a.	n.a.	1.0-3.0

* Development products have VP in the product name. Commercialization depends on feedback from the market.

4.3 Surface treated titanium dioxide

In certain applications, it may be necessary to use a surface modified titanium dioxide. With chemical treatment, a hydrophilic titanium dioxide can be changed to a hydrophobic material. AEROXIDE® TiO$_2$ T 805 is a commercially available fumed titanium dioxide with octyl groups on the surface. It is characterized especially by its good dispersability and low moisture absorption. It also has the following properties:

- High UV absorption
- High photostability
- Easily dispersed, especially in non-polar liquids
- Reduced chemical reactivity
- Lower thickening effect
- Improved flow property and stabilization of the electrostatic charge of toner powders for photocopiers and laser printers

Because of these properties, AEROXIDE® TiO$_2$ T 805 is the perfect additive for toners and is also used as a thermal stabilizer for silicones.
Other titanium dioxide mixed oxides and mixed oxides containing titanium dioxide that are hydrophobized with various alkylsilanes include AEROXIDE® STX 501, AEROXIDE® STX 801, AEROXIDE® TiO$_2$ NKT 90, and VP NKT 65. These products are used mainly to adjust the electrostatic charge, flow behavior, and stability of toners for copiers and laser printers.

The physico-chemical data for the individual hydrophobic titanium dioxides is aggregated in table 12.

Table 12
Physico-chemical data for surface modified hydrophobic fumed titanium dioxide types. These are typical values and not specifications.

Property	Unit	AEROXIDE® TiO$_2$ T 805	AEROXIDE® STX 501	AEROXIDE® STX 801	AEROXIDE® TiO$_2$ NKT 90	VP* NKT 65
BET specific surface area	m^2/g	35-55	25-45	45-65	50-75	30-60
pH (4 % eq. dispersion)		3.0-4.0	6.0-9.5	6.0-9.0	3.0-4.0	3.0-7.0
Loss on drying (2 h @ 105 °C)	%	≤ 1.0	≤ 1.0	≤ 1.0	≤ 1.0	≤ 1.0
Tamped density	g/l	approx. 200	approx. 130	approx. 130	n.a.	n.a.
C content	%	2.7-3.7	0.2-1.0	0.7-1.1	2.5-4.5	1.0-4.0

* Development products have VP in the product name. Commercialization depends on feedback from the market.

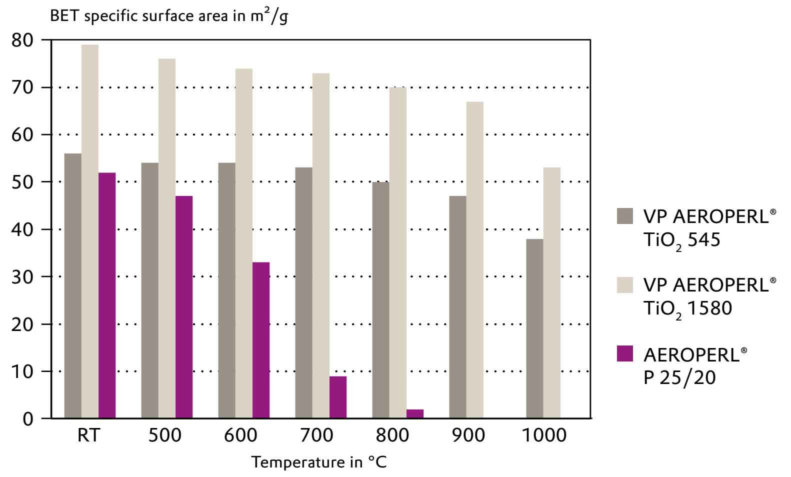
4.4 Granulated titanium dioxide

A selection of titanium dioxides and titanium dioxide-silicon dioxide mixed oxides is also available as granules under the brand name AEROPERL®. These products have several advantages over powder products (see Section 2.4). As well as being easier to handle, the porosity plays an important role for catalytic applications.

Pure titanium dioxide granules are available as VP AEROPERL® P 25/20. This product is used as a carrier or adsorbent in numerous applications. Average particle size of this product is approx. 20 µm and, at 700 g/L, tamped density is much higher than the non-granulated starting powder.

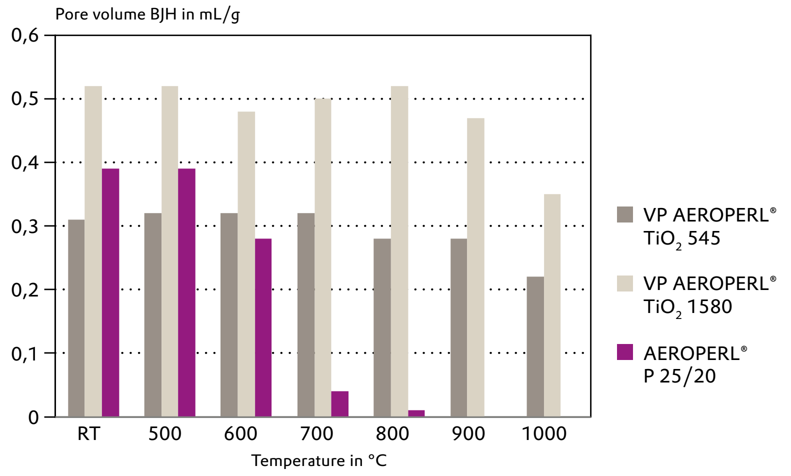
VP AEROPERL® TiO$_2$ 545 and VP AEROPERL® TiO$_2$ 1580 are granulated forms of the corresponding titanium dioxide-silicon dioxide mixed oxides (see also Section 4.2). These AEROPERL® types differ from each other mainly as regards their specific surface areas and amount of silicon dioxide (Table 13). Compared to the pure titanium dioxide VP AEROPERL® P 25/20, these products have a higher thermal stability (Figure 35). Even at higher temperatures there is no noticeable change in the crystal structure of anatase to rutile and, as a result, there is also no change in the specific surface area (see also Section 4.6.1). Thermal and hydrothermal aging effects can be effectively suppressed for titanium dioxide-based catalyst carriers with high specific surface areas. As opposed to VP AEROPERL® P 25/20, the porosity also remains unchanged at high temperatures (Figure 36).

Figure 34



Thermal stability (specific surface area, BET) after 3 h at the specified temperature of VP AEROPERL® P 25/20, VP AEROPERL® TiO_2 545 and VP AEROPERL® TiO_2 1580

Figure 35



Thermal stability (mesopores determined by nitrogen adsorption) after 3 h at the specified temperature of VP AEROPERL® P 25/20, VP AEROPERL® TiO_2 545 and VP AEROPERL® TiO_2 1580

The properties of AEROPERL® products, which are based on titanium dioxide and titanium-silicon mixed oxides are listed in Table 13.

Table 13
Physico-chemical data of AEROPERL® products based on titanium dioxide and titanium-silicon mixed oxides. These are typical values and not specifications.

Property	Unit	VP* AEROPERL® P 25/20	VP* AEROPERL® TiO_2 545	VP* AEROPERL® TiO_2 1580
BET specific surface area	m²/g	35-65	35-55	60-90
pH (4 % eq. dispersion)		3.0-4.5	3.0-4.5	3.0-4.5
Loss on drying (2 h @ 105 °C)	%	≤ 2.5	≤ 2.5	≤ 2.5
Tamped density	g/l	approx. 700	approx. 600	approx. 550
Concentration of SiO_2	%	n.a.	approx. 5	approx. 15
Concentration of TiO_2	%	n.a.	approx. 95	approx. 85

* Development products have VP in the product name. Commercialization depends on feedback from the market.

4.5 Titanium dioxide dispersions

Dispersions of the titanium dioxide types can also be a benefit for customers for applications such as catalyst carrier materials or coatings. Direct use of dispersions in coating processes avoids the time-consuming handling of dusty powders. Production of dispersions of fumed titanium dioxide products, such as AEROXIDE® TiO_2 P 25, requires a high energy input and, with conventional dispersion units, it is often the case that large agglomerates remain, which prevent homogeneous particle distribution (see Figure 37).

AERODISP® W 740 X and VP Disp. W 2730 X are highly filled dispersions of the titanium dioxide products AEROXIDE® TiO_2 P 25 and AEROXIDE® TiO_2 P 90. They are especially suitable for applying layers on carrier materials, for instance, to utilize the (photo-) catalytic activity of the titanium dioxide.

Table 14
Physico-chemical data of selected aqueous titanium dioxide dispersions.
These are typical values and not specifications.

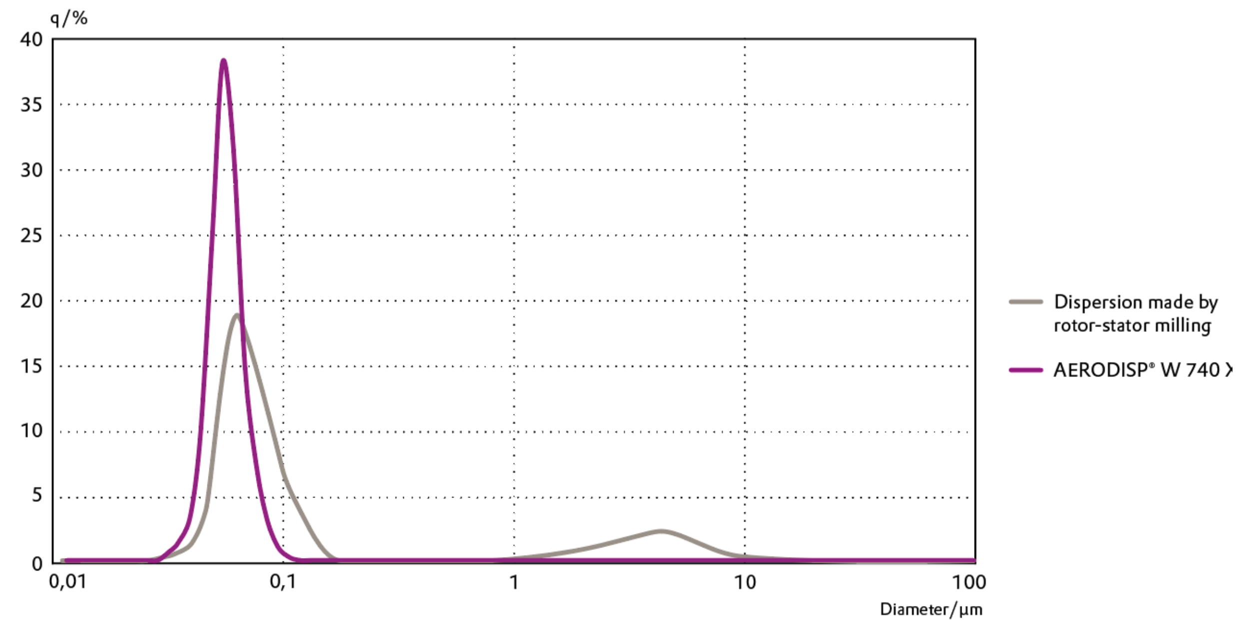
Property	Unit	AERODISP® W 740 X	VP Disp. W 2730 X
TiO_2 type		AEROXIDE® TiO_2 P 25	AEROXIDE® TiO_2 P 90
Solid content	%	ca. 40	ca. 30
pH		5.0-7.0	6.0-8.0
Viscosity	mPas	≤ 30	≤ 5000
Density	g/cm³	1.41	1.28
Aggregate size (d50)	nm	70	≤ 100

* Development products have VP in the product name.
Commercialization depends on feedback from the market.

Evonik's own dispersion technology enables dispersions of these metal oxides to be produced with an average aggregate diameter of less than 100 nm. This ensures a high degree of transparency with thin layers. Figure 37 shows the effect of this high-energy milling, using AEROXIDE® TiO_2 P 25 as an example.

If a 40 % titanium dioxide dispersion is produced using only a rotor-stator unit, the average particle size is 80 nm, but with bimodal distribution, it has a high proportion of aggregate sizes in the range of several micrometers. After high-energy milling, which is used for AERODISP® W 740 X, the average particle size is reduced to 70 nm and the coarse proportion is completely removed. This dispersion is now storage-stable and can also be used in transparent coatings.

Figure 36



Effect of the high energy milling on a 40% titanium dioxide dispersion.

4.6 Application-specific effects

The most important applications are described briefly below. This information does not claim to be complete and is intended only to illustrate the many different applications that are possible with these products.

4.6.1 Catalyst carriers

Titanium dioxide is a popular carrier material and active component for exhaust gas catalytic converters and process catalysts. For example, titanium dioxide, together with vanadium pentoxide is an indispensable component in SCR catalysts for selective catalytic reduction of nitric oxides in exhaust gases. In other cases, titanium dioxide is used as an inert, extremely chemically resistant carrier. The high tolerance of titanium dioxide to sulfur oxides is particularly important.

For many catalytic applications, the titanium dioxide types must have a large surface area and a high level of chemical purity. The phase structure is also important; in general, anatase-rich products are preferred. For all these reasons, AEROXIDE® TiO_2 P 25 and AEROXIDE® TiO_2 P 90 are outstanding starting materials for the production of catalysts. Both types have an extremely high degree of chemical purity; in particular, because of the flame hydrolysis process they contain no sulfur contamination. The large surface area is easily accessible for catalytic processes. Users can adjust the porosity flexibly, for example, in the production of molded bodies for process catalysts or washcoats for exhaust gas catalytic converters.

Alternatively, Evonik also offers finished molded bodies as extrudates with various diameters and BET specific surface areas under the brand name AEROLYST®. These can be supplied in mainly anatase or almost complete rutile modifications. The molded bodies have outstanding physico-chemical characteristics (wear resistance, pressure resistance, etc.). The fact that the pore volume consists completely of mesopores is especially worthy of mention. As a result, these extrudates offer optimum transportation properties for the diffusion of educts and products. In some applications, AEROLYST® can be used directly as a catalyst or also after it has been loaded with an active component. Evonik can also manufacture the catalyst.

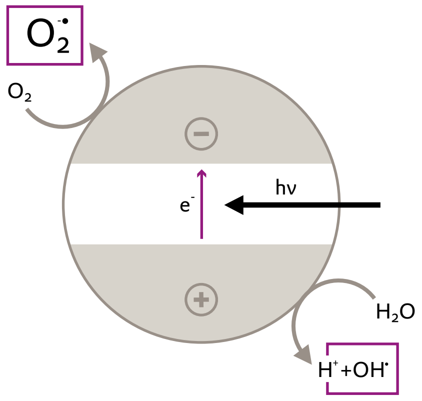
In some cases, customers want to manufacture the application form of the catalysts, such as molded bodies and washcoats, themselves but would still prefer to avoid handling powder materials with low bulk density. For these cases, Evonik has developed micro granules and dispersions, which are marketed under the names AEROPERL® and AERODISP® (see also Sections 4.4 and 4.5).

However, one particular challenge when using titanium dioxide as a catalyst carrier is temperature resistance. As described in Section 4.2, the surface area of AEROXIDE® TiO_2 P 25 is reduced from 50 m^2/g to just 2 m^2/g and there is an almost complete phase conversion to rutile when material is heated to 800 °C over three hours. But when small quantities of silicon dioxide are added, the thermal stability of titanium dioxide is considerably improved. Especially the silicon-titanium mixed oxides VP TiO_2 545 S and VP TiO_2 1580 S described in Section 4.2 have outstanding thermal stabilities. Fumed titanium dioxide types with a small proportion of silicon dioxide to increase thermal stability are also available as AEROPERL® variants. Details are described in Section 4.4.

4.6.2 Photocatalytic reactions

Titanium dioxide is a semiconductor. According to the energy band model, with which the conductor, isolators, and semiconductors can be described, the band gap between the valence band and the conduction band of titanium dioxide in the anatase crystal modification corresponds to the energy content of light quanta up to 3.26 eV or a wavelength of 380 nm. The rutile modification has a band gap that corresponds to the energy content of a light quantum with a wavelength of approximately 410 nm. This is why titanium dioxides are able to absorb UV light and trigger numerous follow-up processes.

Figure 37



Schematic description of a photocatalytic mechanism

In a review article, Carp et al. summarize the current scientific knowledge regarding the photoinduced reactivity of titanium dioxide [11]. Accordingly, we have to distinguish between three processes: photovoltaic effect, photoinduced super hydrophilia, and photocatalysis. The latter can be differentiated further into photocatalytic decomposition reactions (removal of contaminants and / or disinfection) and special reactions, such as photocatalytic water splitting.

A mechanism discussed in literature [12] as to how reactive species can occur on the surface of titanium dioxide with the effect of light and water is described in the following simplified diagram. An electron from the valence band of titanium dioxide is excited into the conduction band by a light quantum. From there it can be transferred to an oxygen molecule, which leads to the formation of a reactive superoxide radical anion. The electron gap in the valence band can be closed by an electron from a water molecule, which also forms a reactive hydroxyl radical.

In paints and coatings photocatalysis usually is suppressed. To prevent contact between organic compounds and the titanium dioxide surface, practically all pigment titanium dioxides are treated with inorganic oxides (e.g. silicon or aluminum oxide). This effectively prevents "chalking" of coatings.

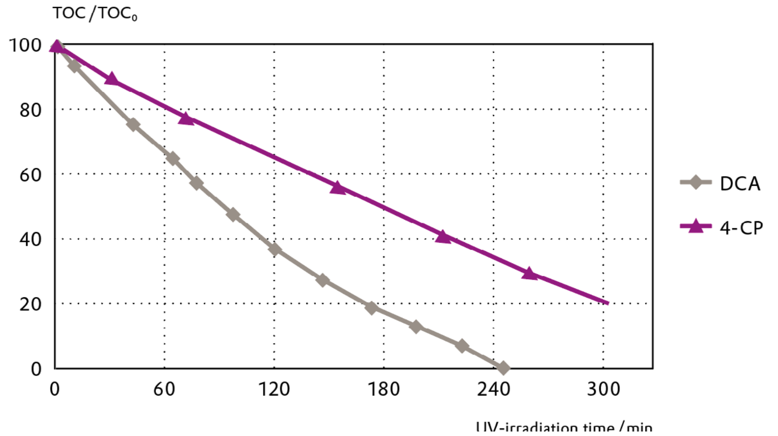
Titanium dioxides produced by the flame hydrolysis method have a surprisingly high level of photoactivity, which can be attributed mainly to two factors: on the one hand, the very high specific surface area and, on the other, the unique crystal structure.

The effect of the crystal structure has been analyzed in several studies: Smirniotis et al. [13] showed that the synergy between the anatase and rutile phases (as with AEROXIDE® TiO_2 P 25) is not universal, while Gray et al. [14] explained that rutile takes over an antenna function. This extends photoactivity in the visible wavelength range and the structural features of the similarly formed TiO_2 crystallite results in catalytic "hot spots" on the anatase / rutile phase boundary.

The photocatalyst can be fixed to the surfaces of various substrates, for example, by using titanium dioxide dispersions. When dispersing in a liquid system, no isolated primary particles can be generated, only more or less small aggregates and agglomerates. Primarily, their size distribution depends on the intensity of the dispersion process (see also Section 4.5). With the help of high energy dispersion techniques, Evonik has developed low-viscosity but still highly filled aqueous titanium dioxide dispersions with aggregate sizes milled to < 100 nm. With dip coating it is then possible to easily coat glass materials, for example. Almost transparent or translucent coatings are possible, depending on the layer thickness. Other options are coatings on stainless steel through the use of activated carbon / epoxy binders with the help of Raschig rings and also "in-mass application" in cement-based construction materials. The work of Kiwi et al. is interesting, according to which photocatalytic properties can be implemented on cotton textiles through TiO_2 bonding [15] [16]. The exceptional position of AEROXIDE® TiO_2 P 25 was confirmed in a comparison of the antibacterial effect of numerous commercially available titanium dioxides [15].

AEROXIDE® TiO_2 P 25 is ideally suited as a catalyst in wastewater treatment, as the photocatalytic activity helps decompose various chlorophenols (Figure 39).

Figure 38

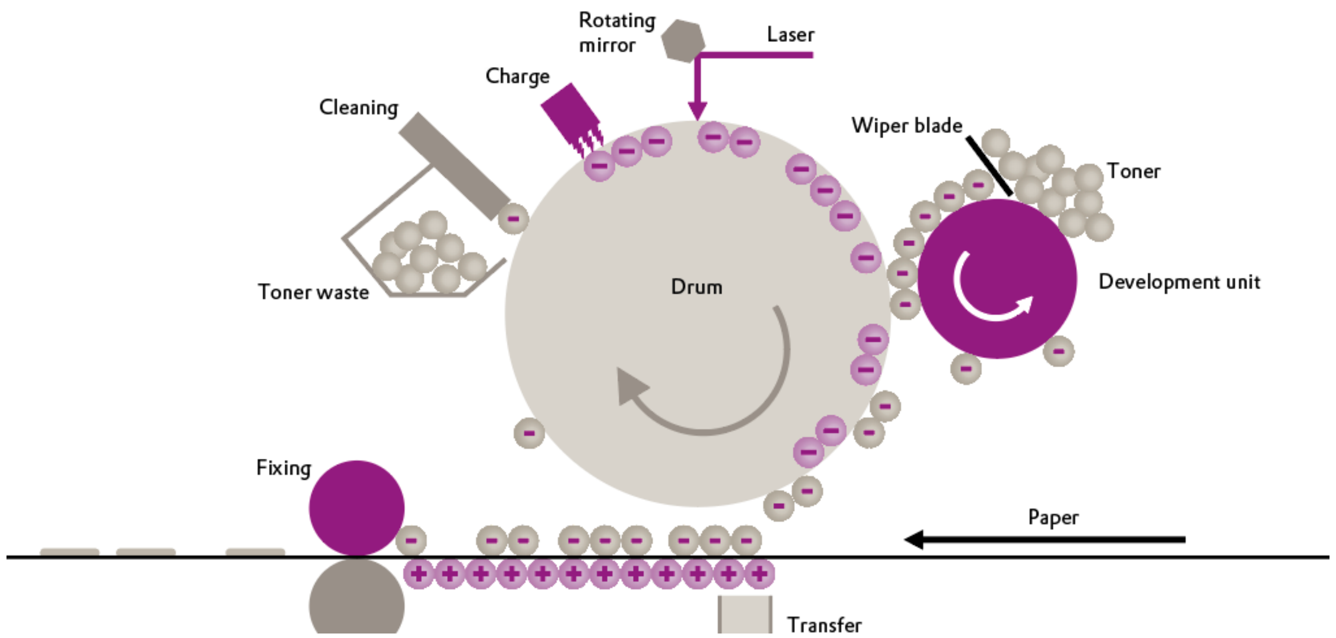


Photocatalytic decomposition of 4-chlorophenol (4-CP) and dichloroacetic acid (DCA) using AEROXIDE® TiO_2 P 25

4.6.3 Toners

Toner particles are the color-bearing particles in print processes, such as in laser printers, copiers, and fax machines. As opposed to inks, where the black or colored components are applied to the medium in a liquid form, toners contain a dry powder. The diagram below shows the main processes of toner printing (electrophotographic process, xerographic print):

Figure 39



Schematic description of the main processes of toner printing

The main components of toners are thermoplastic resins, pigments, waxes, organic additives, and external additives. External additives play an important role in toners which is not obvious at first. These substances allow triboelectric charging (electric charging through friction) of the toner particles to be controlled. Charging is the basis for xerographic printing, as the process functions only when the charge on the toner particle surface is specifically controlled. These additives also improve the flow of the powder, even in case of high humidity, to prevent lumps forming in the toner, which would have a negative effect on the print image. Various fumed oxides, AEROSIL® and AEROXIDE® types, are used as external additives.

Improving flow in toners

Two effects ensure that toner particles treated with AEROSIL® or AEROXIDE® powders have much better flow properties: on the one hand, these fumed metal oxides can interrupt the liquid film on the surface of toners (water adsorbed with high humidity), which largely stops the individual particles sticking to each other. On the other hand, these additives act like a sort of spacer between toner particles. This reduces interparticle adhesion forces (the general principle of flow improvement is also described in Section 3.6.4, Figure 19)

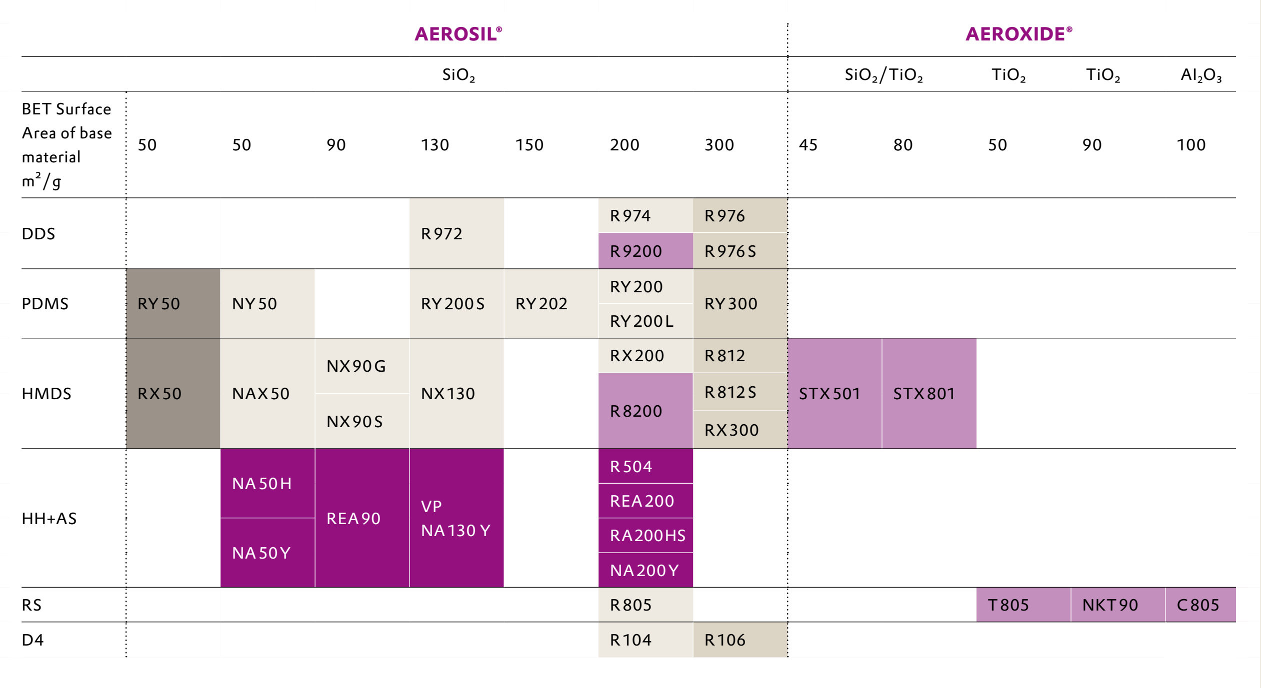
In the case of toner particles that contain components with low glass transition temperatures, a frequent problem is that additives on the surface migrate to the inside of the particles because of the plasticity of the toner and can then no longer acts as spacers. This problem can be avoided with low surface area, coarser AEROSIL® particles. These particles remain on the surface and also prevent fine-particle additives losing their effect as a result of plastic toner particles colliding.

Controlling triboelectric properties

AEROSIL® and AEROXIDE® products have a high degree of purity and a low water content. Because of these properties, the electric resistance of the powders is very high, which means that they can have high electric charge densities, which, in turn, means that the toner particles have outstanding charging properties. With suitable, subsequent surface treatment of the AEROSIL® particles it is possible to improve charge control even more; for example, hydrophobic types have a higher negative charge density than the hydrophilic products, although they have similar surface areas. With the right choice of post-treatment reagent, it is also possible to achieve "pole reversal" and generate positively charged AEROSIL® particles: One example of this is AEROSIL® R 504, which, is post-treated with an aminosilane.

Table 15

Overview of suitable AEROSIL® and AEROXIDE® types for use in toners and their triboelectric properties.



	AEROSIL®							AEROXIDE®				
	SiO_2							SiO_2/TiO_2		TiO_2	TiO_2	Al_2O_3
BET Surface Area of base material m^2/g	50	50	90	130	150	200	300	45	80	50	90	100
DDS				R 972		R 974 R 9200	R 976 R 976 S					
PDMS	RY 50	NY 50		RY 200 S	RY 202	RY 200 RY 200 L	RY 300					
HMDS	RX 50	NAX 50	NX 90 G NX 90 S	NX 130		RX 200 R 8200	R 812 R 812 S RX 300	STX 501	STX 801			
HH+AS		NA 50 H NA 50 Y	REA 90	VP NA 130 Y		R 504 REA 200 RA 200 HS NA 200 Y						
RS						R 805				T 805	NKT 90	C 805
D4						R 104	R 106					

DDS = Dimethyldichlorosilane,
PDMS = Polydimethylsiloxane,
HMDS = Hexamethyldisilazane,
HH = HMDS or PDMS,
AS = Amminosilane,

RS = Alkylsilane,
D4 = Tetra (dimethylsiloxane).

Developmental products are labeled with the VP designation.

R 504	Positive
NKT 90	Weakly negative
RY 50	
R 972	
RX 300	Strongly negative

Non-SiO_2-based particles are also used to control charge distribution and for charge stability. AEROXIDE® products such as AEROXIDE® STX 801 and AEROXIDE® STX 501 especially show their full potential in cases such as these. These special hydrophobic types are titanium dioxide particles surrounded by a layer of silicon dioxide. These core-shell products combine the triboelectric properties of pure TiO_2 with the surface properties of SiO_2. Table 16 shows the application differences between pure silicon dioxide, pure titanium dioxide, and a corresponding mixed oxide of SiO_2/TiO_2:

Table 16
Comparison of the electrification of pure fumed silica, the mixed oxide AEROXIDE® STX 801, and pure fumed titanium dioxide.

	Fumed silica	**AEROXIDE® STX 801**	**Fumed titanium dioxide**
Triboelectric charge	high	medium	low
Charge distribution	wide	medium	narrow
Speed of charge	fast	fast	slow
Charge stability	low	high	medium

AEROSIL® and AEROXIDE® powders are also used to improve other properties. To obtain a good print image, it is necessary to remove toner residues adhering to the drum. Products such as AEROSIL® RX 50 can be used as a cleaning agent, since, due to their structure, they remove surplus toner particles from the surface of the drum. More information about using AEROSIL® and AEROXIDE® products in toners can be found in Technical Information 1222 [17].

4.6.4 Thermal stabilizer for silicones

Compared to other elastomers, silicones have several special features that make them very suitable for certain applications. These include their high resistance to cold and heat, their mechanical properties, and high resistance to chemicals and weather effects. From a chemical aspect, silicone rubber consists of polydimethylsiloxanes (PDMS), in other words, of chains that consist alternately of oxygen and silicon atoms where the remaining silicon valencies are saturated with methyl groups. Many silicones have too little mechanical strength for specific applications. But this can be compensated for with suitable active fillers, such as hydrophilic or hydrophobic AEROSIL® types.

Silicones can be classified in three product groups:

- RTV silicones (RTV = Room Temperature Vulcanization),
- High-consistency rubber (HCR),
- Liquid silicone rubber (LSR).

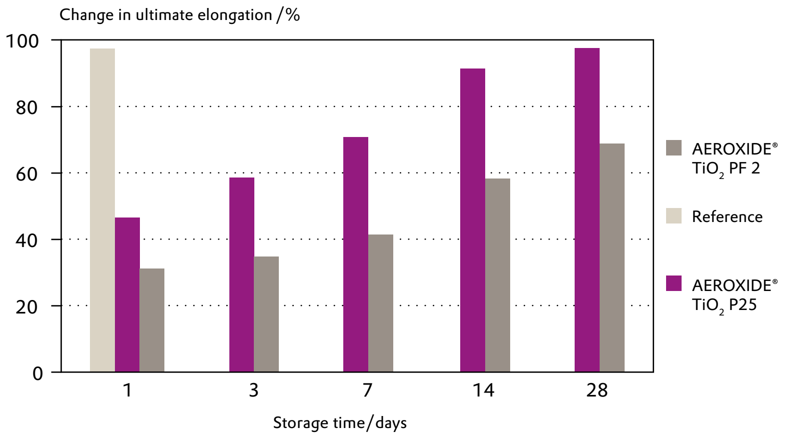
Molded bodies that are subject to high temperatures, such as gaskets, cables, and hoses in the automotive and aerospace industries, are made of high-temperature vulcanizing silicone rubber (HCR or LSR).

From temperatures of about 200 °C, heat aging begins with HCR, which is noticeable by the fact that mechanical properties such as elasticity and tear resistance are reduced. This is due to oxidation processes or thermal chain scission, which results in the rearrangement or elimination of smaller segments.

There are various additives that improve the thermal stability of silicones. Adding 0.5-5.0 % AEROXIDE® TiO_2 P 25 or 0.5-3.0 % AEROXIDE® TiO_2 PF 2 has proved to be a good solution. The reason for the high effectiveness is the ability of AEROXIDE® TiO_2 types to acquire free electrons, forming titanium (III) ions, and, as a result, inhibit hydroxyl radicals. The suitability of AEROXIDE® TiO_2 to stabilize silicone as regards thermal aging is illustrated in the figures below.

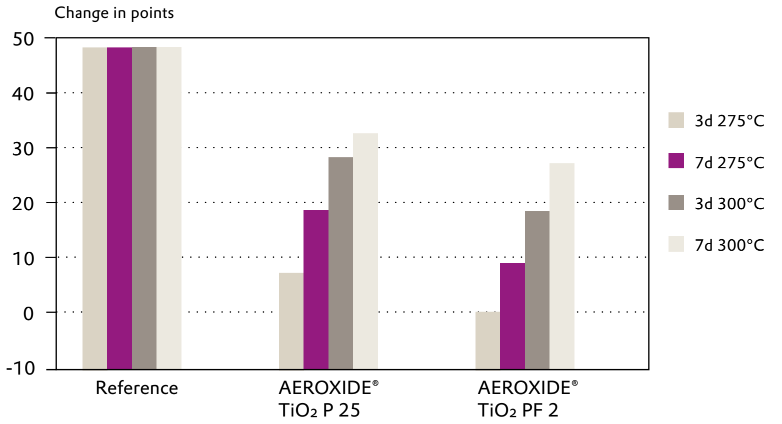
Figure 41 shows the change in ultimate elongation when HCR is stored at 275 °C without a thermal stabilization additive (reference) and with AEROXIDE® TiO_2 P 25 (1.5 %) and AEROXIDE® TiO_2 PF 2 (1.5 %). It can be seen that the reference decomposed strongly after just 24 hours and after three days no measurement was possible. The change in ultimate elongation when using AEROXIDE® TiO_2 PF 2 is less compared to the sample with AEROXIDE® TiO_2 P 25. This shows that AEROXIDE® TiO_2 PF 2 is more effective for the specific silicone and the specific temperature. When samples were stored for seven days at 275 °C, 50 % of the original ultimate elongation was maintained with the addition of 1.5% AEROXIDE® TiO_2 PF 2.

Figure 40



Change in ultimate elongation when HCR is stored at 275 °C without a thermal stabilization additive (reference) and with AEROXIDE® TiO_2 P 25 (1.5 %) and AEROXIDE® TiO_2 PF 2 (1.5 %).

Figure 41



Change in Shore-A hardness when LSR is stored at 275 °C and 300 °C without a thermal stabilization additive (reference) and with AEROXIDE® TiO_2 P 25 (5 %) and AEROXIDE® TiO_2 PF 2 (2 %).

The change in Shore-A hardness when LSR is stored at 275 °C and 300 °C without a thermal stabilization additive (reference) and with AEROXIDE® TiO_2 P 25 (5 %) and AEROXIDE® TiO_2 PF 2 (2 %) is shown in Figure 42. Here, too, it can be seen that AEROXIDE® TiO_2 PF 2 is most effective for the specific silicone and the specific temperature.

For users, it is important that the thermal stabilization agent does not have an adverse effect on the colorability of the finished product. This is illustrated in Figure 43: on the left, an HCR sample without a thermal stabilizing additive, in the middle with 1.5 % AEROXIDE® TiO_2 P 25, and on the right with 1.5 % AEROXIDE® TiO_2 PF 2. By using the two products to stabilize thermal aging, processors also have the possibility to color the silicone item specifically.

Figure 42

Samples without (left) and with a thermal stabilization additive (middle and right)

4.6.5 Other applications

Fumed titanium dioxide can be used as a starting material for the manufacture of lithium titanate (LTO, $Li_4Ti_5O_{12}$), an anode material in lithium-ion batteries (LIB). Some initial studies have also been conducted where pure TiO_2 (AEROXIDE® TiO_2 P 25) was used as an anode active material, as it can also reversibly give and take Li-ions.

Fumed titanium dioxide, especially AEROXIDE® TiO_2 P 25, is mentioned often in various scientific publications and other studies when basic catalytic reactions with titanium dioxide are being investigated. This model substance character can be attributed to the high specific surface area, the purity, and commercial availability.

You demand quality, and not just on paper?

Quality and Product Reliability

Quality control | Product reliability

5. Quality and Product Reliability

5.1 Quality control

All AEROSIL® and AEROXIDE® products worldwide are manufactured according to strict quality standards and Evonik goes to great lengths to ensure that this compliance is maintained. For example, all production sites are certified to the ISO 9001 quality management system, as are all research and application sites. Regular external and internal audits and constant systematic improvement of the quality of our products, services, and processes supports adherence to the high quality standards.

Every invoice recipient receives an certificate of analysis for the related product and a copy of the agreed product specification. Before products are released for dispatch to customers, tests are performed in the quality control lab of the production plant to ensure that the products comply with specification limits. All analyses data is stored.

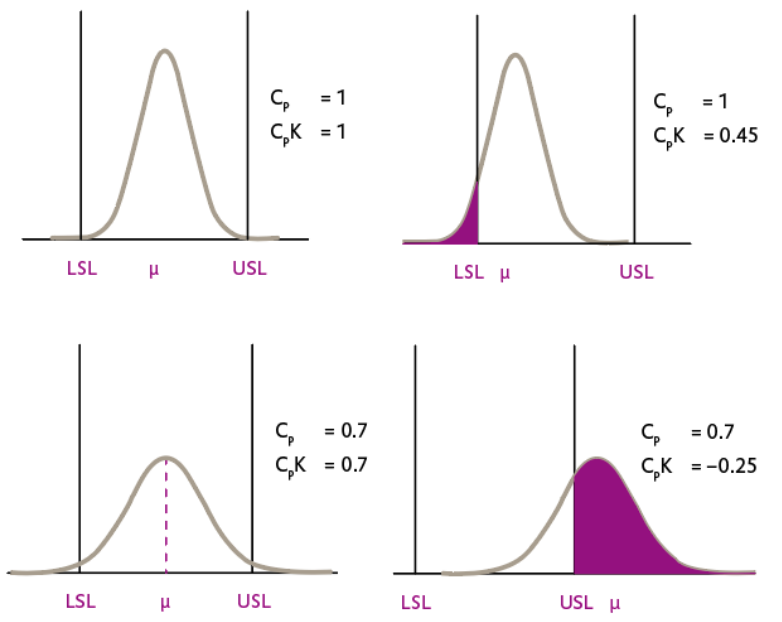
The data is also evaluated regularly as part of statistical quality control (SQC). This involves determining the mean average μ and standard deviation σ, in addition to the values for Cp and CpK. The process capability indices Cp and CpK are key figures that are used to statistically evaluate a process in production technology. They indicate how specified targets can be reached in accordance with the specification.

While the Cp value only indicates the relationship between the specified tolerance and the process distribution, the CpK value also includes the position of the mean value in relation to the specified tolerance midpoint. The CpK value is thus always smaller than or equal to the Cp value.

Figure 44 shows four distributions of measured values relative to the specification limits. The related Cp and CpK values are also shown.

In the simplest case, the aim is that all products achieve a Cp and CpK value of 1 or higher. This means that at least 99.73 % of the produced quantity meets the specifications in terms of the respective quality features. However, current requirements are higher than this, and CpK values of 1.33 or 1.67 are expected.

Figure 43



Examples of process capability indices. LSL = lower specification limit; USL= upper specification limit

5.2 Product reliability

Biological effects and occupational safety

The metal oxides Al_2O_3 and TiO_2 exhibit no toxicity after one-time oral ingestion. Al_2O_3 and TiO_2 have no irritating or sensitizing effects and are not genetically harmful. TiO_2 is also not toxic or sensitizing with UV radiation.

When experiments were carried out on rats, tumors formed when their lungs were overloaded (overload phenomenon), which, however, specialist scientists believe is species-specific. No similar effects have been found in humans to date. However, the International Agency for Research on Cancer (IARC) evaluated the rat studies as adequate proof for carcinogenicity in animal experiments. According to the IARC there is no adequate proof that titanium dioxide has a carcinogenic effect on humans. The overall assessment of titanium dioxide by the IARC led to "possibly carcinogenic to humans" (Group 2B).

As regards the other metal oxides, to date there has been no indication of potential risks for human health. In Germany, when the metal oxides are being processed, the general dust limits of 1.25 mg/m^3 for the respirable fraction and 10 mg/m^3 for the inhalable fraction must be observed. Other countries have defined dust limit values for metal oxides.

Fine powders can form electrostatic charges when they are being conveyed and processed. Therefore, suitable safety precautions must be taken, such as adequate grounding of the systems and using inert gas. Information about technical safety precautions and personal protective equipment can be found in the respective safety data sheets. The latest safety data sheets are automatically included with the first delivery.

Other metal oxides are assessed according to their composition. Information about safe handling can be found in the respective safety data sheet.

Our metal oxides are listed in the following chemical inventories:

Table 17
Listing of metal oxides in chemical inventories

		TiO_2	Al_2O_3
CAS no.		13463-67-7	1344-28-1
Australia	AICS (Australian Inventory of Chemical Substances)	registered	registered
Canada	DSL (Domestic Substance List)	registered	registered
China	IECSC (Inventory of Existing Chemical Substances)	registered	registered
Europe	EC (European Community)	236-675-5	215-691-6
Europe	REACH (Registration, Evaluation, Authorisation and Restrictions of Chemicals)	registered	registered
Europe	C&L inventory (classification and labelling inventory)	notified	notified
Japan	ENCS (Existing and New Chemical Substances)	registered	registered
Korea	KECI (Korea Existing Chemicals Inventory)	registered	registered
New Zealand	NZIoC (New Zealand Inventory of Chemicals)	registered	registered
Philippines	PICCS (Philippine Inventory of Chemicals and Chemical Substances)	registered	registered
Taiwan	CSNN (Chemical Substances Nomination and Notification)	registered	registered
USA	TSCA (Toxic Substances Control Act)	registered	registered

You are looking for international, reliable customer service that exceeds expectations?

Handling and Packaging

Handling AEROXIDE® products | Packaging for AEROXIDE® products | Storage of AEROXIDE® | Safety precautions | Worldwide availability

6. Handling and Packaging

6.1 Handling of AEROXIDE® products

Because there is increasing emphasis on automation, rationalization, and hygiene at work, handling of AEROXIDE® is of key importance. In this context, over the past decades, Evonik has continuously expanded its activities to protect employees and fulfill environmental standards.

Handling refers to the techniques required to move the products in the customer's plant.

The following can be considered focal points:

- Emptying containers
- Transferring to storage
- Internal transportation
- Metering
- Putting the material into the customer's processing machines

Handling also covers the measures required to perform the above steps:

- Filter technology
- Level measurement technology
- Weighing technology
- Discharge technology

Evonik endeavors to help customers plan new handling systems or resolve handling problems. Where business relationships already exist, Evonik provides the services described here throughout the world. The type and the scope of consultation depends on the customer's particular issue.

Evonik operates a technical handling center at Wolfgang Industrial Park in Hanau, Germany in which handling of AEROXIDE® is continuously optimized (see Figure 45). This technical center is available for customers for demonstrations and handling experiments. Most handling steps can be shown here. The handling department may also assist with trials at the customer's own premises in special cases.

Planning dust-free and automated systems requires knowledge of our products and experience in process engineering. As this combination of skills cannot always be provided by the machinery and equipment suppliers, our handling technicians and engineers consult and assist our customers personally – either at the Evonik site in Hanau or, if necessary, at the customer's premises. Where necessary, trials (such as trials for pneumatic dense phase conveying) may also be arranged at external pilot plants (e.g. at the plant manufacturer's factory).

In addition, basic information on handling the products has been published, for example in the brochure "Handling synthetic silicas and silicates" [18] and in a Technical Information series to address specific subjects.

Figure 44

The handling technical center of the Silica Business Line of Evonik Resource Efficiency in Hanau.

6.2 Packaging for AEROXIDE® products

Standard packaging
The standard package for AEROXIDE® is a multi-layer paper valve bag, which, in some cases, is equipped with a PE-coated liner. In a few cases, intermediate layers of PE film are used. Depending on the AEROXIDE® type and tamped density, the filled weight of the bags is between 10 kg and 20 kg.

Flexible Intermediate Bulk Container (FIBC)
Semi-bulk packaging is currently offered only for AEROXIDE® TiO_2 P 25. FIBCs (Flexible Intermediate Bulk Containers), which simplify handling large amounts, are used. These are flexible containers made from polypropylene fabric with loops on the corners to lift them. A discharge nozzle is in the middle of the base and can be connected to all conventional FIBC emptying stations. For the other AEROXIDE® products, we have no filling possibilities for large containers at present.

Packaging for AERODISP® dispersions

AERODISP® dispersions are delivered in 60 kg canisters, 220 kg drums, and 1000 kg Intermediate Bulk Containers (IBC). In the colder season, the containers are protected all over against the cold with metalized bubble wrap. The insulation packaging may vary depending on the type of containers and shipping. In winter, we also transport our AERODISP® dispersions in temperature-controlled trucks. In North America, Evonik does not use these protective hoods, but instead in winter every container has a freeze check indicator, which immediately shows an interruption of the transportation chain in heated trucks or containers. More details about handling of and packaging for AERODISP® products can be found in Technical Information 1278 [19].

6.3 Storage of AEROXIDE®

AEROXIDE® is largely chemically inert and with suitable storage conditions it will not change chemically even after decades. Because of the high surface area of AEROXIDE® there is a possibility of vapor and/or gas adsorption. In particular, interactions may occur with compounds containing amine or hydroxyl groups. With water, adsorption is reversible. Loss on drying of hydrophilic AEROXIDE® can increase with rising humidity and fall again as the humidity decreases. With hydrophobic AEROXIDE®, adsorption capability is significantly lower and moisture absorption much less. The described adsorption processes can have an effect on the application properties of the product. Therefore, it is recommended that AEROXIDE® always be stored away from sources of contamination.

The storage temperature should not exceed 50 °C. With typical tamped densities of 50 to 200 g/l, AEROXIDE® products have a packing factor of just 3 to 10 %. It cannot be ruled out that AEROXIDE® products compress when they are stored for a long time. This can increase the tamped density and change the structure.

Although, in principle, correctly stored AEROXIDE® can be considered as long-term storage-stable (no risk of aging or decomposition), we recommend that you use the products within two years of the production date. The production date is printed on the control number and on every certificate of analysis.

More information about storing AEROXIDE® can be found in Technical Information 1373 [20].

AERODISP® dispersions should be protected against heat and frost and should be used within 6 or 12 months after production. The production date is contained in the control number that is printed on every package.

6.4 Safety precautions

AEROXIDE® is a powder. If dust cannot be completely avoided during handling, an extraction system is recommended.

In the presence of high dust concentrations employees should wear a dust mask with particle filter (see safety data sheet).

When fumed metal oxides are being processed, electrostatic charges can occur when bags are being emptied, for example. Therefore, to eliminate any risks when handling the material, measures should be taken to prevent electrostatic charges, such as grounding and, if necessary, rendering the container inert. More information can be found in a special brochure [21].

The hydrophilic fumed metal oxides Al_2O_3 and TiO_2 are not flammable. Therefore, a dust explosion of the pure oxides is not to be expected.

However, with some surface-treated AEROXIDE® products, such as AEROXIDE® TiO_2 NKT 90, there is a risk of a dust explosion. Suitable safety precautions must be taken when these products are being handled. For more information, please refer to the safety data sheet and Technical Information 1363 [22]. There, you will find information about safety measures based on the safety characteristics.

To counteract the feeling of dryness when the material comes into contact with skin, the fumed metal oxides should be washed off with water and a moisturizer should then be applied to the skin.

Spilled material should be cleared away without raising dust and be collected in a suitable container.

6.5 Worldwide availability

With numerous production facilities for precipitated and fumed silica and metal oxides in Europe, the USA, Asia and more than 100 distribution offices worldwide, Evonik has a unique service and production network. This guarantees a very high level of delivery reliability and short delivery routes. The right product can be delivered to anywhere in the world in excellent quality.

Key:

- ● Applied Technology
- ● Innovation / R&D
- ● Sodium Silicate
- ● Production, Precipitated
- ● Production, Fumed

You would like more details on properties, references, and technical terms?

Annex

List: Physico-chemical characteristics
of fumed metal oxides | References | Glossary

7. Annex

7.1 List: Physico-chemical characteristics of fumed metal oxides

Table 18
Physico-chemical characteristics of hydrophilic fumed metal oxides. These are typical values and not specifications.

Test method	Unit	AEROXIDE® Alu 65	AEROXIDE® Alu C	AEROXIDE® Alu 130	AEROXIDE® TiO_2 P 25	AEROXIDE® TiO_2 P 90
Metal oxide type		Al_2O_3	Al_2O_3	Al_2O_3	TiO_2	TiO_2
BET specific surface area	m^2/g	55-75	85-115	110-150	35-65	70-110
pH 4 % dispersion		4.5-6.0	4.5-5.5	4.4-5.4	3.5-4.5	3.2-4.5
Loss on drying (2 h at 105 °C)	%	≤ 5.0	≤ 5.0	≤ 5.0	≤1.5	≤4.0
Tamped density	g/l	approx. 50	approx. 50	approx. 50	approx. 140	approx. 120
Screen oversize (according to Mocker 45 µm)	%	≤0.05	≤0.05	≤0.05	≤0.05	≤0.05

Table 19
Physico-chemical characteristics of hydrophilic fumed mixed oxides and oxide mixtures.
These are typical values and not specifications.

Test method	Unit	AEROSIL® COK 84	AEROSIL® MOX 80	AEROSIL® MOX 170	AEROSIL® MOX 170 V	VP* TiO_2 1580 S	VP* TiO_2 545 S	AEROXIDE® TiO_2 PF 2	VP* Alu 560 S	VP* Alu 590 S
Metal oxide type		SiO_2/Al_2O_3	SiO_2/Al_2O_3	SiO_2/Al_2O_3	SiO_2/Al_2O_3	TiO_2/SiO_2	TiO_2/SiO_2	TiO_2/Fe_2O_3	Al_2O_3/SiO_2	Al_2O_3/SiO_2
BET specific surface area	m^2/g	155-215	60-100	140-200	140-200	65-95	40-55	45-70	40-80	70-110
pH 4 % dispersion		3.6-4.3	3.6-4.5	3.6-4.5	3.6-4.5	3.0-4.5	3.5-4.5	3.5-4.5	4.5-6.5	4.5-6.5
Loss on drying (2 h at 105 °C)	%	≤1.5	≤1.5	≤1.5	≤ 1.5	n. a.	n. a.	≤2.0	n. a.	n. a.
Tamped density	g/l	approx. 50	approx. 60	approx. 50	approx. 130	approx. 60	approx. 100	approx. 80	approx. 50	approx. 40

*VP = Development product. Commercialization depends on feedback from the market.

Table 20

Physico-chemical characteristics of hydrophobic AEROXIDE® types. These are typical values and not specifications.

Test method	Unit	AEROXIDE® Alu C 805	AEROXIDE® TiO_2 T 805	VP* NKT 65	AEROXIDE® TiO_2 NKT 90	AEROXIDE® STX 501	AEROXIDE® STX 801
Metal oxide type		Al_2O_3	TiO_2	TiO_2	TiO_2	TiO_2	TiO_2
BET specific surface area	m^2/g	75-105	35-55	30-60	50-75	25-45	45-65
pH 4 % dispersion		3.0-4.5	3.0-4.0	3.0-7.0	3.0-4.0	6.0-9.5	6.0-9.0
Loss on drying (2 h at 105 °C)	%	≤ 2.0	≤1.0	≤1.0	≤1.0	≤1.0	≤1.0
C content	%	3.5-4.5	2.7-3.7	1.0-4.0	2.5-4.5	0.2-1.0	0.7-1.1
Tamped density	g/l	approx. 50	approx. 200	n.a.	n.a.	approx. 130	approx. 130

*VP = Development product. Commercialization depends on feedback from the market.

Table 21

Physico-chemical characteristics of AEROPERL® granulated fumed metal oxides. These are typical values and not specifications.

Test method	Unit	AEROPERL® 3375/20	VP AEROPERL® P 25/20	VP AEROPERL® TiO_2 545	VP AEROPERL® TiO_2 1580	VP AEROPERL® Alu 100/30	VP AEROPERL® Alu 560	VP AEROPERL® Alu 590
Metal oxide type		SiO_2/Al_2O_3	TiO_2	TiO_2/SiO_2	TiO_2/SiO_2	Al_2O_3	Al_2O_3/SiO_2	Al_2O_3/SiO_2
BET specific surface area	m^2/g	60-80	35-65	35-55	60-90	85-115	50-80	70-100
pH 4 % dispersion		3.5-6.5	3.0-4.5	3.0-4.5	3.0-4.5	4.0-6.0	4.0-6.0	4.0-6.0
Loss on drying (2 h at 105 °C)	%	≤ 2.0	≤ 2.5	≤ 2.5	≤ 2.5	≤ 2.5	≤ 2.5	≤ 2.5
Tamped density	g/l	approx. 600	approx. 700	approx. 600	approx. 550	approx. 500	approx. 575	approx. 500

*VP = Development product. Commercialization depends on feedback from the market.

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7.3 Glossary

A – F

Adsorption
A substance adhering to the inner and/or outer surface of a solid (as defined in DIN 28400).

Adsorption isotherms
Adsorption isotherms show the relation between the amount of substance adsorbed on the adsorbent and the concentration or partial pressure of the substance / gas being adsorbed in a state of equilibrium at a constant temperature.

AEROSIL®
Registered trademark of Evonik Industries AG or its subsidiaries for synthetic amorphous fumed silica that are manufactured according to the high-temperature hydrolysis method.

AERODISP®
Registered trademark of Evonik Industries AG or its subsidiaries for dispersions of fumed silica and fumed metal oxides (trade name AEROSIL® in aqueous or organic media, such as ethylene glycol).

AEROPERL®
Registered trademark of Evonik Industries AG or its subsidiaries for a spherical granulate made from AEROSIL® or metal oxides with high tamped density and consistently large surface area. The microgranulate displays good flow properties and low-dust handling.

AEROXIDE®
Registered trademark of Evonik Industries AG or its subsidiaries for fumed aluminum and titanium oxides produced using the high temperature hydrolysis method.

Affinity
When two elements or compounds join, the more heat that is released, the stronger their affinity (THOMSEN-BERTHELOT principle).

Agglomerates
Loose collections of aggregates that can be split up during dispersion (as defined in DIN 53 206).

Aggregates
As defined in DIN 53206, a merged group of particles positioned next to one another in one plane, with a surface smaller than the total surfaces of the → *primary particles.*

Amorphous
Shapeless, structureless, as opposed to → *crystalline.*

Anatase
Anatase is one of the three crystal modifications in which titanium dioxide occurs, the other two being → *rutile* and → *brookite.* It is a relatively commonly occurring mineral that crystallizes in the tetragonal crystal system.

Band gap
Energy-related distance between the valence band and the conduction band of a semiconductor.

BET
→ *Specific surface area* **B**runauer, **E**mmet, **T**eller, in: Journal of the American Chemical Society 60 (1938) p. 309.

BET method
Method to measure the specific surface area on the basis of gas adsorption.

Brookite
Brookite is one of the three crystal modifications in which titanium dioxide occurs, the other two being → *anatase* and → *rutile.* It is named after British mineralogist H. J. Brooke (1771–1857).

Catalysis, heterogeneous
In heterogeneous catalysis, the catalyst and educts or products are present in different phases (e.g. catalyst, solid – reacting substances, gaseous).

Chemisorption
A gas, liquid, or dissolved solid attaching or adhering to the surface of a solid or a liquid with a chemical bond being formed.

Chromatography
A physical separation technique in which material is distributed between a stationary and a mobile phase.

Coalescence
Separate colloidal particles merging (in this context, it refers to droplets merging in AEROSIL® particle genesis).

Coehn's rule
Rule named after Alfred Coehn for electrostatic charge through friction, according to which substances with higher permittivities are usually charged positively by friction.

Conduction band
Energy band of a semiconductor above the valence band that has no electrons. A semiconductor becomes electrically conductive when electrons from the valence band are excited into the conduction band.

Covalence, covalent bond
A covalent bond (also atomic bond) is a type of chemical bond responsible for holding atoms firmly together in molecular compounds.

Crystalline
A substance is crystalline if its components are arranged in regular crystal lattices. The opposite of → *amorphous.*

Disagglomeration
Method (usually mechanical) in which relatively loosely connected aggregates are broken up (for example during dispersion).

Desorption
A substance being separated or released from the inner and / or outer surface of a solid. The opposite of → *adsorption.*

Diffusion
The process of different gases, liquids, or solids being brought into contact and gradually mix together without external stimulus.

Dioctyl adipate
Abbreviated as DOA: according to DIN EN ISO 1043-3: 2000-01, dioctyl adipate/bis(2-ethylhexyl)-adipate is a plasticizer. A colorless liquid with barely any odor that belongs to the group of dicarboxylic acid esters (adipates), which is highly soluble in acetone, diethyl ester, and ethanol.

Dipole
A molecule with asymmetrically distributed charge.

Dipole-dipole interaction
Forces that act as the result of dipoles being present.

Dispersing
Using dispersion machines to evenly distribute powdered substances in liquids.

Dispersion
From the Latin dispersio (scatter). As defined in DIN EN ISO 862:1995-10, a system (a disperse system) consisting of several phases, with one continuous phase (the dispersing agent or dispersant) and at least one finely distributed phase (the dispersed phase). Example of dispersions: emulsions (immiscible liquid phases), aerosols, suspensions. Forms of energy that can be used to form a dispersion include chemical, electrochemical, electrical, and mechanical energy.

Dissolver
Dissolvers are used to disperse substances, usually in liquids. The dissolver provides the energy required for → *disagglomeration.*

Doping
In semiconductor production, doping is the standard term for intentionally contaminating extremely pure germanium and silicon crystals by adding minute amounts of foreign material.

Educt
The starting material in a chemical reaction.

Flame hydrolysis
Reaction of, for example, silicon tetrachloride with the water that forms in the oxyhydrogen flame.

Fumed
Produced in a flame.

H–S

Handling
Measures and practices implemented to produce specific operating procedures, particularly those involving powdered raw materials, in compliance with regulatory guidelines and limit values.

Highly dispersed
Finely distributed.

High temperature form
→ *Modification* that is formed preferentially at higher temperatures.

Homogeneous
Of the same kind, consisting of the same substance.

Hydrolysis
Cleaving a chemical compound by reacting it with water.

Hydrophilic
Attracted to or able to be wetted by water. The opposite of → *hydrophobic.*

Hydrophobic
Water-repellent. The opposite of → *hydrophilic.*

Inert
Inactive, not chemically reactive.

Inerting
Turning substances into chemically inactive (inert) compounds.

Infrared (IR) spectroscopy
An optical procedure that uses the absorption spectra of mainly organic solid, liquid, or gaseous compounds in the infrared range for qualitative or quantitative analysis, to determine the structure, etc.

Irreversible
A chemical reaction that cannot be reversed, → *reversible.*

Lewis acid
Electron-pair acceptor, in other words, a molecule or ion to which a free electron-pair from another particle can attach.

Lewis base
Electron-pair donor, in other words, a molecule or ion that is able to provide a free electron-pair to another particle.

Macropores
IUPAC defines macropores as pores in a solid with diameters > 50 nm. → *micropores* <2 nm and → *mesopores* between 2 and 50 nm.

Mesopores
IUPAC defines mesopores as pores in a solid with pore diameters in range of 2-50 nm. → *micropores* < 2 nm and → *macropores* > 50 nm.

Metastable
A state between stable and unstable. A metastable state is stable with regard to minor changes but unstable with regard to larger charges.

Micropores
IUPAC defines micropores as pores in a solid with a pore diameter in the < 2 nm range. → *mesopores* 2-50 nm and → *macropores* > 50 nm.

Microporous (paper industry)
As opposed to the general definition of micropores as pores < 2 nm, in the paper industry, the term microporous is used for paper coatings – e.g. silica-based color-receiving layers for water-based inks – with pores in the micrometer range.

Modification
Various states of chemical elements or compounds with different physical properties despite having the same composition.

Morphology
Study of the origin and development of shapes and forms.

Nanometer
One millionth of a millimeter = 1 nm.

Oxyhydrogen reaction
Gaseous hydrogen (H_2) reacting with oxygen (O_2) in which water is produced as a reaction product. The conversion (detonation) normally produces a loud bang.

Pascal second
Unit of dynamic viscosity [Pa*s].

Paste-like
Of a liquid, (highly) viscous.

Phases
Here: the various crystal forms in which a pure chemical substance can occur.

Photocatalysis
A chemical reaction in which a catalyst is activated by light.

Primary particles
As defined in DIN 53206, the smallest particle (individual particle) that a powdered solid can consist of. Such a particle can be recognized as an individual unit under an electron microscope. Primary particles of fumed or precipitated silica or metal oxides never occur isolated but always are fused together tightly to aggregates and agglomerates.

PU
Abbreviation for Polyurethane.

Reversible
Reversible chemical reaction. The opposite of → *irreversible.*

Rheology
The study of flow. A branch of physics concerned with describing, explaining, and measuring the phenomena that occur as bodies deform in flow.

Rotor-stator device
A device used to break up a pigment or a filler material, consisting of an outer stationary ring and an inner concentric rotating ring. Both rings have openings (holes or slits) that the liquid has to pass through under a high shear load.

RTV
Room Temperature Vulcanization.

Rutile
Rutile is one of the three crystal modifications in which titanium dioxide occurs, the other two being → *anatase* and brookite. It is a relatively commonly occurring mineral that crystallizes in the tetragonal crystal system.

Sedimentation
Settling behavior.

SEM image
Abbreviation for Scanning Electron Microscope image.

Silanes
In the stricter sense, silanes are binary compounds of silicon with hydrogen, with the general formula $S_{in}H_{2n+2}$. They are thus the Si equivalents of alkanes. The term silane is also used more broadly, to refer to derivatives in which some or all of the hydrogen atoms are replaced by other groups.

Silanol groups
Surface-resident groups on the silica surface with the formula ≡ Si-OH.

Silicone rubber
Highly viscous silicone oils that can be cured with peroxides or by other principles to form elastomers. The basic polymer for silicone rubber is dimethylpolysiloxane.

Silica
Collective term for compounds with the chemical formula SiO_2. We distinguish between → *fumed*, e.g. → *AEROSIL®*, and → *precipitated silica.* The different forms of silica differ in their physico-chemical properties, such as the size of the → *specific surface area*, the size of the particles, the loss on drying, or loss on ignition. → *silica gel,* → *electric arc silica.*

Siloxane groups
Si-O-Si units produced by the condensation of → *silanol groups.*

Sintering
Sintering involves compacting individual solid particles (such as primary particles, aggregates, etc.) at high temperatures. The sintering process is performed below the melting temperature, so no actual melting takes place. The solid particles gain a certain degree of plasticity that allows them to be firmly joined after they have collided without merging completely (for example, as droplets would).

Sinter neck
The connection point between two or more particles, created during the sintering process.

Specific surface area
As defined in DIN 66131, the surface area of a solid in relation to its mass, measured in m^2 / g. It is generally measured on the basis of the → *BET method* (Brunauer, Emmett, Teller, in: Journal of the American Chemical Society 60 (1938) p. 309).

S–Z

Structure modification
A method to alter the structure (generally breaking down the structure) of fumed metal oxides. The microscopic 3D network of aggregates and agglomerates is changed to create products with new properties. The main characteristics of these products are a reduced thickening effect and increased tamped density.

Surface functionality
Functional (organic) group that can be accessed from the outside, which is found on the surface of particles.

TEM image
Abbreviation for Transmission Electron Microscope image.

Tamped density
ISO 787-11 defines tamped density as a measured variable that describes the amount of volume lost by a powdered solid when it is shaken or packed down firmly.

Tetrahedron
A solid with four faces, all of which are equilateral triangles.

Thixotropy
The extent to which a liquid's → viscosity decreases in relation to the shear intensity and shear duration and returns to its original state when the shear stress has been removed.

Toxicology
The study of substances that are harmful and, in some cases fatal, in excess doses.

Triboelectricity
Static electricity. The generation of voltage when two different isolators become electrically charged with opposite polarities when they are rubbed together. Often characterized as a quotient of charge per mass.

UP
Abbreviation for unsaturated polyester resins.

Valence band
The highest energy band of a semiconductor with electrons. Above the valence band is the conduction band, separated by the band gap.

Van der Waals forces
Named after Johannes Diderik van der Waals. Intermolecular forces that occur as weak bonding forces between inert atoms and saturated molecules, mainly in real gases but also in liquids and in solids.

Viscosity
DIN 13342 defines viscosity as substance's ability to absorb a shear stress that is dependent on the shear rate through shear deformation.

X-ray analysis
Physical technique for chemical analysis, where the sample is exposed to → *X-rays.*

X-ray diffraction
Technique for analyzing crystal structure, where → *X-rays* are diffracted by the electrons of lattice atoms. Superposing the diffraction waves produces regular → *diffraction rings.*

X-rays
Short-wave electromagnetic radiation, with a wavelength of approximately 10-6 to 10-12 cm.

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