Basics in Chemistry

Materials, Mixtures, Elements, Atoms, Compounds

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Chemistry – Definition

Chemistry is the Science of material properties and their interactions

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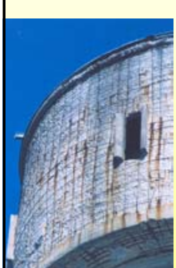
Tasks for a Chemist in Construction Industry



- Product Development
- Development of New Technologies
- Analysis of Damages
- Quality Control

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Material properties

1. Odour
2. Taste
3. .....
4. Thermal conductivity
5. Electrical conductivity
6. Density
7. Solubility
8. ....

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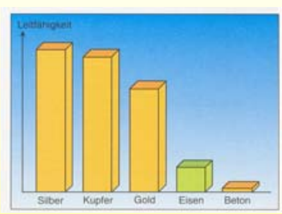
Electrical Conductivity



Electrical conductivity is decisive for the rate of corrosion of the reinforcement.

$$\sigma = \frac{1}{\rho}\left[\frac{1}{\Omega \cdot m}\right]$$

Electrical conductivity is the reciprocal value of the electrical resistance

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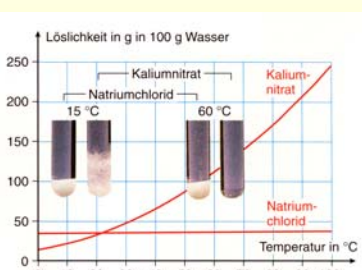
Solubility

$$\text{Solubility} = \frac{\text{Mass of material}}{\text{Volume Solvent}}$$



$$L = \frac{m}{V}\left[\frac{kg}{m^3}\right]$$

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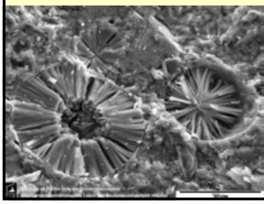
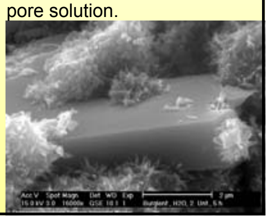
Solubility – in practice

Example: **Ettringite formation**
In hardened cement paste insoluble ettringite is formed in the presence of sulphate which precipitates in the pores.



Example: **Alkaline depot**
During the cement hydration calcium hydroxide is formed. Only a small amount of $Ca(OH)_2$ is dissolved in the pore solution.



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Materials

Definition: **Materials**
It`s a kind of substance and a uniform shape of matter.

Example: Iron

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Material – in Practice

Example: **Styropor (polystyrene)**
Styropor is a polymer formed by polymerisation of monomers

Element

Mercury (Hg)

Definition: **Element**
An element is a material, which can not be separated by chemical techniques.

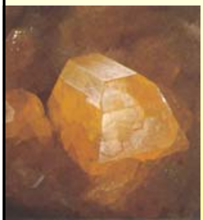
The Periodicity of Elements

DÖBEREINER-*TRIPPLES* (1816)
Formulation of Tripples (similar properties), dependence to atom mass
NEWLAND – *OKTAVES* (1865)
Arrangement of elements which are similar in chemical behaviour and by increasing atom mass.
MEYER und MENDELJEWS - *„PSE“*
(1868 alternatively 1869)
Arrangement of elements by atom mass and density (Meyer) and similar chemical behaviour (Mendeljew), forecast of later found elements.

The Periodic Table of Elements

Alkaline metals : melting point Li=168 °C ➔ Cs=29°C
Noble gas: very inactive regarding reactivity
Metals:Ti, V, Cr, **semi-conductors**: Si, Ge, As, ...

Elements



Sulphur (S)

Today 112 elements are known,
91 elements can be found in nature

Each element is named and characterised by a symbol
Ca = Calcium
Si = Silicon
O = Oxygen
C = Carbon
...

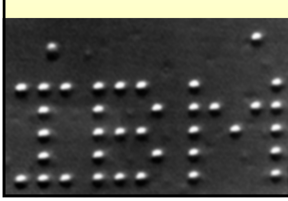
Structure of Matter – Element

Silicon
Semi-conductors: 1 Atom per 10^9 Atoms

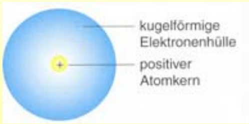
Definition: **Element**
A chemical element is build-up by atoms with the same chemical properties.

Structure of Matter – Atom

Definition: **Atom**
An atom is the smallest part of an element having all chemical properties of the element.

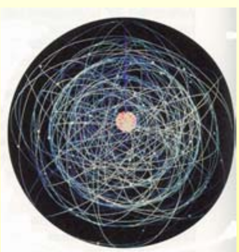


Structure of Atoms



An atom is build-up by a positive core and a ball-shaped electron sheath.
The diameter of the atomic core is $1 \cdot 10^{-15}$m (Femtometer)
The diameter of an atom is approx. $100\text{-}400 \cdot 10^{-15}$m (Picometer)

The structure of an Atomic Core

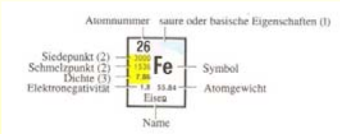


The atomic core is build-up by positive charged **protons** and non-charged **neutrons**.
The mass of the atom (99.8%) is located in the atomic core.
The atomic core is surrounded by negative charged **electrons**.

The Periodic Table of Elements

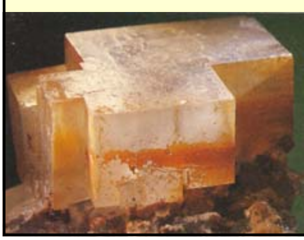
Alkaline metals: Melting point Li=168 °C ➔ Cs=29°C
Noble gas: Very inactive regarding reactivity
Metals: Ti, V, Cr, **semi-conductors**: Si, Ge, As, ...

The Structure of the Atomic Core



- The atomic core of elements differ in their number of protons. The amount of protons is called atomic number which defines the position of the element in the periodic table of elements.
- The amount of protons is also the amount of electrons.
- The amount of neutrons can vary in elements. Elements with different amount of neutrons are called isotopes.

Chemical Compound



Definition: **Compound**
A compound is made of different elements which were bond together. These Compounds can be decomposed in their elements by chemical techniques.

Chemical Compounds in practice

Example: **Polymer tube**
Due to a chemical reaction, the so called polymerisation, monomers build up polymers.

Chemical Compound


Ion bond


Molecular bond


Metal bond

Ion bond

Reaction of Chlorine with Sodium

Sodium reacts with chlorine gas under heat release. Thereby a crystalline compound called sodium chloride is formed.

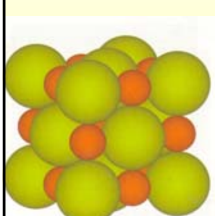
 +  ➔ 

Sodium + **Chlorine** ➔ **Sodium chloride**

Na + **Cl** ➔ **NaCl**

Formation of Sodium Chloride

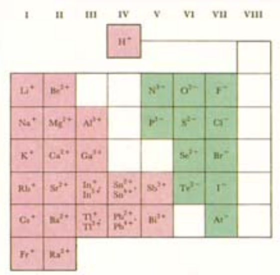
$$Na + Cl \rightarrow Na^{+} + Cl^{-}$$


Natriumchlorid: NaCl (s)

As a result of the **EMITATION** of electrons **POSITIVE** sodium ions are formed (***Cation***)
und
As a result of the **uptake** of electrons **NEGATIVE** Chloride ions are formed (***Anion***)

Cation or Anion ?

The „PTE“ shows, if an element is an anion or cation in an ionic compound.



Some elements (Fe, Cr, Cu,..) can form more than one ion

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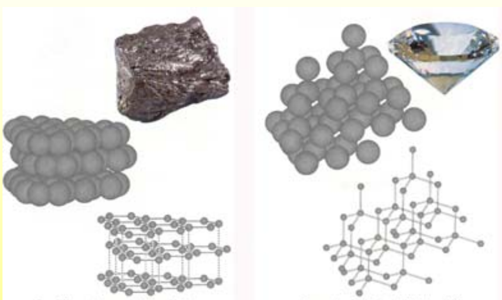
Crystal structure and materials properties



Graphit – schwarzer Kohlenstoff *Diamant – funkelnder Kohlenstoff*

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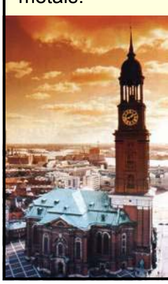
Metal bond

Most of all elements are metals. More than 50% of the main group elements of the PSE and all **transition elements** are metals!



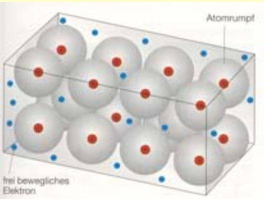
Properties of Metals

- Thermal and electrical conductivity
- Ductility
- Metallic luster

Electron Gas-Model

Electrical conductivity: Transport of electrons by the action of an electric current.

Heat transfer: Heat is transformed to kinetic energy.



Ductility:
The cation layers are moved by mechanical stress.

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Molecular Bond

Most of all chemical compounds are characterised by material properties which are quite different to the properties of ionic or metallic compounds.

Material properties

- Gas, liquid or solid
- High vapour pressure
- Ductile deformable

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The Covalent Bonding

The covalent bond is formed by an electron pair, which is participated by two atoms (Lewis, 1916)

According to LEWIS an electron pair is located between the atomic core and attracts the atomic core which leads to the bond of the atoms.

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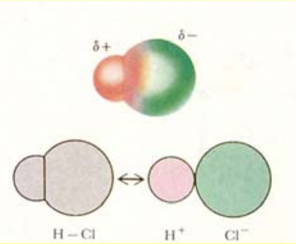
The Electric Dipole

An electric dipole is characterised by a positive charge which is located next to a negative charge with the same value.



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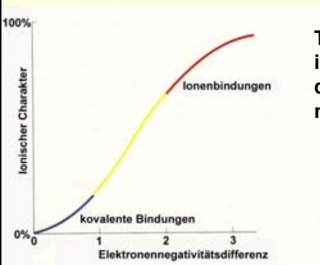
The Dipole Character of a Molecule



The polarity of bonds increases with the rising difference in the electro negativity of the elements.

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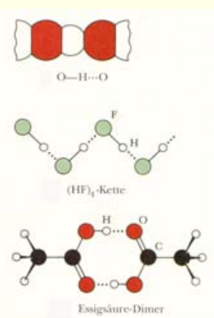
Hydrogen-Bond



Experimental Results:
H_2O boils at 100 C, H_2S boils at – 60 C°. The reason for that is the formation of hydrogen-bonds.

Hydrogen-bonds are formed by hydrogen atoms located between two atoms with high electro negativity.

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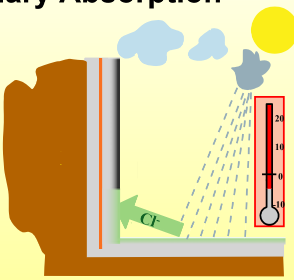
Transport of Aggressive Chemicals by Capillary Absorption



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Liquids

Three forms of water are important in construction:

- Fluid
- Vapour
- Ice

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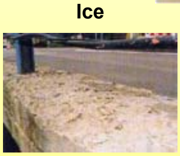
Impacts of Water in Construction

Water may damage material in all this physical conditions:

Fluid

Ice



Vapour

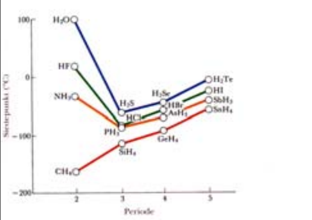
Hydrogen Bond

In the strong hydrogen Bonds the relevant characteristics for construction are founded:

-Water vapour ➔ High boiling point

-Water ➔ Dissolving power for salts

-Ice ➔ Volume Increase while freezing



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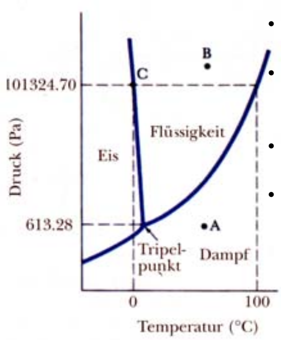
Chemistry of water – Anomaly of water



- **Melting point curve has a negative gradient („Vats“)**
- **Ice (0.916 g/cm³) has a lower density than water (0.999 g/cm³)**
- **The highest density of water is at 4 °C, not at 0 °C**
- **Volume of ice is 9-10% in excess of water**

➔ Freezing of watercourses

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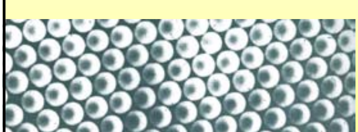
Properties of fluids – Surface tension

- **Fluids tend to minimize their surface.**
- **This State is reached by a Sphere (largest Volume with lowest Surface)**

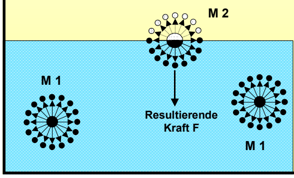
➔Gravitation is the cause of water drops being not spherically



Chemistry of water – Surface Tension

- Fluids aspire to minimum surfaces (sphere)
- Inside the fluid act cohesion forces in all directions
- At the surface there is a force directed inside

$$SurfaceTension\,\sigma = \frac{\Delta E}{A}\,in\,N/m$$



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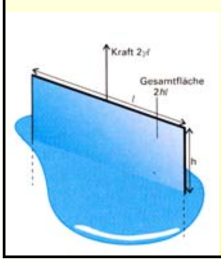
Chemistry of Water – Surface Tension

Altering Surface for an infinitesimal amount *d*A requires the Work *d*w.



$$dw = \sigma \cdot dA$$

Factor of Proportionality σ is Surface Tension

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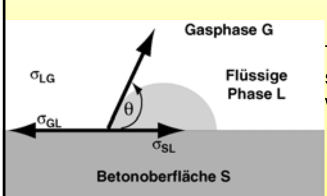
Wetting of Surfaces

Wetting of surfaces of SOLIDS caused by FLUIDS depends on the INTENSITY of the cohesion forces (Ion-Ion- or Ion-Dipole-Interaction)



The degree of wet-ability of a surface is the contact- or wetting-Angle

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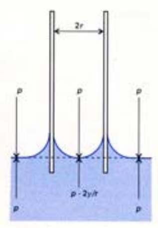
Capillary Absorption

Stands a capillary in a wetting Fluid a hunched down fluid surface is formed. From the Laplace-Equation a negative pressure p above the surface is received.



$$p_{Laplace} = p_{Atmosphäre} - \frac{2\sigma}{r}$$

Capillary-internal-pressure $p_{Laplace}$

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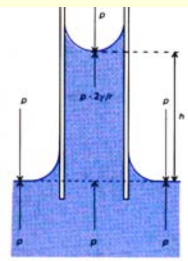
Capillary Absorption

The capillary negative pressure $p_{Laplace}$ the weight force p_{weight} is opposed. The climb-altitude of the fluid results from their effort to build an equilibrium.



Capillary negative pressure $p_{Laplace}$

$$p_{Laplace} = p_{Atmosphäre} - \frac{2\sigma}{r}$$

Weight-Force p_{Weight}

$$p_{Weight} = \rho \cdot \pi \cdot r^2 \, h \cdot g$$

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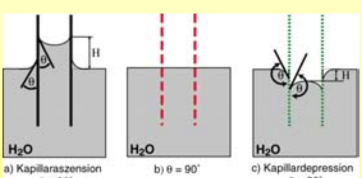
Capillary Absorption

Adhesion forces between Water and surface of the capillary is leading to ascension of the fluid
Hydrophilic = water-liking,
Hydrophobic = water-repellent

Calculation of Altitude h: $$h = \frac{2\sigma}{\rho \cdot g \cdot r} \quad in\ m$$



Impact:
Climbing moisture in masonry

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Important Reactions

- Acid-base-reaction
- Precipitation-reaction
- Reduction-oxidation-reaction

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Acid-Base-Reaction - Definitions

There are numerous definitions for acids and bases

- Arrhenius ➔ 1887 „Chemische Theorie der Elektrolythe", (Chemical Theory of Electrolytes)
- Brönsted ➔ 1923 Brönsted independent of Th. Lowry
- Lewis ➔ 1938 Base has a free pair of electrons, acid is able to accept a free pair of electrons $Cu^{2+} + 4\,NH_3 \rightarrow [Cu(NH_3)_4]^{2+}$

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Acid-Base-Reactions – Definition of Arrhenius

Arrhenius defines acids containing hydrogenatoms and emitting them as H^+-Ions
bases are defined to be able to release in aqueous solution OH^- -Ions.

•Example:
•CO_2 in H_2O ➔ „H_2CO_3" ➔ Acid
•$Ca(OH)_2$ in H_2O ➔ Base

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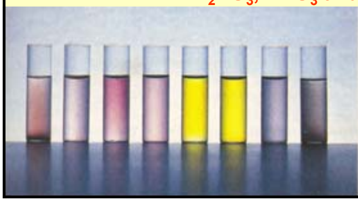
Important Arrhenius-Acids and -Bases

Hydrochloric acid (HCl) and nitric acid (HNO_3) are an organic acids.
Acetic acid (CH_3COOH) is an organic acid.

Important acids for construction:
H_2CO_3, HNO_3 and H_2SO_4



CH_4 (Methane) is no Acid

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Acid-Base-Reactions - Neutralisation

Neutralisation is a reaction between acid and base under formation of salt and water

$$HCl + NaOH \rightarrow NaCl + H_2O$$

Bases are defined to be able to release OH^--Ions.

A neutralisation-reaction is often associated with a Precipitation Reaction.

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Acid-Base-Reactions – Neutralisation Reactions between cement based materials and acid

Reaction between acid (HNO_3) and base (cement stone and calcium hydroxide) under formation of salts and water.

Acid-base-reactions according to Arrhenius

ACID: $HCl \rightarrow H^+ + Cl^-$
BASE: $Ca(OH)_2 \rightarrow Ca^{2+} + 2OH^-$

➔ $NH_3 + H_2O \rightarrow NH_4^+ + OH^-$ (?)

➔ BRÖNSTED-Definition for acids and bases

Acids and Bases according to BRÖNSTED

1923 Brönsted and Lowry suggested the following Definitions:
Acids are PROTON-DONOR („Contributor“)
Bases are PROTON-ACCEPTOR

Typical Representatives of BRÖNSTED-Acids and -Bases

ACID: $HCl + H_2O \rightarrow H_3O^+ + Cl^-$ (Dissociation)
H_2O is a Proton-Acceptor ➔ H_3O^+ (BASE)
HCl is a Proton-Donor ➔ Cl^- (ACID)

BASE: $Ca(OH)_2 \rightarrow Ca^{2+} + 2OH^-$
$OH^- + H_3O^+ \rightarrow 2\ H_2O$ „Proton-Acceptor“

CaO:
➔ $O^{2-} + H_2O \rightarrow 2\ OH^-$ „Proton-Acceptor“
➔ $NH_3 + H_2O \rightarrow NH_4^+ + OH^-$ „Proton-Acceptor“

The Ionic-Product of Water

$H_2O + H_2O \Leftrightarrow H_3O^+ + OH^-$

H_2O is simultaneously Brönsted-acid and - Base

The equilibrium-reaction is called AUTOPROTOLYSE:

$$k = \frac{[H_3O^+]\cdot[OH^-]}{[H_2O]^2}$$

1 Litre water is approximately equivalent 55 mol/l and is scarcely changed by autoprotolyse

$$k_W = [H_3O^+]\cdot[OH^-]$$

K_w= Ionic-product of water

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The Ionic-Product of Water

$H_2O + H_2O \Leftrightarrow H_3O^+ + OH^-$

$$k_W = [H_3O^+]\cdot[OH^-]$$

$$10^{-14} = 10^{-7}\cdot 10^{-7}$$

The Ionic-product of water is independent from the Concentration of the several Ions

$[H_3O^+]$ >> ➔ $[OH^-]$ <<

$[H_3O^+]$ << ➔ $[OH^-]$ >>

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Concentration of H_3O^+ -Ions – the pH-Value

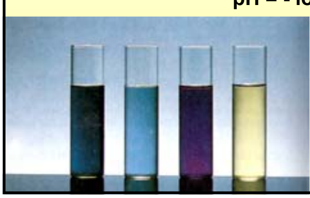
$H_2O + H_2O \Leftrightarrow H_3O^+ + OH^-$

The H_3O^+-Concentrations diversify over a large spectrum:

$[H_3O^+]$ ... 10^{-2} .... 10^{-12}

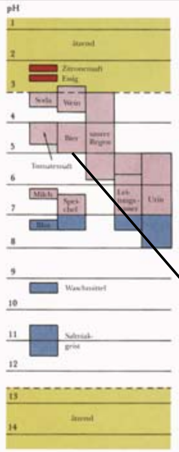
Definition of the pH-Value:

$pH = -\log [H_3O^+]$



Sörensen defined the pH-Scale (Brewing)

sruhe
schaft



pH-Value of Everyday-Life-Materials

Sörensen defined the pH-Scale (Brewing)

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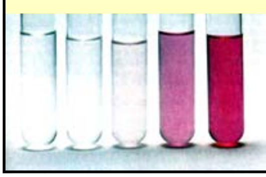
Measurement of pH-Value

Measurement of pH-Value may take place by several Methods:
•Potentiometric Measuring Methods
•Fluid Indicators

Phenolphthalein



pH-Meter

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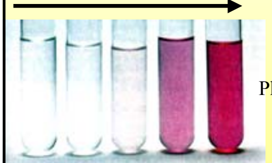
Measurement of pH-Value – Fluid Indicators

Fluid Indicators are organic compounds, whose colour in Solution are pH-Value dependent.

For Example Phenolphthalein, Bromthymolblau or Methylorange

pH-Wert

7.0 → 9.5



Phenolphthalein

Typical Fluid Indicators

Indikator	Farbe der sauren Form	pH-Bereich des Farbumschlags	pK_{In}	Farbe der basischen Form
Thymolblau	rot	1.2 bis 2.8	1.7	gelb
Methylorange	rot	3.2 bis 4.4	3.4	gelb
Bromphenolblau	gelb	3.0 bis 4.6	3.9	blau
Bromkresolgrün	gelb	3.8 bis 5.4	4.7	blau
Methylrot	rot	4.8 bis 6.0	5.0	gelb
Bromthymolblau	gelb	6.0 bis 7.6	7.1	blau
Lackmus	rot	5.0 bis 8.0	6.5	blau
Phenolrot	gelb	6.6 bis 8.0	7.9	rot
Thymolblau	gelb	8.0 bis 9.6	8.9	blau
Phenolphthalein	farblos	8.2 bis 10.0	9.4	pink
Alizaringelb R	gelb	10.1 bis 12.0	11.2	rot
Alizarin	rot	11.0 bis 12.4	11.7	violett

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Analysis of concrete-corrosive Water

Grenzwerte für die chemischen Merkmale der Expositionsklassen XA1–XA3 nach DIN EN 206-1

Chemisches Merkmal	Referenzprüfverfahren	XA1	XA2	XA3
Grundwasser				
SO_4^{2-} mg/l in Wasser	EN 196-2	≥ 200 und ≤ 600	> 600 und ≤ 3000	> 3000 und ≤ 6000
pH-Wert	ISO 4316	≤ 6,5 und ≥ 5,5	< 5,5 und ≥ 4,5	< 4,5 und ≥ 4,0
CO_2 mg/l angreifend	PrEN 13577	≥ 15 und ≤ 40	> 40 und ≤ 100	> 100 bis zur Sättigung
NH_4^+ mg/l	ISO 7150-1 oder ISO 7150-2	≥ 15 und ≤ 30	> 30 und ≤ 60	> 60 und ≤ 100
Mg^{2+} mg/l	ISO 7980	≥ 300 und ≤ 1000	> 1000 und ≤ 3000	> 3000 bis zur Sättigung
Boden				
SO_4^{2-} mg/kg insgesamt [1]	EN 196-2 [2]	≥ 2000 und ≤ 3000 [3]	> 3000 [3] und ≤ 12.000	> 12.000 und ≤ 24.000
Säuregrad in ml/kg	DIN 4030-2	> 200 Baumann-Gully	in der Praxis nicht anzutreffen	

[1] Tonböden mit einer Durchlässigkeit von weniger als 10^{-5} m/s dürfen in eine niedrigere Klasse eingestuft werden.

[2] Das Prüfverfahren beschreibt die Auslaugung von SO_4^{2-} durch Salzsäure; Wasserauslaugung darf statt dessen angewandt werden, wenn am Ort der Verwendung des Betons Erfahrung hierfür vorhanden ist.

[3] Falls die Gefahr der Anhäufung von Sulfationen im Beton – zurückzuführen auf wechselndes Trocknen und Durchfeuchten oder kapillares Saugen – besteht, ist der Grenzwert von 3000 mg/kg auf 2000 mg/kg zu vermindern.

DIN EN 206-1 allows analysis of Concrete-corrosive Water at Construction site.

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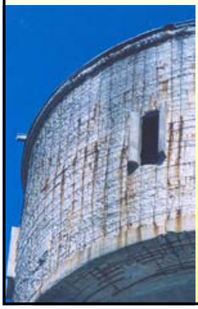
Carbonation of reinforced Concrete



A short historic Abstract

- **1879 Cement-Coating anticipates Rust**
- **1908 Perception, that alkaline environment anticipates Corrosion**
- **1916 „Corrosion for safety reasons of highest interest“**
- **1919 1.5 cm Concrete-Coating should be enough to prevent Reinforcement Corrosion**

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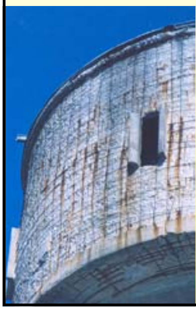
Carbonation of reinforced concrete

The reaction of the CSH-phases with CO_2 is called CARBONATION



The $Ca(OH)_2$ (approx. 20 mass-%) which is build up by the hydration of cement and KOH & NaOH in the pore solution are responsible for the pH of approx. 12.3 to 13 of the concrete.

$$Ca(OH)_2 + CO_2 + H_2O \rightarrow CaCO_3 + 2\,H_2O$$

Reasons for damages by carbonation

- Low cement content
- Minor dimension of cover concrete
- CO_2-content of the air
- Additional pollutants (NO, NO_2, NO_3)
- Insufficient manufacture of th concrete

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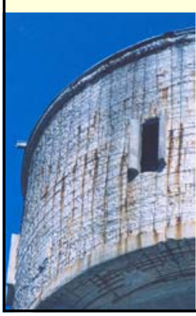
Reaction steps of the carbonation

Carbonation is a coupled process:
Transport & chemical reaction



1. Diffusion of CO_2 into the cement rock

2. Solution of CO_2 in the pore solution
$CO_2 + H_2O \rightarrow H_2CO_3 \rightarrow 2\,H^+ + CO_3^{2-}$

3. Reaction of $Ca(OH)_2$ with H_2CO_3
$Ca(OH)_2 + H_2CO_3 \rightarrow CaCO_3 + 2\,H_2O$
Carbonation of the alkaline hydroxides
$2\,NaOH + CO_2 \rightarrow Na_2CO_3 + H_2O$
$Na_2CO_3 + Ca(OH)_2 \rightarrow CaCO_3 + 2NaOH$

4. Decomposition of cement rock
$C_xSH_y + xCO_2 \rightarrow xCaCO_3 + SiO_2 \cdot y\,H_2O$

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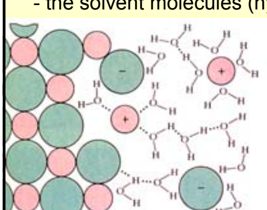
Solubility

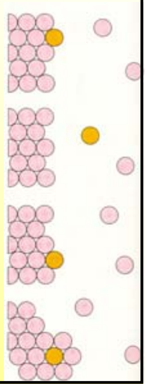
During a dissolution process, we there is a competition regarding the formation of bonding between
- the bonding between the solid phase molecules.
- the solvent and the molecules of the solid phase (hydrogen bonding)
- the solvent molecules (hydrogen bonding)



Saturation and Solubility

In a saturated solution a dynamic equilibrium exists between dissolved matter an a solid phase. The **Solubility** is the concentration of a saturated solution.

Verification:
AgI ➔ ^{127}I and ^{131}I
Detection of radioactivity



Consequences of Carbonation

The CARBONATION has positive and negative effects on reinforced concrete.

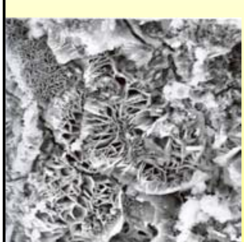
POSITIVE:
Increase of density of the structure of the concrete (ΔV=11%)

NEGATIVE:
Disintegration of the passivation layer (approx. 50 nm) consisting of Iron oxides – and hydroxides on the steel surface
➔ Steel corrosion

Corrosion of the reinforcement

Conditions for the steel corrosion

- **Presence of electrolytes**
- **„Break down“ of the passivation layer**
- **Sufficient amount of oxygen**
- **Formation of von local spots of corrosion**



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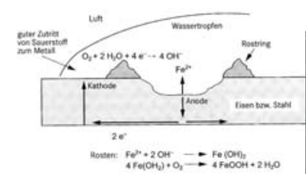
Mechanisms of the corrosion of the reinforcement

The corrosion of the reinforcement is an electrochemical process

Electrochemical reaction steps:

Anode:	$2\,Fe \rightarrow 2\,Fe^{2+} + 4\,e^-$
Cathode:	$O_2 + 2\,H_2O + 4e^- \rightarrow 4\,OH^-$
Reaction:	$2\,Fe + O_2 + H_2O \rightarrow 2\,Fe(OH)_2$
Further reaction:	$4\,Fe(OH)_2 + O2 \rightarrow 4\,FeOOH + 2\,H_2O$



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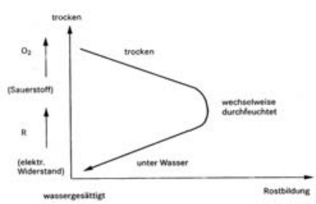
Corrosion of the reinforcement – important factors

The following factors take influence on the corrosion of the reinforcement:

- **Amount of oxygen (quality of the concrete, humidity)**
- **Electrical resistance (humidity, salts)**
- **...**



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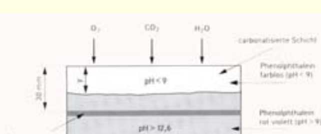
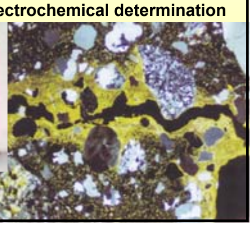
Determination of the depth of Carbonation



Carbonation depth can be measured by ...

- **Liquid indicators**
- **Microscopy**
- **Wet chemical measurement**
- **Electrochemical determination**



Calculation of carbonation depth

Carbonation is a diffusion controlled process:

1. Fick's law

$$\frac{dm}{dt} = D \cdot F \cdot \frac{dc}{dy}$$

Mass balance

$$dm = m_0 \cdot F \cdot dy$$

m	**=**	CO_2 mass transported through the concrete surface [kg]
t	**=**	Time of admission [a]
D	**=**	Diffusion coefficient [m^2/s]
c	**=**	CO_2 concentration in the air and in the pore structure [kg/m^3]
y	**=**	Thickness of carbonated layer [m]
m_o	**=**	Absorbed CO_2 mass per volume unit of concrete [kg]
F	**=**	Area of carbonating concrete [m^2]

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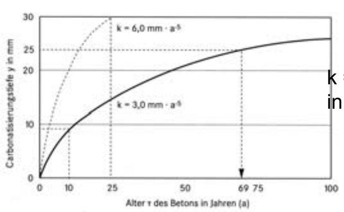
Calculation of carbonation depth – √t-law

Solution of the diffusion equation:

$$y = \sqrt{\frac{2 \cdot D \cdot c_0 \cdot}{m_0}} \cdot \sqrt{t}$$



$$y = k \cdot \sqrt{t}$$

k = Carbonation coefficient in $mm/a^{0.5}$

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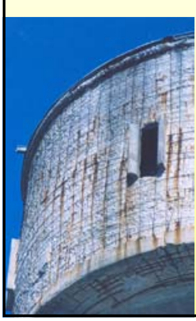
Factors affecting the depth of carbonation



- **Concentration of CO_2**
- **Humidity**
- **Concrete quality (W/C-ratio)**
- **Type of cement**
- **Aftercare**
- **Aggregates, additives, admixtures**
- **Temperature**